PLENARY LECTURES

2026 PAUL H. EMMETT AWARD PLENARY LECTURE BY DAVID FLAHERTY

Monday, June 9, 2025 8:00 AM - 9:00 AM
Centennial Ballroom

Chair: Enrique Iglesia, Purdue University

Charting New Waters: Activities, Active Sites, and Reactive Structures in Dynamic Environments.

David W. Flaherty
School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA

Catalytic reactions on solid materials form the foundation of chemical manufacturing, many phenomena that impact these systems challenge current understanding. We demonstrate that solvent-surface interactions change activities of reactive species within pores of molecular dimensions, form new reactive structures in-situ, and open reaction pathways distinct from those at gas-solid interfaces.

ADV CHARAC - NEW AND ADVANCED METHODS IN CATALYST CHARACTERIZATION

ADV CHARAC - EMERGING ADVANCED CHARACTERIZATION TECHNIQUES

Monday, June 9, 2025 9:30 AM - 11:30 AM
Hanover Hall CDE

Chair: Amrit Venkatesh, University of Virginia

Co-Chair: Dongmin Yun, SK Innovation

Operando Magic Angle Spinning NMR Spectroscopy for Catalytic Reactions and Materials Characterization.

Jian Zhi Hu[1,2], *Sungmin Kim*[1], *Wenda Hu*[2], *Nicholas Jaegers*[3], *Huamin Wang*[1,2], *Yong Wang*[1,2], *and Johannes Lercher*[1,4]
(1)Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA, (2)The Gene and Linda Voiland School of Chemical Engineering and Bioengineering, Washington State University, Pullman, WA, (3)University of California at Berkeley, Berkeley, CA, (4)Technical University of Munich, Garching b. München, Germany

High resolution operando magic angle spinning NMR spectroscopy capable of operating at pressure from below 1 atm to above 50 atm, temperature from -20 to 250 °C and sample spinning rate up to 15 kHz will be presented with examples of application in a variety of reaction systems.

Monitoring Lignin Catalysis Reactions By Operando Spectroscopy and Scattering.

Marcus Foston
Energy, Environmental & Chemical Engineering, Washington University, Saint Louis, MO

This study utilizes operando NMR and in situ SANS to investigate lignin catalytic disassembly, revealing key pathways including O-methylation, α-dehydroxylation, and chain scission to phenolic monomers. Structural dynamics, including lignin polymer coil generation, depolymerization, and condensation, were characterized, providing insights critical for designing efficient catalysts and optimizing biomass conversion processes.

A Spatial-Resolved Online MS Study on OCM Reaction for $CH_3\cdot$ Coupling Mechanistic Insight.

Yong Yang*, Junyu Lang, Danyu Wang, and Ningxujin Ding*
Schoolof Physical Science and Technology, ShanghaiTech University, Shanghai, China

Oxidative coupling of methane (OCM) is a promising reaction for methane to ethylene conversion through direct gas-phase methyl radical coupling. This study provide a new spatial-resolved online MS setup for analysis of the products distribution and insight of intermediates formation correlating to the short-life radical at high temperatures (600-800 ℃).

Spatially and Temporally Resolved Characterization of an Iron Catalyst Bed during Fischer-Tropsch Pretreatment *via In Situ* ^{57}Fe Synchrotron Mössbauer Spectroscopy.

Adli Peck[1]*, Michael Claeys*[1]*, Giovanni Hearne*[2]*, Gustavo Pasquevich*[3]*, Deogratias Tumwijukye*[2]*, and Christopher Mullins*[1]
(1)Department of Chemical Engineering, Catalysis Institute, University of Cape Town, Cape Town, South Africa, (2)Department of Physics, University of Johannesburg, Johannesburg, South Africa, (3)Instituto de Física La Plata, CONICET, Universidad Nacional de La Plata, La Plata, Argentina

Utilizing novel *in situ* ^{57}Fe synchrotron Mössbauer spectroscopy, we monitored phase transformations in an iron catalyst bed during Fischer-Tropsch reduction and carburization. This technique offers qualitative and quantitative insights into iron phases as a function of spatial and temporal coordinates under industrially relevant conditions.

Mapps & CT-Tric: In Situ UV-Vis Methods for Assessment of Particle Size, Charge Transfer, and Adsorbate Location on Heterogeneous Catalysts.

Alejandra Torres Velasco[1,2]*, Priya D. Srinivasan*[1,2]*, and Juan Bravo-Suarez*[2]
(1)Center for Environmentally Beneficial Catalysis, The University of Kansas, Lawrence, KS, (2)Chemical & Petroleum Engineering, The University of Kansas, Lawrence, KS

MaPPS and CT-TRIC offer in situ UV-Vis techniques for estimating charge transfer changes, particle sizes, and identifying adsorption site locations inaccessible by other techniques. These

methods enhance understanding of redox processes in supported metals and/or metal oxides, enabling advances in catalytic systems' characterization under operando conditions.

Toward *in Situ* top Atomic Layer Surface Analysis with High Sensitivity Low Energy Ion Scattering (HS-LEIS).

*Nathanael Ramos[1], Haoran Ding[1,2], and **Adam Holewinski**[2]*
(1)Renewable and Sustainable Energy Institute, University of Colorado Boulder, Boulder, CO, (2)Chemical and Biological Engineering, University of Colorado Boulder, Boulder, CO

We will discuss our recent progress in the development of methods using HS-LEIS for high-fidelity top atomic layer analysis of surfaces exposed to reactive environments

AI - AI-DRIVEN CATALYSIS

AI - TACKLING COMPLEXITY IN THE CATALYST'S ENVIRONMENT AND STRUCTURE

Monday, June 9, 2025 9:30 AM - 11:30 AM
Centennial Ballroom IV

Chair: Thomas Senftle, Rice University

Co-Chair: Fanglin Che, University of Massachusetts Lowell

Initial Lessons Learned in Developing an Integrated Platform to Predict Degradation of Catalysts for Sustainable Conversion of Alternate Feedstocks to Fuels and Chemicals.

***Simon Bare**[1], Sarah Hesse[1], Adam Hoffman[1], Christopher J. Tassone[1], Kirsten Winther[2], Anastassia Alexandrova[3], Matteo Cargnello[4], Phillip Christopher[5], Ashley Head[6], Matthew Kanan[7], Shyam Kattel[8], Ambarish Kulkarni[9], Robert Rallo[10], Robert Rioux[11], and Judith Yang[6]*
(1)Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, Menlo Park, CA, (2)SLAC National Accelerator Laboratory, Menlo Park, CA, (3)Department of Chemistry and Biochemistry, University of California - Los Angeles, Los Angeles, CA, (4)Department of Chemical Engineering, Stanford University, Stanford, CA, (5)Chemical Engineering, University of California, Santa Barbara, Santa Barbara, CA, (6)Brookhaven National Laboratory, Upton, NY, (7)Department of Chemistry, Stanford University, Stanford, CA, (8)Florida A&M University, Tallahassee, FL, (9)Chemical Engineering, University of California, Davis, Davis, CA, (10)Pacific Northwest National Laboratory, Richland, WA, (11)Department of Chemical Engineering, The Pennsylvania State University, University Park, PA

We are developing a cutting-edge platform to predict catalyst sintering and long-term performance based on based on short-term experiments. We are leveraging ML and AI in an active learning workflow, whereby steady state and dynamic testing, operando and in situ characterization, and theoretical modeling are used as input parameters.

AI-Enabled Multiscale Modeling of Catalyst Cluster and Adsorbate Dynamics.

Piaoping Yang[1]*, Alfred Worrad*[1]*, Salman A. Khan*[2]*, and Dionisios Vlachos*[2]
(1)University of Delaware, Newark, DE, (2)Delaware Energy Institute, University of Delaware, Newark, DE

We develop actively trained machine learning potentials (MLPs) with global optimization methods to predict the structure of Pt clusters/Al_2O_3-supported, adsorbates on them, spillover, and particle isomerization. We will report data for H and CO adsorbates and introduce a method for computing dynamic spectroscopy.

KEYNOTE: Accelerating computational catalysis with machine learned potentials.

John Kitchin
Chemical Engineering, Carnegie Mellon University, Pittsburgh, PA

Computational catalysis has relied on density functional theory for several decades. Over the past two decades we have seen a series of advances from the Behler-Parinello neural network potentials to the GAP potentials, and most recently the graph neural network machine learned potential architectures.

Multiscale Modeling of Nanostructured Electrocatalyst for Alkaline Water Electrolysis Via Graph Neural Network.

Jinuk Moon[1]*, Jiwon Kim*[2]*, Jinwoo Lee*[2]*, and Jeong Woo Han*[1]
(1)Department of Materials Science and Engineering, Research Institute of Advanced Materials, Seoul National University, Seoul, Korea, Republic of (South), (2)Department of Chemical and Biomolecular Engineering, KAIST, Daejeon, Korea, Republic of (South)

Integrating GNN with evolutionary algorithms, we developed a framework to analyze catalyst structures and activities at the nanometer scale. This approach enabled us to identify catalysts with significant activity. The framework is broadly applicable to any catalytic reactions where their global optimal structures are unknown yet critical in their reactivity.

Predicting the Chemical (Dis)Order in Multicomponent Materials with High-Throughput Simulations and Representation Learning.

Jiayu Peng
University at Buffalo, Buffalo, NY

Multicomponent materials offer broad tunability and diverse applications, including heterogeneous catalysis, yet the complexity of their chemical ordering complicates and hinders their design and optimization. This presentation discusses our physics-informed, data-driven methods to understand and predict chemical (dis)order using high-throughput atomistic simulations and symmetry-aware geometric deep learning.

Foundational Interatomic Potentials for Modelling Complex Catalyst Systems.

Victor Fung
Georgia Institute of Technology, Atlanta, GA

Here we show how foundational models can be created for the materials science domain via physics-informed pre-training strategies, and how they can then be fine-tuned to become highly effective interatomic potentials and property predictors with excellent data efficiency over bespoke models.

BIOMASS - BIOMASS AND WASTE VALORIZATION CATALYSIS

BIOMASS - BIOMASS TO FUELS 1

Monday, June 9, 2025 9:30 AM - 11:30 AM
Regency Ballroom VI

Chair: Stephen Schuyten, Johnson Matthey Inc.

Co-Chair: Luke Roling, Iowa State University

Upcycling Polypropylene to Jet Fuel over Ru_1-ZrO_2 Catalyst.

Xiang WANG
Dalian University of Technology, Dalian, Liaoning, China

We report that processing 100 grams of post-consumer polyethylene and polypropylene yields 85 mL of liquid in a solvent-free hydrocracking over atomic Ru-doped ZrO_2. The liquid (C_5-C_{20}) comprises ~70% jet-fuel-ranged branched hydrocarbons (C_8-C_{16}), while the gas product is liquefied-petroleum-gas (C_3-C_6) without methane and ethane.

Valorization of Ethanol to Sustainable Aviation Fuels Via n-Butene-Rich Intermediate over Cu-MO_x/SiO_2 Catalysts.

Martin Affandy[1]*, Robert A. Dagle*[1]*, Libor Kovarik*[2]*, Yong Wang*[3]*, and Vanessa Lebarbier Dagle*[2]
(1)Pacific Northwest National Laboratory, Richland, WA, (2)Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA, (3)The Gene and Linda Voiland School of Chemical Engineering and Bioengineering, Washington State University, Pullman, WA

This work provides insight into a promising new catalytic system for the direct conversion of ethanol to butene-rich olefins, with excellent yield to desired product while maintaining remarkable stability. These characteristics provide a baseline for scale-up investigations and a bridge towards piloting and eventual commercial adaptation.

From Concept to Commercial: Developing and Scaling Lanzajet's Catalytic Alcohol-to-Fuels Pathway.

Jacob Miller*, Prafulla Dinkarrao Patil, Kathryn Bjorkman, and Edwin Yik*
LanzaJet, Deerfield, IL

LanzaJet has scaled conversion of ethanol to a SAF blendstock. We outline the pathway and discuss how data obtained at different scales have guided the development of our SAF technology. We present examples of the role fundamental reaction engineering and reactor modeling play in implementation of our technology at scale.

Effects of Metal Precursor and Pd Nanoparticle Size on Lignin Biomass Hydrodeoxygenation.

Chigozie Ezeorah[1]*, Aaron Vannucci*[1]*, and John Regalbuto*[2]
(1)Chemistry and Biochemistry, University of South Carolina, Columbia, SC, (2)Chemical Engineering, University of South Carolina, Columbia, SC

We hypothesized that smaller catalyst particle size would lead to greater product selectivity with respect to catalytic hydrodeoxygenation of oxygenated aromatic molecules that can be derived from lignin. HDO of benzyl and vanillyl alcohols using Pd/SiO_2 catalyst of different sizes revealed visible size effects.

Catalytic Conversion of Captured Monoterpenes to Sustainable Aviation Fuel.

Ajibola Lawal[1]*, Andrew D. Sutton*[2]*, and Kim Tutin*[3]
(1)Chemical Process Scale-Up, Oak Ridge National Laboratory, Oak Ridge, TN,
(2)Manufacturing Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN,
(3)Chemicals, Captis Aire LLC, East Point, GA

Captured monoterpene conversion to aromatics and cycloalkanes, as suitable hydrocarbon component in sustainable aviation fuel blends.

Opening Pathways for the Conversion of Woody Biomass into Sustainable Aviation Fuel Via Catalytic Fast Pyrolysis and Hydrotreating.

Mike Griffin[1]*, Steven Rowland*[1]*, Kristiina Iisa*[1]*, Abhijit Dutta*[1]*, Xiaolin Chen*[1]*, Cody Wrasman*[1]*, Calvin Mukarakate*[1]*, Matthew Yung*[1]*, Mark Nimlos*[1]*, Luke Tuxworth*[2]*, Xavier Baucherel*[2]*, and Susan Habas*[1]
(1)National Renewable Energy Laboratory, Golden, CO, (2)Johnson Matthey, Newcastle, United Kingdom

Integrated experimental campaigns highlight opportunities to produce high-quality sustainable aviation fuel from woody biomass via catalytic pyrolysis and hydrotreating. Lifecycle assessment indicates GHG emission reductions exceeding 85% compared to petroleum jet fuel, and phosphorous modification of technical ZSM-5 catalysts reveal opportunities to reduce coking and improve carbon efficiency.

Site Specific Deactivation Pathways of Mixed Oxide Catalyst in Presence of Oxygenates during Aldol Condensation of Ketones to Produce Sustainable Aviation Fuel (SAF).

Udishnu Sanyal[1]*, Laura C. Meyer*[1]*, Yang He*[2]*, Mond F. Guo*[1]*, and Karthikeyan Ramasamy*[3]

(1)Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA, (2)Energy & Environment, Pacific Northwest National Laboratory, Richland, WA, (3)Pacific Northwest National Laboratory, Richland, WA

Our study highlights the importance of understanding catalyst deactivation mechanism to develop robust catalyst system for upgrading biomass feedstock to sustainable aviation fuel (SAF). By unraveling the deactivation species and their underlying fundamental reaction mechanism is critical to design sustainable catalyst which further improves the efficiency of overall process.

Process Development, Scale-up and Commercialization of a Sustainable Biobased Material.

Keith Hutchenson[1]*, Kevin Gu*[2]*, Morgan Hahnert*[1]*, James Lin*[2]*, Daniel Slanac*[1]*, and Shunzu Wang*[2]
(1)Covation Biomaterials LLC, Newark, DE, (2)Covation Biomaterials, Shanghai, China

Covation Biomaterials has developed and will commercialize a sustainable, biobased material derived from a 2nd generation biomass. This presentation will provide an overview of the new monomer process for this material as well as the scale-up methodology employed to develop this sustainable, economically viable manufacturing process.

Impact of K and ZrO_2 Sequential Addition on Red Mud-Based Catalysts for CO_2 Hydrogenation.

Mahbuba Aktary[1]*, Md. Nasiruzzaman Shaikh*[1,2]*, and Atif Alzahrani*[1,3]
(1)Materials Science and Engineering, King Fahd University of Petroleum and Minerals, Dhahran, Eastern Province, Saudi Arabia, (2)Interdisciplinary Research Center for Hydrogen Technologies and Carbon Management (IRC-HTCM), King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia, (3)Interdisciplinary Research Center for Sustainable Energy Systems (IRC-SES), King Fahd University of Petroleum & Minerals, Dhahran 31261, Saudi Arabia, Dhahran, Saudi Arabia

The addition sequence of active metal and promoter has a substantial impact on the performance of red mud-based catalysts in CO_2 hydrogenation. This study investigates the effect of adding promoter (KNO_3) and ZrO_2 in a different order on the conversion of CO_2 and the product's selectivity.

Hydrotreatment of Waste Vegetable Oil for Advanced Biofuels Production.

Paula Marmol[1]*, Patricia Reñones*[1]*, Silvia Morales de la Rosa*[2]*, and* ***Jose Miguel Campos Martín***[1]
(1)CSIC, Instituto de Catalisis y Petroloequímica, Madrid, Spain, (2)Instituto de Catálisis y Petroleoquímica, Spanish National Research Council (CSIC), Madrid, Spain

Biofuel production from waste biomass offers a zero-emission alternative to fossil fuels. Hydrotreatment involves hydrodeoxygenation (HDO) and hydroisomerization (HISO) steps,

using efficient catalysts like TMP and nickel-based systems. Studies reveal an optimal balance of metal and acid sites enhances fuel conversion and stability. Scaled-up tests confirm industrial viability.

C2+ - CATALYSIS OF C2+ CHEMISTRY

C2+ | C2+ OLEFIN HYDROGENATION AND OXIDATION REACTIONS

Monday, June 9, 2025 9:30 AM - 11:30 AM
Centennial Ballroom III

Chair: Dongxia Liu, University of Delaware

Co-Chair: Victor Gabriel Baldovino Medrano, Centro de Investigaciones en Catálisis (CICAT), Universidad Industrial de Santander

KEYNOTE: Catalytic Active Site Design for Chemoselective Hydrogenation Using Multinary Intermetallics.

Robert Rioux
Department of Chemistry, The Pennsylvania State University, University Park, PA; Department of Chemical Engineering, The Pennsylvania State University, University Park, PA

Multinary intermetallic compounds produced as bulk materials are used to demonstrate the active site requirements, in terms of nuclearity, composition (binary to multinary) and facet preferencing for chemoselective hydrogenation. Utilizing acetylene semi-hydrogenation as a reference chemistry across all intermetallic catalysts, we demonstrate electronic effects can be disentangled from ensemble effects.

Effect of Pt Particle Size and Electronic Properties on the Hydrogenation of Ethylene..

Sara Haidar[1]*, Md Raian Yousuf*[1]*, Hung-Ling Yu*[1]*, Stephen Porter*[2]*, Sagar Sourav*[3]*, Eli Stavitski*[4]*, Dionisios Vlachos*[5]*, Abhaya Datye*[2]*, and Ayman M. Karim*[1]
(1)Department of Chemical Engineering, Virginia Polytechnic Institute and State University, Blacksburg, VA, (2)Department of Chemical and Biological Engineering and Center for Micro-Engineered Materials, University of New Mexico, Albuquerque, NM, (3)Department of Chemical Engineering, Indian Institute of Technology Madras, Chennai, Tamil Nadu, India, (4)National Synchrotron Light Source II, Brookhaven National Laboratory, Upton, NY, (5)Delaware Energy Institute, University of Delaware, Newark, DE

This study examines how Pt particle size, ranging from single atoms to nanoparticles on CeO_2, influences electronic properties and catalytic activity for ethylene hydrogenation. The findings reveal a volcano-shaped activity trend, highlighting the critical interplay between electronic and geometric properties, offering pathways to optimize catalysts for hydrogenation reactions.

Chemical and Structural Requirements for Dioxygenase-Type Reactivity in Selective Ethene Oxidation on Ag Catalysts.

Andrew Hwang[1]*, Andrey Karpov*[2]*, Carlos Lizandara-Pueyo*[2]*, and Enrique Iglesia*[3,4]

(1)Department of Chemical and Biomolecular Engineering, University of California, Berkeley, Berkeley, CA, (2)BASF SE, Ludwigshafen, Germany, (3)University of California, Berkeley, Berkeley, CA, (4)Purdue University, West Lafayette, IN

Kinetic and mechanistic studies that clarify the roles of Cs and Re promoters and Cl moderators in effecting dioxygenase-like reaction channels during aerobic ethene epoxidation on Ag-based catalysts will be described.

High-Valent Early-Transition Metal Chlorides for the Catalytic Gas-Phase Cyclotrimerization of Acetylene to Benzene.

Jonathan Moritz Mauß *and Ferdi Schüth*
Department of Heterogeneous Catalysis, Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr, Germany

Various high-valent early-transition metal chlorides exhibit promising reactivity in the catalytic gas-phase cyclotrimerization of acetylene to benzene. Coupled with sustainable acetylene production via an electric plasma-assisted methane pyrolysis process of biomethane or hydrogenated carbon dioxide with renewable energies this would offer a possible pathway for direct sustainable benzene production.

Effects of Pd Site Structure and Interconversion on Wacker Oxidation of Ethylene over PdCu/Zeolites.

Deepak Sonawat*, Patrick Granowski, Tara T. DuBridge, and Siddarth Krishna*
Chemical and Biological Engineering, University of Wisconsin-Madison, Madison, WI

Steady-state kinetics reveals similar Wacker oxidation rates over PdCu/zeolites containing varying fractions of Pd ions and PdO clusters, showing they are nearly equivalent active site precursors. *In situ* XAS quantifies the fraction of redox-active Pd and Cu, providing new insights into active site structure, redox, and regenerability for Wacker oxidation.

ELECTRO PHOTO - ELECTROCATALYSIS AND PHOTOCATALYSIS

ELECTRO PHOTO - ORGANIC ELECTROCHEMICAL TRANSFORMATIONS 1

Monday, June 9, 2025 9:30 AM - 11:30 AM
Centennial Ballroom I

Chair: Juliana Carneiro, Columbia University

Co-Chair: Samji Samira, Virginia Tech

Automated Cohp Calculations for the Prediction of Stability and Catalytic Activity in Mixed Transition Metal Oxides.

*Kirsten Winther[1], **Ruchika Mahajan**[2], and Michal Bajdich[3]*
(1)SLAC National Accelerator Laboratory, Menlo Park, CA, (2)Chemical Engineering, Stanford

University, Palo Alto, CA, (3)SUNCAT Center for Interface Science and Catalysis, SLAC National Accelerator Laboratory, Menlo Park, CA

This work focuses on finding affordable, stable and active catalysts for ORR/OER in hydrogen technologies. By leveraging ICOHP-based bulk descriptors and automating high-throughput DFT calculations with AutoCatLab python library, we efficiently screen ternary oxides. Finally Prediction models like GPR and GNN help predict bulk stability, accelerating discovery of effective catalysts.

Propane Activation on Pt Electrocatalyst at Room Temperature: Quantification of Adsorbate Identity and Coverage.

Ashutosh Bhadouria and ***Brian M. Tackett***
Charles D. Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN

This talk will describe the quantification of adsorbate coverage and the adsorbate identity during propane activation at Pt electrocatalysts in aqueous electrolyte at room temperature.

Electrochemical Dehydrogenation of Benzyl Alcohol for Hydrogen Release Under Ambient Temperature.

Moses Chilunda[1]*, Alexander von Rueden*[2,3]*, Mal Soon Lee*[3]*, Juan A. Lopez-Ruiz*[3,4]*, and Elizabeth Biddinger*[1]
(1)Chemical Engineering, The City College of New York, New York, NY, (2)Chemical and Biological Engineering, University of Wisconsin-Madison, Madison, WI, (3)Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA, (4)WSU-PNNL Bioproducts Institute, Pacific Northwest National Laboratory, Richland, WA

Electrochemical dehydrogenation (ECD) of benzyl alcohol to form benzaldehyde serves as a model for studying primary alcohols that can be used as liquid organic hydrogen carriers. This work explores how the molecular interactions at electrocatalyst-electrolyte interface influence the selective ECD of benzyl alcohol by tuning parameters affecting the interfacial environment.

Direct Propylene Epoxidation By Water Oxidation over $PdPtO_x$ Electrocatalysts.

Jason S. Adams[1]*, Minju Chung*[2]*, Justin Bui*[3]*, Yuriy Roman*[2]*, and Karthish Manthiram*[4]
(1)Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, CA, (2)Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, MA, (3)Department of Chemical and Biomolecular Engineering, University of California, Berkeley, Berkeley, CA, (4)Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, CA

We develop and characterize $PdPtO_x$ catalysts and elucidate their mechanisms for electrochemical propylene epoxidation using a combination of x-ray techniques, kinetic studies, and isotopic measurements. We find that equimolar PdPt catalysts annealed at 500°C lead to the highest partial currents (>25 mA cm^2) and faradaic efficiencies (~60-70%) of epoxidation.

Kinetics of Alkaline Aldehyde Electrooxidation and Anodic Hydrogen Generation.

Nathanael Ramos[1,2]*, Hudson Neyer*[1,2]*, J. Will Medlin*[2]*, and Adam Holewinski*[1,2]
(1)Renewable and Sustainable Energy Institute, University of Colorado Boulder, Boulder, CO,
(2)Chemical and Biological Engineering, University of Colorado Boulder, Boulder, CO

At low potential, H_2 is formed at Au, Ag, and Cu anodes during aldehyde oxidation in alkaline media. Using rotating disk electrode, reaction kinetics are discussed including Au and Ag having much higher peak carboxylate and H_2 formation rates than Cu at only slightly higher overpotential.

Enhancement of Steam-Methane Reforming By Joule Heating of Ni/ZrO_2-Fecral Wire: Potential Electrocatalytic Effect.

Elmer Ledesma*, Meghana Idamakanti, Praveen Bollini, and Michael Harold*
William A. Brookshire Department of Chemical and Biomolecular Engineering, University of Houston, Houston, TX

Joule heating of Ni-coated FeCrAl is effective for SMR. Joule heating of Ni/ZrO_2 wire coil exhibits enhanced performance over conventional heating and over Joule heating of a similarly-shaped wire coated with Ni/Al_2O_3. This enhancement stems from electrical conductivity differences of the supports, with ZrO_2 being more conductive than Al_2O_3.

FUNDAMENTALS - FUNDAMENTALS OF CATALYSIS AND SURFACE SCIENCE

FUNDAMENTALS - ELECTROCHEMICAL AND PHOTOCATALYSIS

Monday, June 9, 2025 9:30 AM - 11:30 AM
Centennial Ballroom II

Chair: Thomas Schwartz, University of Maine

Co-Chair: Benjamin Jackson, Pacific Northwest National Laboratory

Quantifying Electrochemical Potential during Gas-Phase Heterogeneous Catalysis with Solid Electrolyte Potentiometry.

Deiaa Harraz[1]*, Kunal Lodaya*[1]*, Cole Cadaram*[1]*, Bryan Tang*[2]*, and Yogesh Surendranath*[1]
(1)Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA,
(2)Chemistry and Chemical Biology, Harvard University, Cambridge, MA

Measurement of the electrochemical potential of metallic catalysts has revolutionized our understanding of a several transformations in liquid phase catalysis. Using solid electrolyte potentiometry, we have developed a technique to measure catalyst electrochemical potential during gas phase catalysis, elucidating electrochemical mechanisms operative in absence of a bulk liquid phase.

Wireless Potentiometry of Thermochemical Heterogeneous Catalysis.

Neil Razdan[1]*, Karl Westendorff*[2,3]*, and Yogesh Surendranath*[2,3]
(1)Chemical & Biochemical Engineering, University of California Berkeley, Berkeley, CA, (2)Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, MA, (3)Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA

We establish a facile, non-invasive method to quantify the electrochemical potential of metal nanoparticles supported on non-conductive oxides (e.g., silica) during solid-liquid heterogeneous catalysis. This approach enables, for the first time, measurement of the kinetic relevance of electron-transfer events during heterogeneous redox catalysis—as we demonstrate for HCOOH oxidative dehydrogenation.

Elucidating the Role of Electric Fields on Fe Oxidation Via Multiscale Models and an Environmental Atom Probe.

Naseeha Cardwell[1]*, Sten Lambeets*[2]*, Isaac Onyango*[1]*, Mark G. Wirth*[2]*, Eric Vo*[2]*, Yong Wang*[2]*, Pierre Gaspard*[3]*, Cornelius F. Ivory*[1]*, Daniel Perea*[2]*, Thierry Visart De Bocarmé*[3]*, and* ***Jean-Sabin McEwen***[1,2]
(1)The Gene and Linda Voiland School of Chemical Engineering and Bioengineering, Washington State University, Pullman, WA, (2)Pacific Northwest National Laboratory, Richland, WA, (3)Université Libre de Bruxelles, Brussels, Belgium

This work quantifies the effect of intense applied electric fields on Fe oxidation when a single catalytic grain is exposed to oxygen. We demonstrate how external high electric fields applied to nanoscale catalytic systems can be utilized to dynamically exploit reaction dynamics towards desired products at mild reaction conditions.

Surface Coverage Analysis Reveals Potential-Determining Heterolytic Reactions during Thermocatalytic Aerobic Glucose Oxidation.

Minju Chung[1]*, Karl O. Albrecht*[2]*, Joshua M. Terrian*[2]*, and David W. Flaherty*[3]
(1)School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA, (2)Archer Daniels Midland, Decatur, IL, (3)Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA

Concurrent interpretations of catalyst potential (E_{cat}) and steady-state kinetics reveal mechanistic insights into chemical phenomena at solid-liquid interfaces. The coverages of surface intermediates primarily govern the scaling relationship between E_{cat} and turnover rates. Each elementary step exhibits unequal kinetic and E_{cat} relevance in the reaction network oxidizing glucose.

KEYNOTE: Single Crystal Electrochemistry and Its Relevance to Electrocatalysis: Case Studies.

Bingjun Xu

Catalysis Center for Energy Innovation, Department of Chemical and Biomolecular Engineering, University of Delaware, Newark, DE

This talk discusses adsorption/desorption behaviors of organic and polymeric species on single crystal Pt surfaces and their implications for electrocatalytic reactions on more practical Pt-based materials.

The Dynamics of the Active Sites for Hydrogen Evolution Reaction over 2D-Layered Ti_2c Mxene.

Lin Chen
Department of Physics, Chemistry and Biology, Linköping University, Linköping, Sweden

MXene, a new 2D materials with many potential applications, for example, hydrogen evolution reaction (HER). Here, the mechanism of HER activity over Ti2C MXene and the dynamics of the active sites is revealed by advanced constant potential approach in combination of ab initio thermodynamics and kinetic analysis.

Moving Beyond the Langmuir Model.

Peijun Hu
Chemistry, Shanghaitech University, Shanghai, Shanghai, China

I will present some of our work on the topic of active sites. I will demonstrate that different reactions occur at different sites on catalytic surfaces; there is a correlation between the valence of reactants and the coordination of active sites. A model beyond the Langmuir model is proposed.

MONNIER - JOHN MONNIER MEMORIAL SESSIONS

MONNIER - JOHN MONNIER MEMORIAL SESSION 1

Monday, June 9, 2025 9:30 AM - 11:30 AM
Hanover Hall FG

Chair: John Regalbuto, University of South Carolina

Co-Chair: Benjamin Egelske, University of South Carolina Columbia

The Growth of Supported Nanoparticle Sizes Via Controlled Electroless Deposition.

John Meynard Tengco[1], *Haiying Zhou*[1], *Wen Xiong*[1], *Benjamin Egelske*[1], *Akkarat Wongkaew*[2], *John Regalbuto*[1], *and John Monnier*[1]
(1)Chemical Engineering, University of South Carolina, Columbia, SC, (2)Chemical Engineering, Burapha University, Bangsaen, Thailand

The controlled growth of supported nanoparticles from a starting seed catalyst was demonstrated using the method of electroless deposition, through regulated addition of metal allowing for

slower and more uniform deposition. Multilayer depositions of Pt, Pd, and Ag were achieved, resulting in larger particles, confirmed by various characterization methods.

Renewable Hydrogen Production Using Bimetallic Catalyst with Controlled Composition and Structure.

An Zhang, Kun Yang, and ***Weijian Diao***
Chemical Engineering, Villanova University, Villanova, PA

Bimetallic Pd-Ir catalysts were synthesized and tested for catalytic decomposition of sulfuric acid in the Hybrid Sulfur water-splitting reaction for hydrogen production. We have found that selective placement of Pt on Ir metal core with higher surface free energy results in active and stable Pt catalysts for SO_3 decomposition.

Learnings about Supported Metal Catalysts.

Stuart Soled[1]*, Chris Kliewer*[2]*, and Michael Lanci*[3]
(1)Materials and Catalysis, ExxonMobil Technology and Engineering Co, Annandale, NJ, (2)ExxonMobil, Clinton, NJ, (3)ExxonMobil Corporation, Annandale, NJ

This talk is dedicated to the memory of John Monnier, a wonderful friend and colleague. It will focus on bimetallic catalyst preparation, the role of surface enrichment and how oxidative regeneration affects changes in structure.

Novel Carbon Support Systems for Metal Catalyzed Cross Coupling Applications.

Frank Gupton
Chemical and Life Science Engineering, Virginia Commonwealth University, Richmond, VA

Recent work has demonstrated that novel carbon support systems such as graphene and multi-wall carbon nanotubes depart unusual and advantageous catalytic properties to palladium nanoparticles that have been deposited onto the surface of these substrates. We have been able to create essentially a solid-state ligand system for the metal nanoparticles.

The Poisoning of Silica Supported Pd (but not Pt!) By Residual Chloride for Hydrogen Chemisorption.

Haiying Zhou, Alaba Ojo, Santosh Kiran Balijepalli, John Monnier, and ***John Regalbuto***
Chemical Engineering, University of South Carolina, Columbia, SC

We have identified that the cause of a systematic discrepancy between chemisorption estimates versus STEM and XRD estimates of supported Pd nanoparticles size is residual chloride, which blocks the Pd surface. This does not occur on Pt.

Characterization of Zeolite-Based Catalysts for Plastic Upcycling By Use of Positron Annihilation Spectroscopy.

Anne Gaffney
Idaho National Laboratory, Idaho Falls, ID

Catalysts: HZSM-5 and MESO-Y, play a pivotal role in upgrading plastics thereby transforming existing plastic materials into simpler, higher-quality value-added products. Here we present studies of various zeolites used as catalysts undergoing deactivation processes. Positron Annihilation Lifetime Spectroscopy (PALS) is excellent for examining sub-nano-meter size morphology of these catalysts.

SYNTHESIS - CATALYST SYNTHESIS AND MANUFACTURING

SYNTHESIS - SINGLE-ATOM CATALYST SYNTHESIS, STABILITY, AND REACTIVITY

Monday, June 9, 2025 9:30 AM - 11:30 AM
Regency Ballroom VII

Chair: Eswar Iyyamperumal, Ketjen Corporation

Co-Chair: Jennifer Lee, Harvard University

Hydrothermally Stable Single Atom Cu on CeO_2 for Ethanol Upgrading.

Jesse Larence[1], *Abhaya Datye*[2], *Hien N. Pham*[2], *Andrew T. DeLaRiva*[2], *Ryan Alcala*[3], *Vanessa Lebarbier Dagle*[4], *Huamin Wang*[5], *Benjamin Moskowitz*[4], *Martin Affandy*[5], *Robert A. Dagle*[4], *Ted Kim*[6], *and Jeffrey T. Miller*[6]
(1)University of New Mexico, Albuquerque, NM, (2)Department of Chemical and Biological Engineering and Center for Micro-Engineered Materials, University of New Mexico, Albuquerque, NM, (3)Department of Chemical & Biological Engineering and Center for Micro-Engineered Materials, University of New Mexico, Albuquerque, NM, (4)Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA, (5)Pacific Northwest National Laboratory, Richland, WA, (6)Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN

In this study we utilize various characterization techniques to demonstrate bulk single atom Cu stabilized on CeO_2 is hydrothermally stable when subjected to high temperature under H_2 and steam to simulate conditions seen in alcohol to jet fuel processes (ATJ) and compare to real conditions seen in the ATJ reaction.

Optimizing Pd Single-Atom Catalysts in Pyrene-Based Cofs: Purification Strategies and Catalytic Performance in Ethylene and Acetylene Hydrogenation..

Hridita Purba Saha[1], ***Ruby Deeter***[2], *Hani M El-kaderi*[2], *and Ayman M. Karim*[1]
(1)Department of Chemical Engineering, Virginia Polytechnic Institute and State University, Blacksburg, VA, (2)Department of Chemistry, Virginia Commonwealth University, Richmond, VA

This study highlights the critical role of purification in optimizing the activity of Pd single atoms within the imine-linked Pyrene COF structure, emphasizing the need for a fundamental understanding of how binding site modifications and Pd ligand environment variations influence catalyst activity and selectivity.

Diluted Atomic Layer Deposition (DALD): A Facile Method for the Synthesis of Single Metal Atom Catalysts.

*Kai Shen[1], Ayman M. Karim[2], Dionisios Vlachos[3], Raymond Gorte[1], and **John Vohs**[1]*
(1)Department of Chemical and Biomolecular Engineering, University of Pennsylvania, Philadelphia, PA, (2)Department of Chemical Engineering, Virginia Polytechnic Institute and State University, Blacksburg, VA, (3)Delaware Energy Institute, University of Delaware, Newark, DE

In this talk we will describe a facile two-step method, Diluted-ALD (DALD), for the synthesis of a high concentration of supported single metal atom sites on an oxide surface. Results will be presented for DALD synthesis of single metal atom sites of Ir, Rh, and Pt on several oxide supports.

Covalent Metal-Ester Bonding in Hybrid Catalysts: Enhanced Catalyst Loading and Support-Tunable Reactivity.

Aaron Vannucci *and Joseph Kuchta III*
Chemistry and Biochemistry, University of South Carolina, Columbia, SC

We have designed a new synthetic method for covalently bonding molecular catalysts to metal oxide supports through metal-ester bonds. This synthesis procedure leads to catalyst loadings of two catalyst sites per nm^2 for various supports. Catalyst reactivity can also be correlated to the PZC of the support.

Single-Atom Alloy Formation Via Reaction-Driven Catalyst Restructuring.

Gregory Novotny[1]*, Georgios Giannakakis[1], Yogita Soni[1], E Charles Sykes[2], and Prashant Deshlahra[1]*
(1)Department of Chemical and Biological Engineering, Tufts University, Medford, MA, (2)Department of Chemistry, Tufts Univ, Medford, MA

The vinyl acetate (VA) synthesis reaction causes formation of mobile metal diacetate clusters that drive extensive restructuring of PdCu, leading to single-atom alloy formation, nanoparticle size reduction, and high activity and selectivity for VA synthesis and ethanol dehydrogenation. This approach is scalable and appears to be generalizable to other alloys.

Solid-State Ion Exchange of Transition Metal Chlorides on Mordenite.

*Rio Moore and **James Crawford***
Chemical & Biological Engineering, Montana State University, Bozeman, MT

Solid-state ion exchange of transition metal ions on zeolites is an attractive strategy to obtain well-defined active sites. We report a systematic study of first-row transition metal (II) chlorides on H-mordenite. Our results suggest that for metal chlorides that sublime, vapor pressure influences the exchange process.

ADV CHARAC - NEW AND ADVANCED METHODS IN CATALYST CHARACTERIZATION

ADV CHARAC - ADVANCED TRANSIENT METHODS FOR STRUCTURAL DYNAMICS

Monday, June 9, 2025 1:00 PM - 3:20 PM
Hanover Hall CDE

Chair: Dongmin Yun, SK Innovation

Co-Chair: Yuanyuan Li, Oak Ridge National Laboratory (ORNL)

Resolving Solid-State Oxygen Diffusion with Transient Methods: A Case Study on CrO_x/Al_2O_3.

Jason Malizia[1]*, Shengguang Wang*[1]*, Stephen Kristy*[1]*, Rong Xing*[2]*, Mingyong Sun*[3]*, and Rebecca Fushimi*[1]
(1)Idaho National Laboratory, Idaho Falls, ID, (2)Research and Development, Clariant Corporation, Louisville, KY, (3)Clariant, Louisville, KY

The Temporal Analysis of Products (TAP) reactor system is used to monitor solid-state oxygen diffusion in a CrO_x/Al_2O_3 catalyst. The flux responses of oxygen release under varying reaction conditions provides a dataset from which a diffusion model is built. This model is then applied to more complex phenomenon.

Operando Photoelectron Photoion Coincidence Spectroscopy to Detect Short-Lived Intermediates in Catalysis.

Zihao Zhang[1]*, Patrick Hemberger*[2]*, and Andras Bodi*[2]
(1)School of Natural Resources, University of Tennessee-Knoxville, Knoxville, TN, (2)Paul Scherrer Institute, Villigen, Switzerland

We show how *operando* PEPICO unveils catalytic mechanisms by discerning elusive intermediates, such as methyl radicals (CH_3) and short-lived oxygenates, in the oxidative dehydrogenation of propane, CH_3Cl coupling, and lignin monomer hydrodeoxygenation.

Evidence of Multi-Origin and Topology-Dependent Product Selectivity in the Methanol-to-Olefins Process By Operando CH3OH/CD3OD Switching Experiments.

Luca Maggiulli[1]*, Davide Ferri*[1]*, and Jeroen A. van Bokhoven*[2]
(1)Paul Scherrer Institute, Villigen, Switzerland, (2)Laboratory for Catalysis and Sustainable Chemistry, Paul Scherrer Institute, Villigen, Switzerland

In this work we introduced a transient operando diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS)/gas chromatography (GC) methodology together with a CH_3OH/CD_3OD switching protocol to elucidate the multi-origin of olefins in the methanol-to-olefins (MTO) process process over zeolites ZSM-5 and SSZ-13.

Spatiotemporal X-Ray Absorption Spectroscopy of Ni-Mg-Al Mixed Oxide Catalysts during Dry Methane Reforming.

Sofie Ferwerda[1]*, Valerie Briois*[2]*, Sebastian Weber*[3]*, Michael Kraemer*[3]*, Nils Bottke*[3]*, Matteo Monai*[1]*, and Bert M. Weckhuysen*[1]
(1)Inorganic Chemistry and Catalysis, Institute for Sustainable and Circular Chemistry, Utrecht University, Utrecht, Netherlands, (2)ROCK beamline, Soleil Synchrotron, Saint-Aubin, France, (3)Catalysis Research, BASF SE, Ludwigshafen am Rhein, Germany

Using spatiotemporal X-ray absorption spectroscopy, this study provides new insights into species concentration profiles along millimeter-sized catalyst beds, capturing real-time catalyst transformations. By changing Mg/Al ratios and synthesis conditions, we investigated oxidation state changes, reduction-oxidation propagation, and synthesis-structure-performance relationships in Ni-Mg-Al catalysts during dry methane reforming.

Time-Domain NMR for Characterizing Catalyst Surface Fluid-Interactions.

Murilo Toledo Suekuni[1] *and* ***Alan Allgeier***[2]
(1)Chemical and Petroleum Engineering, The University of Kansas, Lawrence, KS, (2)Center for Environmentally Beneficial Catalysis (CEBC), University of Kansas, Lawrence, KS

Time-domain NMR measurements reflect surface-fluid interaction strength in the mesoporous silicate, KIT6. In the context of 1-hexene and methanol, we demonstrate that the later is repelled from the surface in the presence of water and that its mechanism of NMR relaxation is dominated by intramolecular dipole coupling.

KEYNOTE: Active Sites and Reaction Pathways: How Transient Methods Provide a Unique Perspective to Characterize Essential Catalyst Features .

Rebecca Fushimi
Catalysis and Transient Kinetics Group, Idaho National Laboratory, Idaho Falls, ID

New ways of distinguishing active sites and resolving reaction pathways are presented through transient experiments. The synchronous measurement of time-dependent gas and surface response on the millisecond timescale represents a distinctive achievement.

CO2 - CO2 CAPTURE AND UPGRADING

CO2 - ELECTROCHEMICAL AND THERMAL CO_2 CONVERSION

Monday, June 9, 2025 1:00 PM - 3:20 PM
Centennial Ballroom IV

Chair: Joaquin Resasco, The University of Texas at Austin

Co-Chair: Manish Shetty, Texas A&M University

Understanding the Role of Ionic Liquids and Alkali Metal Cations in Reactive Carbon Dioxide Capture.

***Soumya Chatterjee**, Derek Zhu, and Michael Janik*
Chemical Engineering, The Pennsylvania State University, University Park, PA

Mechanistic role of room temperature ionic liquids in understood for reactive CO_2 capture. Potential dependent reaction energies and activation barriers is computed for electro-reduction of CO_2 in room temperature ionic liquids. Importance of local interactions at electrode-electrolyte interface is investigated to study the impact of ionic liquids in CO_2 reduction.

Oxide-Encapsulated Electrocatalysts for Selective and Stable Carbon Dioxide Transformation Via Reactive Carbon Capture.

***Zhexi Lin**[1], Nathaniel Blake[1], Xueqi Pang[1], Zhirui He[1], Reza Mirshekari[2], Oyinkansola Romiluyi[2], Yoon Jun Son[2], Suryansh Kabra[1], and Daniel Esposito[1]*
(1)Department of Chemical Engineering, Columbia Electrochemical Energy Center, Lenfest Center for Sustainable Energy, Columbia University, New York, NY, (2)Shell International Exploration & Production, Inc., Houston, TX

In situ spectroelectrochemical measurements demonstrate that titania encapsulation blocks undesired species to suppress hydrogen evolution by about 50%, while also working synergistically with a chelating agent to stabilize silver electrodes in impurity-containing electrolytes. This work provides a simple yet effective catalyst design strategy for efficient reactive carbon capture systems.

Microenvironment Engineering to Fine-Tune Selectivity of the Electrochemical CO_2 Reduction on a Copper-Gold Catalyst.

***Seyed Parsa Amouzesh**[1], Taha Baghban-Ronaghi[1], SeyedSepehr Mostafayi[1], Karen A. Castaneda[2], and Mohammad Asadi[1,3]*
(1)Chemical and Biological Engineering, Illinois Institute of Technology, Chicago, IL, (2)Department of Physics, Illinois Institute of Technology, chicago, IL, (3)Chemical and Biological Engineering, Illinois Tech, Chicago, IL

Achieving selectivity in CO_2RR for value-added products like ethanol and ethylene is crucial for commercialization. We developed a pulse current strategy using Au-decorated Cu, demonstrating that pulse conditions control the shift from ethylene to ethanol by optimizing local pH and CO_2 Concentration.

Exploring Design Principles for Tandem Electrochemical CO2 Reduction.

***Lun An**[1], Wenyu Huang[2], and Long Qi[3]*

(1)Ames National Laboratory, Ames, IA, (2)Chemistry, Iowa State University, Ames, IA, (3)Division of Chemical & Biological Sciences, Ames Laboratory, Ames, IA

We coupled the CO_2-to-CO conversion on Ni-N-C with CO reduction on CuNPs, creating a tandem catalysis system for producing ethylene and ethanol. By systematically tuning the spatial distribution of Ni-N-Cs and CuNPs, we effectively modulated the local concentration of CO on CuNPs, thus enhancing the selectivity towards multicarbon products.

Dual-Atom Alloying Strategy for Tuning Copper Catalyst for CO_2 Electrocatalytic Reduction to C_2 Oxygenates.

Isaac Kojo Seim[1]*, Gbolade Kayode*[2]*, Charles Dees*[3]*, Matthew Montemore*[2]*, and Ming Yang*[1]
(1)Chemical and Biomolecular Engineering, Clemson University, Clemson, SC, (2)Chemical and Biomolecular Engineering, Tulane University, New Orleans, LA, (3)Electrical and Computer Engineering, Clemson University, Clemson, SC

The direct electrocatalytic reduction of carbon dioxide to ethanol is a promising route to mitigate greenhouse gas emissions. Here, we demonstrate a dual-atom alloy catalyst that synergistically enhances ethanol selectivity. Experimental and mechanistic insights reveal that yttrium and palladium species uniquely drive CO_2 activation, C–C coupling, and ethanol formation.

High-Temperature CO_2 Electroreduction in Molten Salt Electrolyte for Pure Carbon-Negative Carbon Nanotubes.

Andrew Wong[1] *and* ***Yukun Hu***[2]
(1)Materials Science and Engineering, National University of Singapore, Singapore, Singapore, (2)Chemical & Biomolecular Engineering, National University of Singapore, Singapore, --- None ---, Singapore

The electrochemical CO_2 reduction in molten salt electrolytes enables the production of carbon nanostructures, such as high-purity carbon nanotubes, with >80% Faradaic efficiency. This work presents design principles for achieving pure, high-quality CO_2-derived carbon nanotubes, addressing bottlenecks to profitability and commercialization of carbon-negative electrochemical CO_2 conversion to carbon products.

Structure-Dependent Microkinetic Analysis of r-WGS Reaction on Pt- and Rh-Based Catalysts.

Gabriele Spanò, ***Riccardo Colombo****, Raffaele Cheula, Gabriele Contaldo, and Matteo Maestri*
Laboratory of Catalysis and Catalytic Processes - Dipartimento di Energia, Politecnico di Milano, Milano, Italy

In this work we provide fundamental underpinnings of how catalyst affinity to oxygen dictates the r-WGS reaction mechanism, uncovering transition states and dominant active sites through a structure-dependent microkinetic analysis. These findings pave the way to develop sound kinetic models for r-WGS and effective catalyst optimization.

Zinc Single-Atom Nanozyme As Carbonic Anhydrase Mimic for CO_2 capture and Conversion.

Eslam Hamed[1] *and Sam Li*[2]
(1)Chemistry, National University of Singapore, Singapore, Singapore, (2)National University of Singapore Department of Chemistry, Singapore, Singapore

Single-atom Zn-N-C nanozymes (SANs) mimic carbonic anhydrase, achieving 91% CO_2 conversion to bicarbonate via a biomimetic process. The high metal loading (18 wt%) enhances catalytic activity, enabling CO_2 sequestration and amino acid detection in supplements with remarkable sensitivity, showcasing Zn-SAN's potential in environmental and analytical applications.

Scale-up CO_2 Conversion Technology.

Hanif Choudhury[1]*, Mohamed Sufiyan Challiwala*[1]*, and Nimir Elbashir*[2]
(1)Chemical Engineering, Texas A&M University at Qatar, Doha, Qatar, (2)TEES Gas & Fuels Research Center, Texas A&M University at Qatar, Doha, Qatar

TAMUQ team developed a unique process known as CARGEN(R) technology that produce tunable syngas ratio and require lesser energy. CARGEN(R) technology also produces a valuable biproduct known as multi-walled carbon nanotube which has significant use in the today's world. This study illustrates the scale-up journey of the CARGEN technology.

ELECTRO PHOTO - ELECTROCATALYSIS AND PHOTOCATALYSIS

ELECTRO PHOTO - PHOTOCATALYSIS

Monday, June 9, 2025 1:00 PM - 3:20 PM
Centennial Ballroom I

Chair: Shu Hu, Yale University

Co-Chair: Guoxiang (Emma) Hu, Georgia Institute of Technology

Dynamical Effects in Photocatalytic Activity of Sulfated Titania.

Christian Geci[1]*, Niall Gushue*[1]*, Leah Batoosingh*[1]*, Riley Day*[1]*, Robert Meulenberg*[2]*, Pascal Raybaud*[3]*, Andreas Kafizas*[4]*, Thomas Schwartz*[5]*, and* ***Brian Frederick***[1]
(1)Chemistry/FIRST, University of Maine, Orono, ME, (2)Physics/FIRST, University of Maine, Orono, (3)IFP Energies Nouvelles, Solaize, France, (4)Chemistry, Imperial College London, London, ME, (5)Chemical and Biomedical Engineering, University of Maine, Orono, ME

The enhanced photocatalytic reactivity of sulfated titania for methyl orange degradation has been correlated with the presence of deep electron traps. Transient absorption spectroscopy reveals enhanced carrier lifetimes on millisecond timescale that are significant for photocatalysis. The speciation of sulfur has been determined with X-ray absorption, UV-vis, and DFT calculations.

Probing Spatial Energy Flow in Plasmonic Catalysts.

***Bill Yan**, Rachel Elias, and Suljo Linic*
Chemical Engineering, University of Michigan, Ann Arbor, MI

We developed methodologies to measure the local temperature of the oxide support, plasmonic NP, and molecular adsorbates under light illumination. We revealed the existence of large temperature gradients among these entities, which arose from the process of light-to-heat conversion and appear to be a defining aspect of plasmonic catalytic systems.

Influence of Visible Photon Fluxes on Reactions of Co-Adsorbed CO and H on Pt Surfaces.

***Samji Samira**[1,2], Silvia Marino[1], Anika Jalil[1], Michael Gordon[1], and Phillip Christopher[1]*
(1)Department of Chemical Engineering, University of California, Santa Barbara, Santa Barbara, CA, (2)Department of Chemical Engineering, Virginia Tech, Blacksburg, VA

Visible photon fluxes enable new reaction channels and surface coverages during surface reactions of CO* and H* on Pt. In addition to direct photoexcitation of the Pt–CO bonds under illumination, it is shown that the degree of rate control of the kinetically relevant step decreases, thus allowing excited state transformations.

Elucidating the Role of Nanoscale Electrocatalyst/Semiconductor Interfaces in Photoelectrochemical Water Splitting.

***Ahmet Sert** and Suljo Linic*
Department of Chemical Engineering, University of Michigan, Ann Arbor, MI

In this work, we shed light on the complexities associated with the physical mechanisms underlying the operation of complex photoelectrocatalytic systems by focusing on rigorous investigations of well-defined model systems. We also developed a comprehensive physical framework to describe the experimentally observed behavior.

Photocatalytic Reverse Water-Gas Shift Reaction Using Copper-Based Nanostructures..

***Shivam Kumar**[1] and Ravi Teja Addanki Tirumala[2]*
(1)School of Chemical, Biological, and Materials Engineering, University of South Florida, Tampa, FL, (2)Center for Environmentally Beneficial Catalysis, University of Kansas, Lawrence, KS

This study focuses on developing cost-effective Cu_2O-based catalysts for the reverse water-gas shift reaction (RWGSR), converting CO_2 into valuable CO with ~99% selectivity. Dynamic phase changes between Cu_2O and metallic Cu, confirmed via spectroscopy and XRD, influence reaction rates. Visible light enhances performance, with Cu_2O outperforming Cu at lower temperatures.

Unravelling the Role of Visible Light in the Rwgs Reaction over Cu/Al_2O_3: Not All That Shines Is Good.

Kristijan Lorber[1], Iztok Arčon[2], Matej Huš[3], Nataša Novak Tušar[1], and ***Petar Djinović***[1]
(1)Department of Inorganic Chemistry and Technology, National Institute of Chemistry, Ljubljana, Slovenia, (2)Laboratory for quantum optics, University of Nova Gorica, Nova Gorica, Slovenia, (3)Department of Catalysis and Chemical Reaction Engineering, National Institute of Chemistry, Ljubljana, Slovenia

Illumination of the Cu/Al_2O_3 catalyst negatively affects the CO rate. The rate-slowing scales linearly with irradiance and is wavelength dependent. TD-DFT and in-situ DRIFTS confirmed lower stability of OH groups in the excited state compared to the ground state. Hydroxyl groups appear important in enabling low-energy barrier CO production.

Scalable Solar-Driven Reforming of Alcohol Feedstock to H_2 Using $Ni/Zn_3In_2S_6$ Photocatalyst.

Denny Gunawan[1]*, Cui Ying Toe[1,2], Jason Scott[1], and Rose Amal[1]*
(1)Chemical Engineering, University of New South Wales, Sydney, NSW, Australia, (2)Renewable Energy Engineering, University of Newcastle, Callaghan, NSW, Australia

This work presents solar-driven alcohol reforming for H_2 production, featuring $Ni/Zn_3In_2S_6$ photocatalyst and upscaled photoreactor achieving 1.08% solar-to-H_2 efficiency. Techno-economic analysis highlights solar-to-H_2 efficiency and solar availability as key feasibility factors. Overall, the findings demonstrate the potential of solar-driven reforming to produce cost-effective renewable H_2, contributing to net-zero emissions goals.

ENVIRO AUTO - ENVIRONMENTAL AND AUTOMOTIVE CATALYSIS

ENVIRO AUTO - METHANE OXIDATION CATALYSIS - MECHANISMS AND CATALYST DEACTIVATION

Monday, June 9, 2025 1:00 PM - 3:20 PM
Hanover Hall FG

Chair: Donna Liu, Johnson Matthey

Co-Chair: Petr Koci, University of Chemistry and Technology

Enhancing Oxygen Transfer and Tuning Pd Electronic Properties Via Shape Engineering of Ceria-Supported Catalysts for Lean Methane Oxidation.

Martim Chiquetto Policano[1]*, Jimmy A. Faria[2], and Leon Lefferts[3]*
(1)Chemical Engineering, University of Twente, Enschede, Overijssel, Netherlands, (2)Faculty of Science and Technology, University of Twente, Enschede, Overijssel, Netherlands, (3)Catalytic Processes and Materials (CPM) - TNW Faculty, University of Twente, Enschede, Netherlands

Morphology strongly influences catalytic performance. Pd/CeO_2-r excels due to abundant oxygen vacancies enhancing redox activity, while Pd/CeO_2-c relies on exceptional stability. Elevated Pd^{2+} surface concentrations drive activity. Microkinetic modeling highlights support interactions and reveals reduced oxygen pressure dependence at higher temperatures from enhanced lattice oxygen mobility and metal-oxygen exchange.

Pd-Based Catalysts for Enhanced Low-Temperature Lean Methane Combustion: Experimental and Modeling Insights in a Catalytic Monolith Reactor.

Honghong Shi[1], *Rana Muhammad Haris*[2], *Kenneth Rappe*[3], *Michael Harold*[2], *and Yong Wang*[1]
(1)Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA, (2)William A. Brookshire Department of Chemical and Biomolecular Engineering, University of Houston, Houston, TX, (3)Energy & Environment Directorate, Pacific Northwest National Laboratory, Richland, WA

Two different strategies on catalyst development were presented to address the major shortcomings of the commercial Pd catalysts: poor hydrothermal stability and poor low temperature activity. With combined experimental and 1+1D monolith modeling work, we aim to provide more robust and energy efficient solutions for methane oxidation under practical conditions.

Kinetic Model Development for the Complete Oxidation of Methane on a Practical PtPd/Al_2O_3 Catalyst.

Min Wang[1], ***Haiying Chen***[1], *Yuliana Lugo-Jose*[1], *Joseph M. Fedeyko*[2], *Todd Toops*[1], *and Jacqueline Fidler*[3]
(1)Oak Ridge National Laboratory, Oak Ridge, TN, (2)Clean Air - SEC, Johnson Matthey, Audubon, PA, (3)CONSOL Energy, Canonsburg, PA

A kinetic model is developed for a PtPd/Al_2O_3 catalyst under practically relevant reaction conditions for the abatement of methane emissions from the ventilation air of underground coal mines. The kinetic parameters derived from the model are consistent with the values that are reported in the literature.

Overcoming Deactivation in Wet Methane Combustion Using Pd Catalysts Supported on Physically Mixed Al_2O_3 and ZrO_2..

Do Heui Kim[1] *and* ***Gyu hyun Jang***[2]
(1)Seoul National University, Seoul, Korea, Republic of (South), (2)Seoul National University, Seoul, Seoul, Korea, Republic of (South)

Pd catalysts supported on physically mixed Al_2O_3 and ZrO_2 (Pd/Al_2O_3-ZrO_2) exhibited high catalytic activity and outstanding hydrothermal stability after H_2O treatment at 400 °C for 20 h. This work demonstrates the pivotal role of physically mixed Al_2O_3 and ZrO_2 as supports in mitigating the deactivation mechanism for wet methane combustion.

Enhanced Low-Temperature Methane Oxidation Catalysts with Improved Sulfur Tolerance for High Water Content Emissions Control.

*Melanie Moses-DeBusk[1], **Sreshtha Sinha Majumdar**[2], and Yensil Park[1]*
(1)Buildings and Transportation Science Division, Oak Ridge National Laboratory, Oak Ridge, TN, (2)Oak Ridge National Laboratory, Oak Ridge, TN

The presence of sulfur, high water concentrations, and low exhaust temperatures of lean-burn natural gas engines in hard-to-electrify sectors are a challenge for methane oxidation catalysts (MOC). A new MOC shows improvement over Pd/Al_2O_3 and $PtPd/Al_2O_3$ MOCs providing increased hydrothermal durability and sulfur tolerance at low-temperatures through Mg modification.

Impact of Hydrogen on Methane and NOx Conversion in Three-Way Catalysts for Natural Gas–Hydrogen Blend Exhaust.

***Vitaly Prikhodko**, Min Wang, Yeonshil Park, and Haiying Chen*
Oak Ridge National Laboratory, Oak Ridge, TN

This study demonstrates that the addition of hydrogen significantly enhances the conversion of methane (CH4) and nitrogen oxides (NOx) emissions pollutants in natural gas-powered engine exhaust

Process Scaleup and Validation for Catalytic Oxidation of Ventilation Air Methane from Coal Mining.

***Andrew Palermo**[1], Hai-Ying Chen[2], Phil Evans[3], Joseph M. Fedeyko[4], Jacqueline Fidler[5], Patrick Flynn[5], Kerr Gray[3], Melissa A Hess[4], Yuliana Lugo-Jose[4], and Min Wang[2]*
(1)Catalyst Technologies, Johnson Matthey, Houston, TX, (2)Oak Ridge National Laboratory, Oak Ridge, TN, (3)Catalyst Technology, Johnson Matthey, Stockton, United Kingdom, (4)Clean Air - SEC, Johnson Matthey, Audubon, PA, (5)CONSOL Energy, Canonsburg, PA

A PtPd methane oxidation catalyst was developed for ventilation air methane abatement. The catalyst maintained above 99.5% methane conversion for more than 1000 hours. A field test unit with the capability of handling 1000 scfm gas flow has been fabricated to be tested on a coal mining site.

FUNDAMENTALS - FUNDAMENTALS OF CATALYSIS AND SURFACE SCIENCE

FUNDAMENTALS - REACTION MECHANISMS AND KINETICS

Monday, June 9, 2025 1:00 PM - 3:20 PM
Centennial Ballroom II

Chair: Griffin Canning, Toyota

Co-Chair: Neil Razdan, University of California Berkeley

Catalytic Implications of Solvent Structuring in the Pores of Sn-Beta Zeolites on Meerwein-Ponndorf-Verley Reaction Rates.

Faysal Ibrahim[1]*, Edgard Lebrón Rodríguez*[2]*, Jerome Evans*[1]*, Levi Callahan*[1]*, Fabiola Y. Rodríguez-Rodríguez*[3]*, Christine Kortendick*[1]*, Nelson Cardona-Martinez*[3]*, and Ive Hermans*[1,2,4]
(1)Department of Chemistry, University of Wisconsin - Madison, Madison, WI, (2)Department of Chemical and Biological Engineering, University of Wisconsin - Madison, Madison, WI, (3)Chemical Engineering, University of Puerto Rico - Mayagüez, Mayaguez, PR, (4)Wisconsin Energy Institute, University of Wisconsin - Madison, Madison, WI

By leveraging Modulation Excitation Spectroscopy, key solvent-zeolite interactions were observed for the MPV reduction reaction in Sn-beta zeolites. The accessibility of cyclohexanone to the Sn active site is directly impacted by the clustering of 2-butanol within the pore which this work provides spectroscopic evidence of.

New Insights into the Mechanism of the Haber-Bosch Process.

Simon Hansen*, Benjamin Sjølin, Ivano Castelli, Tejs Vegge, Anker D. Jensen, and* ***Jakob Munkholt Christensen***
Technical University of Denmark, Lyngby, Denmark

The mechanism of catalytic ammonia synthesis has been investigated and we can observe an H2/D2 isotope effect. From quench cooling of the working catalyst we can conclude that this is not due to differences in nitrogen coverage. Instead, the existence of a previously unknown hydrogen-assisted reaction pathway is proposed.

Consequences of Confinement and Acid Strength on Arene Methylation Kinetics and Product Selectivities over Acidic Zeolites.

Andrew Norfleet *and Rajamani Gounder*
Charles D. Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN

Effects of confining five distinct arene methylation transition states within microporous voids are quantified via rate constants as guest-host interactions are varied among aluminosilicate materials of different void size (TON, Beta, FAU, MCM-41), active site distributions among differing voids in a framework (MFI channels or intersections), and heteroatom identity.

Hydrogen Activation on Zeolite-Encapsulated Transition Metal Sulfide Clusters.

Rachit Khare[1]*, Yunxiang Sheng*[1]*, and Johannes A. Lercher*[1,2]
(1)Department of Chemistry, Technische Universität München, Garching, Germany, (2)Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA

Combining kinetic studies with spectroscopy measurements and density functional theory calculations, we show that molecular transition metal sulfide clusters, encapsulated in zeolite

micropores, activate hydrogen on Mo atoms as hydrides. These clusters mimic the active site in nitrogenase and show high activity and exceptional stability for hydrogenation reactions.

Designing Metal-Substituted Oxide Catalysts for Chemoselective Hydrogenation Reactions.

***Mikyung Hwang**, Michael Janik, and Konstantinos Alexopoulos*
Chemical Engineering, The Pennsylvania State University, University Park, PA

Modulating reducibility of a metal oxide surface by substituting a metal cation can provide more active sites and improve catalytic performance during selective hydrogenation. A data-driven model for predicting oxide surface chemistry using open databases suggests a design rule for developing optimized metal-substituted oxide catalysts for targeted C-H bond formation.

Understanding the Promotional Role of Pd in Oxidative Alcohol Coupling Reactions over Dilute PdAu Alloys.

*Oluwatofunmi Akinsanya[1], Deep M. Patel[2], Christopher O'Connor[3], Marta Perxés Perich[4], Jessi E.S. van der Hoeven[4], Christian Reece[5], Luke T. Roling[2], and **Nathaniel Eagan**[1]*
(1)Department of Chemical and Biological Engineering, Tufts University, Medford, MA, (2)Department of Chemical and Biological Engineering, Iowa State University, Ames, IA, (3)Rowland Institute at Harvard, Harvard University, Cambridge, MA, (4)Materials Chemistry and Catalysis, Debye Institute for Nanomaterials Science, Utrecht University, Utrecht, Netherlands, (5)Harvard University, Cambridge, MA

Supported dilute-limit Pd_1Au_x alloys (x=5-200) drive oxidative ethanol coupling, with Pd addition promoting both activity and selectivity. This is attributed to increased ethoxy stabilization and occurs whether Pd atoms isolated or aggregated. DFT calculations further explore the ability of various adsorbates to stabilize Pd in Au surfaces.

Selective Hydrogenation Catalysis with Ternary Intermetallic Catalysts.

***Jin LI**[1], Mustafa Eid[2], Nilanjan Roy[1], Robert Rioux[3,4], and Michael Janik[1]*
(1)Chemical Engineering, The Pennsylvania State University, University Park, PA, (2)Chemistry, The Pennsylvania State University, University Park, PA, (3)Department of Chemical Engineering, The Pennsylvania State University, University Park, PA, (4)Department of Chemistry, The Pennsylvania State University, University Park, PA

Ternary intermetallic compounds offer a wide design space for tuning catalytic hydrogenation activity and selectivity for industrially important reactions. Multiple examples of combing DFT-MKM-experiment will be presented to overview how incorporation of a third element into binary intermetallics can alter catalytic performance.

HOMO - HOMOGENEOUS, MOLECULAR AND SUPRAMOLECULAR CATALYSIS

HOMO - HOMOGENEOUS, MOLECULAR AND SUPRAMOLECULAR CATALYSIS

Monday, June 9, 2025 1:00 PM - 3:20 PM
Regency Ballroom VII

Chair: Tracy Lohr, Shell

Co-Chair: Paul Kim, Shell

Electrolyte Composition Dictates Structure and Behavior of a Molecular Nitrate Reduction Electrocatalyst.

Dean Miller[1]*, Matthew Liu*[1]*, Uran Iwata*[2]*, Neha Sharma*[1]*, Wylie Kau*[3]*, Jinyu Guo*[1]*, Samantha Bunke*[1]*, and William A. Tarpeh*[3,4]
(1)Chemical Engineering, Stanford University, Stanford, CA, (2)Chemistry, Stanford University, Stanford, CA, (3)Department of Chemical Engineering, Stanford University, Stanford, CA, (4)SUNCAT Center for Interface Science and Catalysis, SLAC National Accelerator Laboratory, Menlo Park, CA

Molecularly-precise electrocatalysts are needed to convert dilute reactants in impure feedstocks into valuable products. Co(DIM) is a benchmark molecular electrocatalyst for nitrate reduction to ammonia, but its structure-activity relationships remain unclear. We develop an XAS platform to elucidate electrolyte-dependent intermediate electronic and geometric structures *in situ* that explain voltammetric observations.

Understanding the Electrocatalytic Activity of Pyridine-Alkoxide-Based Cu-Molecular Complexes for PFOA Degradation in Aqueous and Organic Medium.

Prasenjit Sarkar *and Karen L. Mulfort*
Chemical Science and Engineering, Argonne National Laboratory, Lemont, IL

Three Cu-pyridine alkoxide complexes have been utilized to electrocatalytically reduce PFOA. Complex **1** electrocatalytically degrades 35% PFOA within 5 h of cathodic 5 mA electrolysis. In aqueous medium, after 21 hours of anodic 5 mA electrolysis, complexes **2** and **3** degrade PFOA by 74% and 82%, respectively.

First-Principles Insights into Significant Enhancement of Arene Reduction Yields Using Electrochemical Rapid Alternating Polarity.

Kaida Liu[1]*, Rajat Daga*[1]*, Yu Kawamata*[2]*, Phil Baran*[2]*, and* ***Matthew Neurock***[1]
(1)Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN, (2)Department of Chemistry, The Scripps Research Institute, La Jolla, CA

Rapid alternating polarity lead to tremendous increases in the yields for arene reduction reactions of great importance in the synthesis of pharmaceutical intermediates. The integration of ab initio molecular dynamics and kinetic Monte Carlo simulations provide detailed insights into the mechanisms and kinetics that control arene reduction and HER.

Photocatalytic C(sp3)–C(sp3) Cross-Coupling of Carboxylic Acids and Alkyl Halides Using a Nickel Complex and Carbon Nitride.

Gianvito Vilé
Department of Chemistry, Materials, and Chemical Engineering "Giulio Natta", Politecnico di Milano, Milan, Italy

The state-of-the-art in C(sp^3)-C(sp^3)-coupling relies on dual Ir/Ni homogeneous systems, which depends on costly and scarce iridium. This work replaces iridium with a recyclable, earth-abundant nCNx catalyst. The optimized system achieves high yields under mild conditions, with enhanced recyclability. This approach expands photoredox chemistry for the green synthesis of pharmaceuticals.

Nanozymes with Catalytic Triad Active Sites Mimicking Ester and PET Hydrolysis Enzymes.

Hoya Ihara[1]*, Tianwei Yan*[1]*, Matthew Edgar*[1]*, Siddarth Krishna*[2]*, James A. Dumesic*[1]*, and George W. Huber*[1]
(1)Department of Chemical and Biological Engineering, University of Wisconsin-Madison, Madison, WI, (2)Chemical and Biological Engineering, University of Wisconsin-Madison, Madison, WI

We show that it is possible to synthesize the catalytic triad nanozymes which have high catalytic activity for ester hydrolysis, both as synthetic homogeneous complexes and grafted heterogeneous catalysts. Our approach provides new directions to design nanozyme catalysts for a range of applications such as PET recycling.

Designing a New Class of Nanoparticle Catalytic Supports Based on Supramolecular Hydrogen-Bonded Networks.

Kushaan Bahl *and Marcella Lusardi*
Chemical and Biological Engineering, Princeton University, Princeton, NJ

We demonstrate the production of Au nanoparticle catalysts supported on melamine cyanurate (MCA), a supramolecular hydrogen-bonded assembly of melamine and cyanuric acid. We characterize the Au nanoparticle chemical state and size distribution on this new support class and investigate their activity in the selective oxidation of amines in air.

First-Principles Insights into Electrolyte Effects on Electrochemical Reductive Bond Homolysis Selectivity.

Nhu Quach[1]*, Mayank Tanwar*[2]*, Zach A. Nguyen*[3]*, Dylan G. Boucher*[4]*, Kevin M. McFadden*[3]*, Shelley D. Minteer*[3]*, and Matthew Neurock*[2]
(1)Department of Chemistry, University of Minnesota, Minneapolis, MN, (2)Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN, (3)Department of Chemistry, University of Utah, Salt Lake City, UT, (4)Department of Chemistry and Biochemistry, Baylor University, Waco, TX

We examine how the interactions of the electrolyte-DMF solvent systems can govern the selectivity between multiple products in a cobalt-carbon bond homolysis reaction. Mechanistic insights from AIMD simulations reveal that harder cations like Li^+ significantly alter the polar aprotic DMF local solvation environment, enhancing cage-escape bond homolysis and hydrogenation selectivity.

MICRO MESO - MICROPOROUS AND MESOPOROUS MATERIALS

MICRO MESO - SYNTHESIS AND CATALYST DESIGN

Monday, June 9, 2025 1:00 PM - 3:20 PM
Regency Ballroom VI

Chair: Christopher Paolucci, University of Virginia

Co-Chair: Joel Schmidt, Chevron

Green Synthesis of Hierarchical SAPO-34: Using Cellulose Nanocrystals for Enhanced Catalytic Performance in Methanol to Light Olefins Reaction.

Ralph Al Hussami*, Galal Nasser, Tinotenda Mupfure, and Jan Kopyscinski*
Catalytic & Plasma Process Engineering, Department of Chemical Engineering, McGill University, Montreal, QC, Canada

Cellulose Nanocrystals (CNCs) are introduced as a secondary template for mesopore generation in microporous SAPO-34 for the first time. CNCs offer a sustainable, cost-effective, and safe alternative to traditional mesoporogens in the MTO process, demonstrating improved catalyst performance by extending catalyst active lifetime and increasing average light olefins selectivity.

Tuning the Acidity and Altering the Wettability of M-Tud-1 Catalyst for Selective Production of Solketal from Glycerol.

Sathyapal Churipard R., Mikaila Mahnke, Isha Panhale, Sundaramurthy Vedachalam, and ***Ajay Dalai***
Chemical and Biological Engineering, University of Saskatchewan, Saskatoon, SK, Canada

The current work presents the unique catalyst design with synergistic effect of Bronsted (Al) and Lewis (Ti) acidic sites in TUD-1 catalyst. In addition, hydrophobic modification resisted the catalyst deactivation by water and significantly enhanced the catalytic activity in aqueous environment. These interesting findings will be presented at the NAM29.

New Method for Producing Hydrophobic Pure-Silica Zeolites Via Post-Synthetic Treatment of Borosilicate Zeolites.

C.Y. Chen*[1] and Stacey I. Zones[2]*
(1)Chevron Energy Technical Center, Richmond, CA, (2)Chemical and Biomolecular Engineering, University of California, Berkeley, Berkeley, CA

This 2-step method consists of: (1) Borosilicate zeolites are first deboronated to create 4 SiOH groups for each boron T-atom removed; (2) Deboronated zeolites are then calcined at up to 950 °C to anneal one pair of SiOH groups to Si-O-Si, creating hydrophobic pure-silica zeolites useful for adsorption and separations.

Synthesis of Large Mesoporous Y Zeolite Catalysts.

Xuemin Li[1], *Abraham Martinez*[1], *Oleksandr Trybrat*[1], *Jinyi Han*[2], *Yi-sheng Chen*[3], *C.Y. Chen*[3], *Bi-Zeng Zhan*[3], *Howard S. Lacheen*[3], *Alexander Kuperman*[4], *and Alexander Katz*[5]
(1)Department of Chemical and Biomolecular Engineering, University of California - Berkeley, Berkeley, CA, (2)Chevron Energy Technical Center, Richmond, CA, (3)Chevron Energy Technology Company, Richmond, CA, (4)Chevron Energy ompany, Richmond, CA, (5)Chemical and Biomolecular Engineering, University of California, Berkeley, Berkeley, CA

We synthesized large-mesopore USY zeolite catalysts by hydrothermally treating zeolite precursor materials. Our catalyst synthesized at the lowest hydrothermal treatment temperature of 100 °C possesses a mesopore diameter of 9.3 nm (mesopore volume of 0.55 cm^3/g), and is an active acid catalyst for HD exchange and CI-test reactions.

Metal Organic Framework Derived Carbon Materials for CO_2 Reduction Reactions.

Swarit Dwivedi, Rajan Lakshman, Waqar Ahmad, and ***Akshat Tanksale***
Chemical and Biological Engineering, Monash University, Clayton, VIC, Australia

We synthesised MOF-derived materials for CO2 conversion to acetic acid, methanol, and formic acid. We report atomistic mechanisms governing the formation of MOF-derived materials. We rationally tune these materials to achieve a metal-metal oxide dispersion embedded in porous carbon capable of C-C coupling with and without an external methyl source.

Selective Heteroatom Incorporation within MWW-Type Molecular Sieves.

Youngkyu Park[1,2], *Stacey I. Zones*[3], *and Mark E. Davis*[1]
(1)Chemical Engineering, California Institute of Technology, Pasadena, CA, (2)Chemical and Biomolecular Engineering, University of California, Berkeley, Berkeley, CA, (3)Chevron Energy Technology Company, Richmond, CA

Two structurally related organic structure-directing agents (OSDAs) are designed to alter the boron siting within MWW-type borosilicate molecular sieves. It is revealed that the difference in the distribution of framework B sites is primarily due to the strong interaction between the quaternary ammonium within the OSDAs and framework B species.

Elucidating the Effect of Charge Compensating Species on Aluminum-Oxygen Bond Cleavage in the Dissolution of the Faujasite Framework.

Charles Umhey[1], *Zheng Cui*[2], *Daniel Shantz*[2], *and Jean-Sabin McEwen*[3]
(1)Department of Chemical Engineering and Bioengineering, Washington State University,

Pullman, WA, (2)Tulane University, New Orleans, LA, (3)The Gene and Linda Voiland School of Chemical Engineering and Bioengineering, Washington State University, Pullman, WA

Whether double six membered rings (D6MRs) are preserved during the interconversion of Faujasite (FAU) is the subject of debate. FAU dealumination pathways are evaluated to determine the feasibility of preserving D6MRs. Dealumination pathways damaging D6MRs were found to be more favorable than pathways leaving D6MRs intact.

REACTOR - REACTION ENGINEERING AND REACTOR DESIGN

REACTOR - REACTOR DESIGN FOR OXIDATION/DEHYDROGENATION REACTIONS

Monday, June 9, 2025 1:00 PM - 3:20 PM
Centennial Ballroom III

Chair: Canan Karakaya, Oak Ridge National Laboratory

Co-Chair: Udishnu Sanyal, Pacific Northwest National Laboratory

KEYNOTE: Membrane Reactor: Coupling Catalytic Reaction and Separation for Dehydrogenation of Light Alkanes.

Antara Bhowmick[1], Lu Liu[2], Chen Zhang[2], and ***Dongxia Liu***[1]
(1)Department of Chemical and Biomolecular Engineering, University of Delaware, Newark, DE, (2)University of Maryland, College Park, MD

Innovations in inorganic membrane reactors solve the thermodynamic and kinetic challenges in alkane dehydrogenation to achieve high conversion, high product yield, negligible coke formation and system's long-term stability.

Electrified Propane Dehydrogenation in a Washcoated Reactor: Design and Efficiency Considerations.

Hasan Koybasi[1]*, Dongxia Liu[2], and Dionisios Vlachos[3]*
(1)Chemical & Biomolecular Engineering, University of Delaware, Newark, DE, (2)Department of Chemical and Biomolecular Engineering, University of Delaware, Newark, DE, (3)Delaware Energy Institute, University of Delaware, Newark, DE

We modeled propane dehydrogenation reactor featuring Joule-heated wall with an adjacent washcoated catalyst. We employ a pseudo-2D transient model to elucidate the reactor's dynamic behavior and the time to reach steady state. The influence of reactor geometry and operating conditions on transport limitations, temperature uniformity and energy efficiency were investigated.

Continuous Simultaneous Hydrogenation and Acetylation of 4-Nitrophenol to Paracetamol in a Two-Stage Packed Bed Reactor.

Jimin Park[1]*, Marta Hatzell[2], Carsten Sievers[3], and Andreas Bommarius[3]*

(1)School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA, (2)George W. Woodruff School of Mechanical Engineering, Georgia Institute of Technology, Atlanta, GA, (3)School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA

A continuous paracetamol synthesis process in a packed bed reactor uses 5 wt% Pt/C as catalyst. Hydrogenation of 4-nitrophenol and acetylation with acetic anhydride occur simultaneously. The process achieves 98.5% yield and a process mass intensity of 7.2, a significant improvement in Green Chemistry metrics as well as product quality.

Gas-Liquid-Solid Microreactors By Self-Assembly of Amphiphilic Janus Catalysts for the Aerobic Oxidation of Aromatic Alcohols.

Kang Wang[1] *and Marc Pera-Titus*[2]
(1)School of Chemistry, Cardiff university, Cardiff, United Kingdom, United Kingdom, (2)School of chemistry, Cardiff catalysis institute, Cardiff, Wales, United Kingdom

Amphiphilic Janus particles prepared by bottom-up synthesis displayed twofold activity for the aerobic oxidation of various aromatic alcohols compared to non-Janus counterparts. This enhanced activity is attributed to the formation of stable G-L-S microreactors based on oil foams.

Controlling Selectivity Via Spatiotemporal Oxygen Distribution during the Oxidative Dehydrogenation of Ethane.

Austin Morales*, Praveen Bollini, and Michael Harold*
William A. Brookshire Department of Chemical and Biomolecular Engineering, University of Houston, Houston, TX

Oscillation amplitudes during forced dynamic operation of ethane oxidative dehydrogenation are used to control spatiotemporal distributions of oxygen thereby leading to dynamic ethylene selectivities which surpass those of conventional steady state operation. Dynamic operation achieves this by accessing catalytically stored oxygen distributions which are unachievable under steady state conditions.

Highly Efficient Oxidation of Glycerol to Formic and Glycolic Acid Using an Innovative Jet-Loop Reactor.

Jakob Albert*, Ira-Christina Wirth, and Daniel Niehaus*
Chemistry, University of Hamburg, Hamburg, Germany

Using a jet loop reactor for the selective oxidation of glycerol to formic and glycolic acid drastically improves space-time yields up to 30.0 g FA L-1h-1 compared to classical stirred-tank reactors allowing for very mild reaction conditions of 115°C and 5 bar O2 pressure under kinetically-controlled conditions.

ADV CHARAC - NEW AND ADVANCED METHODS IN CATALYST CHARACTERIZATION

ADV CHARAC - ADVANCED IN SITU AND OPERANDO X-RAY BASED METHODS
Monday, June 9, 2025 3:40 PM - 5:40 PM
Hanover Hall CDE

Chair: Jae Jin Kim, Shell International Exploration and Production Inc.

Co-Chair: Renqin Zhang, Clariant

Novel Approach Using Operando X-Ray Techniques to Monitor Catalyst Temperature While Tracking Sintering of Dispersed Rh Species during the Reverse Water-Gas Shift Reaction.

Anastassiya Khan[1], *Zhihengyu Chen*[1], *Adam Hoffman*[1], *Sarah Hesse*[1], *Emily K. Schroeder*[2], *Phillip Christopher*[3], *Christopher J. Tassone*[1], *and Simon Bare*[1]
(1)Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, Menlo Park, CA, (2)Department of Chemical Engineering, University of California, Santa Barbara, Santa Barbara, CA, (3)Chemical Engineering, University of California, Santa Barbara, Santa Barbara, CA

Our findings highlight the importance of *operando* characterization in capturing a catalyst's dynamics under varying length and time scales. Identification of excess heat produced during the catalyst's activation and subsequent rapid catalyst sintering provides an important insight into tuning reactor operating conditions to target specific catalyst structures.

First Observation of Propyl-Ga(III) Active Sites during Non-Oxidative Propane Dehydrogenation, By X-Ray Absorption Spectroscopy.

Jason Chalmers[1], *Adam Hoffman*[2], *Fernando Vila*[3], *Simon Bare*[2], *and Susannah Scott*[1]
(1)Department of Chemical Engineering, University of California, Santa Barbara, Santa Barbara, CA, (2)Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, Menlo Park, CA, (3)University of Washington, Seattle, WA

We investigate the Ga speciation in Ga-based propane dehydrogenation catalysts with operando X-ray absorption spectroscopy. We quantify the Ga sites under reaction conditions and correlate their abundance directly with the rate. Here we report the first observation (by XAS) of a propylGa(III) intermediate in the propane dehydrogenation catalytic cycle.

Real-Time Chemical Gradient Mapping in Ammonia Slip Catalysts Using Operando Spectrotomography.

Srashtasrita Das[1], *Vasyl Marchuk*[1,2], *Dmitry Doronkin*[1,3], *Dario Sanchez*[4], *Jan-Dierk Grunwaldt*[1,3], *and Thomas Sheppard*[1]
(1)Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany, (2)European Synchrotron Radiation Facility (ESRF), Grenoble, France, (3)Institute of Catalysis Research and Technology (IKFT), Karlsruhe Institute of Technology (KIT), Eggenstein-Leopoldshafen, Germany, (4)Swiss Light Source, Paul Scherrer Institute (PSI), Villigen, Switzerland

Hard X-ray *operando* spectrotomography using synchrotron radiation was performed to probe chemical gradients in dual-layer washcoated ammonia slip catalysts which are used in catalytic converters to mitigate excess ammonia emissions produced during selective catalytic reduction of NO_x. Local composition and structural variations were correlated to catalyst performance for various configurations.

Understanding Anomalous Thermal Oxidation Behavior of γ-Al_2O_3 Supported Pd Nanoparticles Via in-Situ Pair Distribution Function Analyses..

Siddhant Singh[1]*, Graham King*[2]*, and Robert W.J. Scott*[1]
(1)Department of Chemistry, University of Saskatchewan, Saskatoon, SK, Canada, (2)Brokhause diffraction sector beamlines, Canadian Light Source, Saskatoon, SK, Canada

The oxidation of γ-Al_2O_3 supported Pd nanoparticles to PdO has been studied using a combination of X-ray PDF and XAS analyses. The results demonstrate that the thermal-driven oxidation of Pd nanoparticles is highly dependent on the presence of grain boundaries and induced strain fields in the Pd fcc lattice.

Correlating the *D*-Band Electron Hole Character and Surface Hydroxylation with Hydrogen Activation on Supported Pt Clusters.

Hung-Ling Yu[1]*, Md Raian Yousuf*[1]*, Eli Stavitski*[2]*, and Ayman M. Karim*[1]
(1)Department of Chemical Engineering, Virginia Polytechnic Institute and State University, Blacksburg, VA, (2)National Synchrotron Light Source II, Brookhaven National Laboratory, Upton, NY

This work highlights the critical role of hydroxyl groupin the context of hydrogen activation. In addition, the results of in-situ XAS indicate that other than the L_3 white line intensity, the character of electron holes is an important parameter in H_2 binding and activation.

Residuals from Statistics-Based X-Ray Absorption Spectroscopy Analysis Methods Track Structural Evolutions during *In-Situ* Measurements.

Adam Hoffman[1]*, Florian Meirer*[2]*, Nina Genz*[3]*, and Simon Bare*[1]
(1)Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, Menlo Park, CA, (2)Inorganic Chemistry and Catalysis, Institute for Sustainable and Circular Chemistry, Utrecht University, Utrecht, Netherlands, (3)Paul Scherrer Institute, Villigen, Switzerland

The reduction of NiO/SiO_2 was characterized via *operando* XAS, with the data analyzed using PCA and MCR-ALS. The results showed that non-statistically significant PCA components and the residuals from MCR-ALS contained EXAFS-like structural information that accounted for thermal dampening effects. This workflow may identify transients in other *operando* catalysis measurements.

BIOMASS - BIOMASS AND WASTE VALORIZATION CATALYSIS

BIOMASS - BIOMASS TO FUELS 2

Monday, June 9, 2025 3:40 PM - 5:40 PM
Regency Ballroom VI

Chair: Anurag Kumar, Phillips 66

Co-Chair: Juan Carlos Vega-Vila, University of Maryland

Cu Evolution in Bimetallic Cu-Y/Beta during Ethanol Upgrading: Unveiling the Role of Diatomic Metal-Metal Interactions and Cu-Controlled C-C Coupling in Cascade Reactions.

*Junyan Zhang[1], **Stephen Purdy**[2], Meijun Li[3], Nohor Samad[4], James W. Harris[4], Kinga A. Unocic[5], Evan C. Wegener[6], Shan Jiang[7], Jeffrey T. Miller[7], Felipe Polo-Garzon[1], Dongxia Liu[8], Theodore Krause[9], Zili Wu[1], Andrew D. Sutton[2], Yanran Cui[10,11], and Zhenglong Li[10,11]*
(1)Chemical Sciences Division, Oak Ridge National Laboratory (ORNL), Oak Ridge, TN, (2)Manufacturing Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN, (3)Manufacturing Science Division, ORNL, Oak Ridge, TN, (4)Department of Chemical and Biological Engineering, The University of Alabama, Tuscaloosa, AL, (5)Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, TN, (6)Argonne National Laboratory, Lemont, IL, (7)Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN, (8)Chemical and Biomolecular Engineering, University of Maryland, (9)Chemical Sciences and Engineering Division, Argonne National Laboratory, Lemont, IL, (10)State Key Laboratory of Biobased Transportation Fuel Technology, College of Biosystems Engineering and Food Science, Zhejiang University, Hangzhou, China, (11)Division of Bio-Based Chemicals, Zhejiang University-Quzhou, Quzhou, China

Cu-Y/Beta is an effective catalyst for ethanol upgrading to mixed C_{3+} olefins. This talk details a systematic study of bimetallic interactions between Cu and Y, and the role each plays in the ethanol to olefins cascade reaction network using a mixture of rate measurements and in-situ spectroscopy.

Catalyst Deactivation in an Industrial Green Hydrotreater.

***Elham Nejadmoghadam**[1], Olov Öhrman[2], Derek Creaser[3], and Louise Olsson[3]*
(1)Chemical Engineering, Chalmers university of technology, Göteborg, Sweden, (2)Preem AB, Gothenburg, Sweden, (3)Chemical Engineering, Chalmers University of Technology, Gothenburg, Sweden

The findings suggest designing a guard bed upstream from a catalytic reactor to protect the main catalyst bed from feed impurities or poisons. Adding metals to guard beds can reduce coking, minimizing pressure drop and surface area loss while improving poison trapping, extending catalyst life, and enhancing inorganic compound removal.

Commercial Pathway to Green Fuels and Chemicals – Pilot Scale Demonstration Upgrading Woody Biomass Pyrolysis Oil Using Fluid Catalytic Cracking.

***Lucas Dorazio**[1], James C. Fu[2], Reinhard Seiser[3], and Jessica Olstad[4]*

(1)BASF, Iselin, NJ, (2)Refining Catalyst R&D, BASF Corporation, (3)NREL, Golden, CO, (4)National Renewable Energy Laboratory, Golden, CO

This contribution discusses results from a pilot scale circulating FCC riser study exploring co-processing of woody biomass based pyrolysis oil. We will discuss the impact of catalyst design on reaction chemistry and deoxygenation pathway. We will also describe the impact biooil addition has on the operation of the riser reactor.

Sugars and Polysaccharides As Renewable Feedstocks: The Use of Microwaves and Catalytic Mechanisms for Oxygenates.

Iris Yu
Civil & Environmental Engineering, National University of Singapore, Singapore, Singapore, Singapore

Energy-efficient processing and selective production are key to biomass valorization. We explore the potential of microwave-assisted processing in offering superheating, which concentrates energy on activating target chemical bonds. Furthermore, understanding the behaviors of bio-based molecules on catalyst surfaces will guide the future catalyst design for high-throughput and selective reactions.

Catalytic Reduction of Esters over Zirconia-Supported Metal Catalysts.

***Javier Chavarrio**, Kyle Kirkendall-Jones, Raka G. Dastidar, and George W Huber*
Department of Chemical and Biological Engineering, University of Wisconsin-Madison, Madison, WI

This study investigates the catalytic reduction of esters in alcohol-rich streams for synthetic diesel production. The authors developed a mechanistic kinetic model for ester hydrogenolysis, demonstrating that Cu/ZrO2 catalysts effectively reduce esters to alcohols. The process can be applied to complex alcohol coupling product streams, achieving 96% ester reduction.

Role of Lewis Acid Sites in Mono- and Trimetallic Zeolites for Ethanol Upgrading to Butene-Rich Olefins..

***Shivangi Nandkumar Borate**[1], Young Gul Hur[1], Meijun Li[2], Stephen Purdy[3], Andrew D. Sutton[3], and James W. Harris[1]*
(1)Department of Chemical and Biological Engineering, The University of Alabama, Tuscaloosa, AL, (2)Manufacturing Science Division, ORNL, Oak Ridge, TN, (3)Manufacturing Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN

Yttrium- and lanthanum-containing dealuminated Beta zeolites catalyze aldol condensation. Trimetallic catalysts containing Y/La, Cu, and Zn were tested for ethanol upgrading to C_{3+} olefins. C-C coupling rates, product selectivities, and catalyst deactivation were assessed. The impact of Cu sintering and coke deposition will be discussed.

CO2 - CO2 CAPTURE AND UPGRADING

CO2 - CO_2 CONVERSION TO HYDROCARBONS

Monday, June 9, 2025 3:40 PM - 5:40 PM
Centennial Ballroom IV

Chair: Lifeng Zhang, Eastman Chemical Company

Co-Chair: Marcella Lusardi, Princeton University

Selective Production of Jet Fuels By Direct CO_2 Hydrogenation on Hybridized K/Fealox-ZSM-5.

***Jong Wook Bae**, Dongming Shen, and Ye Ji Kim*
School of chemical engineering, Sungkyunkwan University (SKKU), Suwon-si, Gyeonggi-do, Korea, Republic of (South)

The production of Sustainable Aviation Fuel (SAF) has been largely investigated worldwide as one of the candidates for solving recent environmental problems. Therefore, hybridized tandem catalysts were investigated for the activation of CO_2 stepwise tandem reactions such as reverse water gas shift (RWGS) and subsequent Fischer-Tropsch synthesis (FTS) reaction.

Bifunctional Heterogeneous Catalyst for the Direct Hydrogenation of CO_2 to C_{2+} Compounds.

***Sankar Meenakshisundaram**[1], Alberto Gonzalez-Fernandez[1], Matthew Lindley[1], Sarah Haigh[2], Chris Hardacre[3], Shashikant Kadam[4], James Paterson[5], Stephen Poulston[6], and Christopher Hawkins[6]*
(1)Cardiff Catalysis Institute, Cardiff University, Cardiff, United Kingdom, (2)Department of Materials, The University of Manchester, Manchester, United Kingdom, (3)Chemical Engineering, The University of Manchester, Manchester, United Kingdom, (4)Applied Sciences, Innovation & Engineering, bp, Saltend, United Kingdom, (5)Fischer-Tropsch, bp, Kingston upon Hull, United Kingdom, (6)Johnson Matthey Technology Centre, Reading, United Kingdom

The transformation of CO_2 into C_{2+} hydrocarbons has emerged as a key area of research in recently, driven by its potential for sustainable chemical production. This study explores the direct conversion of CO_2 into C_{2+} hydrocarbons by the coupling of chemisorbed intermediates to form C–C bonds over a bifunctional catalyst.

Alkali Metal Promoted Fe-Based Catalyst for CO2 Conversion into Hydrocarbons.

***Cong Zhou**[1], Wei Zhang[2], Thuy Le[2], Sungmin Kim[1], Huamin Wang[1], and Johannes Lercher[1]*
(1)Pacific Northwest National Laboratory, Richland, WA, (2)Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA

This study reports a catalyst formulation with high selectivity to hydrocarbons from CO2 transforming it into liquid fuels and high-value-added chemicals. A mechanistic pathway and a strategy for conversion of CO_2 is discussed allowing to minimize methane formation.

Metal Oxide Mobility in Zeolite: Impact on Hydrocarbon Pools and Its Inhibition Via Silicalite-1 Coating during CO_2 Hydrogenation.

Fatima Mahnaz[1], *C D Balaji*[2], *Jasan Robey Mangalindan*[1], *Jenna Vito*[1], *Jithin John Varghese*[3], *and Manish Shetty*[1]
(1)Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX, (2)Department of Chemical Engineering, Indian Institute of Technology Madras, Chennai, India, (3)Department of Chemical Engineering, Indian Institute of Technology Madras, Chennai, Tamil Nadu, India

Efficient conversion of CO_2-to-hydrocarbons over bifunctional oxide/zeolite catalysts rely on the proximity between redox and Brønsted acid sites. This study investigates how metal oxide mobility affects hydrocarbon pool formation within zeolite pores when integrated at nanoscale proximity and explores strategies to inhibit oxide mobility to enhance catalyst performance and reactivity.

Elucidating Cesium Promotional Effects on Hydrogenation of CO/CO_2 to Light Olefins.

Olusola Johnson*, Babu Joseph, and John Kuhn*
Chemical, Biological, & Materials Engineering, University of South Florida, Tampa, FL

Cesium-promoted iron catalyst enables selective and stable CO_2 hydrogenation to light olefins, demonstrating high C_2-C_4 selectivity. The study elucidates cesium's promotional effects through electronic modification of iron and enhanced carbide formation, providing design principles for CO_2-to-olefin catalysis.

Role of Zeolite Acidity and Metal Oxide-Zeolite Proximity Towards Olefins Selectivity in CO_2 Hydrogenation to Olefins over Znzrox-Aei Tandems.

Ahmed Sajid[1], *Julien Devos*[2], *Ibrahim Khalil*[1], *and Michiel Dusselier*[1]
(1)Center for Sustainable Catalysis and Engineering, KU Leuven, Leuven, Belgium, (2)Center for Sustainable Catalysis and Engineering, KU Leuven, Leuven, /, Belgium

This work is dedicated to the improvement of AEI zeolite (SSZ-39) performance by steaming towards olefin selectivity in tandem CO_2 to olefins process. Steamed SSZ-39 showed 10 times higher olefin/paraffin ratio as compared to its un-steamed version, with 4 times slower deactivation in tandem system vs. methanol to olefin reaction.

ELECTRO PHOTO - ELECTROCATALYSIS AND PHOTOCATALYSIS

ELECTRO PHOTO - OXYGEN ELECTROCATALYSIS

Monday, June 9, 2025 3:40 PM - 5:40 PM
Centennial Ballroom I

Chair: William Tarpeh, Stanford University

Co-Chair: Brian Tackett, NIST

M-N-C Electrocatalysts for Oxygen Reduction: Selectivity Origin, Rate-Limiting Step, and New Site Structure.

Yuanyue Liu
The University of Texas at Austin, Austin, TX

Single metal atom embedded in nitrogen doped graphene (M-N-C) is a promising catalyst for oxygen reduction reaction (ORR). Here we used advanced atomistic simulation methods to uncover its selectivity origin, rate-limiting step, and new site structure.

Supported Metal Catalysts Overcome Limitations in Reactivity for Oxygen Electrocatalysis.

Asmee Prabhu, Kah Meng Yam, Chak Sing Bryan Lee, Lavie Rekhi, Luan Q. Le, and ***Tej Choksi***
School of Chemistry, Chemical Engineering and Biotechnology, Nanyang Technological University, Singapore, Singapore

Using density functional theory, we show that interfacial polarization in supported metal catalysts transcends ubiquitous limitations in the reactivity of catalysts for the oxygen reduction reaction. We rediscover the superior performance of experimentally reported supported metal carbides and rationalize why such reactivity limitations are overcome through an electronic structure analysis.

Adsorbate Electric Field Strength Sensitivity Explains Oxygen Reduction pH Dependency.

Jay Bender[1]*, Rohan Sanspeur*[2]*, Nicolas Bueno Ponce*[3]*, Angel Valles*[1]*, Alyssa Uvodich*[1]*, Delia Milliron*[4]*, John Kitchin*[2]*, and Joaquin Resasco*[1]
(1)McKetta Department of Chemical Engineering, The University of Texas at Austin, Austin, TX, (2)Chemical Engineering, Carnegie Mellon University, Pittsburgh, PA, (3)Chemistry and Biochemistry, Texas State University, San Marcos, TX, (4)Chemical Engineering, The University of Texas at Austin, Austin, TX

Over weakly binding catalysts (Au or Ag), oxygen reduction rates increased with electrolyte pH while rates were unaffected by electrolyte pH over strongly binding catalysts (Pt, Ir, Ru). We argue that the adsorbate's sensitivity to electric field strength in the kinetically relevant elementary step explains pH dependency for the ORR.

Electronic and Geometric Activity Promotion in Pdge Intermetallic Electrocatalysts with Enhanced Oxidative Stability.

Majd Matalkeh[1]*, Jin LI*[1]*, Andrew Wong*[1]*, Bryan Vogt*[2]*, Michael Janik*[2]*, and* ***Ezra L. Clark***[1]
(1)Chemical Engineering, Penn State, University Park, PA, (2)Chemical Engineering, The Pennsylvania State University, University Park, PA

A new method for preparing near-surface Pd_xGe_{1-x} intermetallic electrocatalysts is developed that imparts significant oxidative stability and corrosion resistance into the material, which make

it capable of catalyzing reactions that occur at relatively anodic potentials. The catalyst exhibits an O_2 reduction activity roughly an order of magnitude higher than Pd.

On the Geometric Particle Size Effect for Nickel Nanoparticles for Electrochemical Hydrogen Peroxide Production.

*Johannes Hendrik Bitter, **Ivo van Luijk**, and Akbar Asadi Tashvigh*
Wageningen University, Wageningen, Netherlands

Ni on the edges and corners of supported Ni nanoparticles are active and selective towards electocatalytic production of H2O2.

Robust OER Electrocatalysts from Calixarene-Templated Nanoporous Iridium.

***Lara-Pauline Faden**[1], Minkyoung Kwak[2], Shannon Boettcher[3], William Mustain[4], and Alexander Katz[1]*
(1)Chemical and Biomolecular Engineering, University of California, Berkeley, Berkeley, CA, (2)University of California, Berkeley, Berkeley, CA, (3)and Energy Storage and Distributed Resources Division, Lawrence Berkeley National Laboratory, Berkeley, CA, (4)Chemical Engineering, University of South Carolina, Columbia, SC

The highly dispersed nature of nanoporous IrOx is manifested in a high ECSA, making it a promising material to reduce Ir loading in commercial water electrolyzers. We observe robust stability, which we attribute to our electrocatalysts being formed under strain in the presence of bubbles.

FUNDAMENTALS - FUNDAMENTALS OF CATALYSIS AND SURFACE SCIENCE

FUNDAMENTALS - STRUCTURAL EVOLUTION OF CATALYSTS

Monday, June 9, 2025 3:40 PM - 5:40 PM
Centennial Ballroom II

Chair: Andrew Palermo, Johnson Matthey

Co-Chair: Kausthubh Savant, University of California, Los Angeles

MgO-Thin-Film Supported Atomically Dispersed Pt Solid-Solution Catalyst for CO Oxidation: Elucidation of Deep-Surface Pt.

*Yizhen Chen[1], Xiao Zhao[2], Yizhi Zhang[3], Peifen Lyu[4], Bo Yang[3], Hao Chen[5], Marina Leite[4], Haiyan Wang[3], Miquel Salmeron[2], and **Bruce Gates**[6]*
(1)Chemical Engineering, University of California, Davis, Davis, CA, (2)Lawrence Berkeley National Laboratory, Berkeley, CA, (3)Purdue University, West Lafayette, IN, (4)University of California - Davis, Davis, CA, (5)Stanford University, Stanford, CA, (6)Department of Chemical Engineering, University of California - Davis, Davis, CA

IR spectra, AFM images, depth profiling XPS data, STEM images, and ambient-pressure XPS data show how Pt single atoms diffuse into the MgO subsurface and then into the MgO bulk during calcination, determining the details of the chemistry. Spin-coated samples open a new frontier for investigating metal-support interactions in catalysts.

Physical Transformations of Rh/TiO_2 Catalysts Under Reverse Water Gas Shift Conditions That Dictate Stability.

Seunghwa Hong[1], *Emily K. Schroeder*[1], *Selin Bac*[2], *Xiaobo Chen*[3], *Adam Hoffman*[4], *Jake A. Heinlein*[5], *Ashley Head*[3], *Simon Bare*[4], *Matteo Cargnello*[6], *and Phillip Christopher*[2]
(1)Department of Chemical Engineering, University of California, Santa Barbara, Santa Barbara, CA, (2)Chemical Engineering, University of California, Santa Barbara, Santa Barbara, CA, (3)Brookhaven National Laboratory, Upton, NY, (4)Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, Menlo Park, CA, (5)Department of Chemical Engineering, Stanford University, Stanford, CA, (6)Chemical Engineering, Stanford University, Stanford, CA

We explored the effect of initial Rh structure distribution and crystal phase of TiO_2 support on the physical transformations and long-term reactivity degradation in reverse water gas shift reactions at elevated temperatures, revealing a strong structure sensitivity that affects both CO selectivity and catalyst stability.

Understanding Reactant-Induced Sintering in Hydrogenation of Liquid Hydrogen Carriers over Metal Catalysts.

Sara Ahsan[1], *Matthew Edgar*[1], *Jingrui Wei*[2], *Sirinada Chantachaiwat*[1], *Paul Voyles*[2], *and Siddarth Krishna*[1]
(1)Chemical and Biological Engineering, University of Wisconsin-Madison, Madison, WI, (2)Material Science and Engineering, University of Wisconsin-Madison, Madison, WI

We examine how the structure of N-heterocyclic hydrogen carrier molecules impacts catalytic reactivity and stability during hydrogenations over supported metal catalysts. Using flow reactions and post-reaction characterizations, we show that methyl groups promote surface metal migration and sintering, offering insights for designing stable catalysts for efficient long-duration hydrogen storage.

Turnovers Drive Pt Catalyst Particle Surface Reconstruction to Non-Equilibrium Surface Structures.

Silvia Marino[1], *Samji Samira*[1,2], *Ryan Berry*[1], *Michael Gordon*[1], *and Phillip Christopher*[1]
(1)Department of Chemical Engineering, University of California, Santa Barbara, Santa Barbara, CA, (2)Department of Chemical Engineering, Virginia Tech, Blacksburg, VA

CO adsorption on Pt nanoparticles drives surface reconstruction, favoring undercoordinated sites over well-coordinated sites due to faster turnovers. In-situ IR and photolysis experiments show reversible surface roughening induced by rapid CO adsorption-desorption, challenging

equilibrium-based predictions. These findings highlight the impact of CO turnovers on surface restructuring.

The Impact of Coordination Environment on Single-Atom Catalysis.

Ugochukwu Nwosu[1] *and Samira Siahrostami*[2]
(1)Chemistry, Simon Fraser University, Burnaby, BC, Canada, (2)Department of Chemistry, Simon Fraser University - Burnaby Campus, Burnaby, BC, Canada

Using density functional theory calculations, we explore the effect of modifying the identity of metal-coordinating atoms in single-atom catalyst motifs for carbon dioxide reduction and nitrate reduction. We find that the nature of the coordinating sphere can both modify the reactivity metal centre and serve as an active site.

Regenerability of Ga-Si-Al_2O_3 Catalysts for Propane Dehydrogenation.

Melis Yarar[1]*, Zixuan Chen*[1]*, Paula Abdala*[1]*, Christophe Copéret*[2]*, Alexey Fedorov*[1]*, and Christoph R. Müller*[1]
(1)Department of Mechanical and Process Engineering, ETH Zurich, Zurich, Switzerland, (2)Department of Chemistry and Applied Biosciences, ETH Zürich, Zürich, Switzerland

Regenerability of Ga-Si-Al_2O_3 catalysts for propane dehydrogenation was studied to elucidate the role of different interface and speciation. Atomic layer deposition of metals allowed to engineer model surfaces which revealed declining activity correlates with lower reducibility of Ga^{3+} sites and increasing relative fraction of $^{[5,6]}Ga^{3+}$ sites with repeated PDH-regeneration cycles.

HYDRO ECON - CATALYSIS FOR THE HYDROGEN ECONOMY

HYDRO ECON - DEHYDROGENATION

Monday, June 9, 2025 3:40 PM - 5:40 PM
Centennial Ballroom III

Chair: Mohammadreza Karamad, Simon Fraser University

Co-Chair: Kasun Gunasooriya, University of Oklahoma

Quantifying Reaction-Diffusion Phenomena of Ethane Dehydrogenation on Two-Dimensional Metal Carbide Catalysts.

Tobias Misicko[1] *and* ***Yang Xiao***[2]
(1)Louisiana Tech University, Ruston, LA, (2)Department of Chemical Engineering, Louisiana Tech University, Ruston, LA

We developed a two-dimensional Mo_2TiC_2 MXene Pt nanolayer catalyst, which exhibits promising ethane dehydrogenation stability and activity: 24-h without deactivation at 550 °C, turnover frequencies 1.2 s^{-1} and high selectivity (>95%) toward ethylene. The pore size

influences intrinsic kinetics and diffusion of both reactants and products in ethane dehydrogenation.

Controlling the Copper Cluster Size and Cu-O Coordination Enhances Alkanol Dehydrogenation.

Zhiyu Qi[1], *Wenda Hu*[1,2], *Chia-Yu Chang*[3], *Jinshu Tian*[2], *Mingwu Tan*[4], *Hao Xu*[1], *Zihao Zhang*[2], *Jian Zhi Hu*[1,2], *Bing Joe Hwang*[3], *and Yong Wang*[1,2]
(1)The Gene and Linda Voiland School of Chemical Engineering and Bioengineering, Washington State University, Pullman, WA, (2)Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA, (3)Chemical Engineering, National Taiwan University of Science and Technology, Taipei, Taiwan, (4)4Agency for Science, Technology and Research (A∗STAR), Singapore, Singapore

1% Cu/CeO_2 calcined at 800 °C, featuring ~30-atom clusters synergizing with oxygen vacancies, achieves superior propanol dehydrogenation rates compared to other particle sizes and Cu-O coordinations. These findings offer guidance for designing efficient Cu catalysts for alcohol dehydrogenation and related processes, with broader implications for hydrogen production and storage.

Driving Thermochemical Dehydrogenations with Electrochemistry.

Rui Zeng[1] *and Yogesh Surendranath*[2]
(1)Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA, (2)Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, MA

The transition to hydrogen economy is challenged by the sluggish dehydrogenation reactions in hydrogen carriers. A hydrogen-selective membrane can promote them but are limited by low separation efficiency and hydrogen partial pressure. We report an electrochemical approach to circumvent these challenges by pairing a hydrogen-selective membrane with an electrochemical cell.

Formic Acid Decomposition over Supported Pd Alloy Catalysts: Role of Oxygen in Hydrogen Production.

Nandam Hemanth Kumar, Ankit Kumar, Riya Javiya, and ***Abinaya Sampath***
Indian Institute of Technology Gandhinagar, Gandhinagar, India

This study provides fundamental understanding of the effects of Ag on Pd-catalyzed formic acid dehydrogenation under aerobic conditions where water formation is preferred over hydrogen. We conclude that Ag electronically modifies Pd and the Pd-formic acid interaction and promotes hydrogen formation over water without modifying the mechanism of hydrogen production.

KEYNOTE: The Role of Hydrogen in Catalysis and the Role of Catalysis in the Hydrogen Economy.

Maurits van Tol
Johnson Matthey, Royston, United Kingdom

We will share how we see the role of hydrogen develop in the coming decade and we will provide an overview of "the art of the possible" in low-carbon intensity production of chemicals and energy.

Catalyst Acrobatics in the Cryogenic Spin Flipping of Ortho-to-Parahydrogen with Relevance to H_2 Liquefaction and Transport..

Michael Reynolds
Shell Exploration and Production Company, Houston, TX

Hydrogen is a future energy carrier based on its heating value and energy density. However, only liquid hydrogen is economic to transport at scale. This presentation will explain hydrogen liquefaction and discuss catalysts for converting hydrogen's two spin isomers at low temperatures, the apparatus used, and the value to industry.

Iron-Based Catalyst for Production of Hydrogen and Carbon Nanotubes through the Catalytic Decomposition of Methane..

Shashank Shekhar[1] *and K. K. Pant*[2]
(1)Pressure and Catalysis Group, AbbVie, North Chicago, IL, (2)Chemical Engineering Department, Indian Institute of Technology Delhi, New Delhi, India

Catalytic decomposition of methane using Fe and Fe-Ni catalysts achieved 75% methane conversion at 800 °C. While Fe catalysts offer high stability, Ni addition slightly improved conversion and significantly enhanced CNT quality (higher ID/IG ratio). This work highlights cost-effective catalyst development for hydrogen production and high-quality CNTs without greenhouse emissions.

Green Hydrogen Use in Hazardous Process.

Abhineet Raj
Process Safety, Tata Steel Ltd., Jamshedpur, India

Hydrogen injection trial was done in 4 tuyeres via hydrogen tanker. This helped in gaining important answers related to technology required for safe handling and injection of hydrogen in blast furnace.Our company became to inject such large volume of hydrogenin any Blast Furnace

Enhancing Hydrogen Release from Liquid Organic Hydrogen Carriers (LOHCs) and Addressing Catalyst Instability through Cross-Scale Modeling.

Shyam Deo[1]*, Wenyu Sun*[1]*, Tanusree Chatterjee*[1]*, Victoria Ehlinger*[2]*, Thomas Moore*[3]*, Mengyao Yuan*[2]*, Giovanna Bucci*[2]*, Matthew Mcnenly*[2]*, and Sneha Akhade*[1]
(1)Material Science Division, Lawrence Livermore National Laboratory, Livermore, CA,

(2)Engineering Directorate, Lawrence Livermore National Laboratory, Livermore, CA,
(3)Queensland University of Technology, Brisbane, QLD, Australia

LOHC technology revolutionizes hydrogen storage and release. Our Systems-To-Atoms (S2A) framework integrates chemistry and structure to enhance catalyst durability by addressing degradation mechanisms. These advancements ensure efficient, sustainable hydrogen release, unlocking LOHC's potential for a cleaner energy future.

MONNIER - JOHN MONNIER MEMORIAL SESSIONS

MONNIER - JOHN MONNIER MEMORIAL SESSION 2

Monday, June 9, 2025 3:40 PM - 5:40 PM
Hanover Hall FG

Chair: Weijian Diao, Villanova University

Co-Chair: Gregory Tate, Applied Catalysts

Where's the Top? Examining History and Aspects of Ethylene Oxide Catalyst Optimization.

John Lockemeyer
Catalysis, Shell Global Solutions US, Houston, TX

A brief history of ethylene oxide catalyst development will be presented. The aspects of optimization of alkali dopants in catalyst formulations and organic chloride moderator levels in normal operation will be discussed. An emphasis on the relevance to commercial operation will be illustrated with examples of catalyst testing.

Effects of the method of active site characterization for determining structure-sensitivity in Ag-catalyzed ethylene epoxidation [1].

Benjamin Egelske
Chemical Engineering, University of South Carolina Columbia, Columbia, SC

This study investigates the particle size effect reported for silver catalyzed ethylene epoxidation applying electroless deposition to create a series of catalysts with narrow particle size distributions. Our findings indicate an insensitive relationship between particle size and turnover frequency but a direct relationship for particle size and ethylene oxide selectivity.

Understanding Hydrogenation Catalysis with Supported Molecular Calixarene-Ir Clusters.

Alexander Katz
Chemical and Biomolecular Engineering, University of California, Berkeley, Berkeley, CA

This presentation focuses on understanding of hydrogenation catalysis as enabled by protected-but-accessible supported molecular calixarene-Ir catalysts.

Fundamental Studies of Hydrocracking Catalysts in a Vacuum Gas Oil Feed.

Melanie Schaal
Catalysis Applications, Honeywell UOP, Des Plaines, IL

The 'sweet science' of catalysis is crucial for the selective cracking of high molecular weight hydrocarbons to lower MW hydrocarbons. Dr. Monnier believed the reaction itself was the ultimate characterization tool. In his honor, fundamental reaction studies will be presented which demonstrate the importance of metal-acid proximity in hydrocracking catalysts.

Critical Importance of High Pressure and High Selectivity for a Successful Oxidative Coupling of Methane (OCM) Process.

Madan Bhasin
Innovative Catalytic Solutions, Charleston, WV

For commercially successful OCM process, high pressures of >10 atm. and selectivity >80% to C2+ are critically important. Several non-stoichiometric, defect/disordered rare-earth oxycarbonate catalysts (characterized by atomic level resolution techniques) have been discovered that give, for the first time, 70-73% selectivity at 10 atm. in microreactors stable for ~30 days.

Improved Study of the Oxidative Coupling of Methane at Elevated Pressure and Temperature: Investigating Gas Phase OCM Using Calculated Void Volume in Reactor.

Kevin Enyekwe[1]*, John Meynard Tengco*[2]*, John Monnier*[2]*, John Regalbuto*[2]*, Madan Bhasin*[3]*, and Hamid Reza Godini*[4]
(1)chemical engineering, University of South Carolina, columbia, SC, (2)Chemical Engineering, University of South Carolina, Columbia, SC, (3)Innovative Catalytic Solutions, Charleston, WV, (4)C1 Green Chemicals, Berlin, Berlin, Germany

The OCM gas phase reaction was investigated using reactor setups with different void volume. This approach enables us to see the effect of gas phase activity in an OCM catalytic reaction. From the results, there was a significant implication of having different level of void volume in the reactor.

PHARMA - CATALYSIS FOR PHARMACEUTICAL AND FINE CHEMICAL SYNTHESIS

PHARMA - CATALYSIS FOR PHARMACEUTICAL AND FINE CHEMICAL SYNTHESIS

Monday, June 9, 2025 3:40 PM - 5:40 PM
Regency Ballroom VII

Chair: Yujie Sun, University of Cincinnati

Co-Chair: Shane Chen, Johnson Matthey

KEYNOTE: Isotopically Labeled Compound Synthesis through Innovative Catalysis.

Jingwei Li
Merck & Co, Rahway, NJ

Novel catalytic reactions have the potential to significantly transform synthetic organic chemistry in various impactful ways. In my talk, I will showcase how our labeled compound synthesis group has discovered, developed, and implemented novel isotope labeling methodologies through innovative catalytic approaches to facilitate and accelerate delivery of these crucial compounds.

Understanding the Molecular Origin of Performance Enhancements Seen Under Rapidly Alternating Polarity (rAP) in Organic Electrosynthesis.

Megan Kelly[1]*, Asmaul Hoque*[2]*, Shannon S. Stahl*[3]*, and Marcel Schreier*[4]
(1)Chemical and Biological Engineering, University of Wisconsin-Madison, Madison, WI, (2)Chemistry, University of Wisconsin-Madison, Madison, WI, (3)Department of Chemistry, University of Wisconsin-Madison, Madison, WI, (4)Chemical and Biological Engineering & Chemistry, University of Wisconsin-Madison, Madison, WI

We utilize electrochemical reactors which enable precise control of mass transfer to study interfacial phenomena occurring under rapidly alternating polarity (rAP). Our results indicate that mass transfer plays a key role in rAP's ability to mediate interfacial reagent concentrations to enhance reaction performance and chemoselectivity.

Bimetallic Alloy Nanoparticles for Stereoselective Heterogeneous Hydrogenation.

Christina Li
Chemistry, Purdue University, West Lafayette, IN

Bimetallic alloy nanoparticles are important catalysts for selective heterogeneous hydrogenation reactions. Our group recently showed that bimetallic alloys comprising a noble metal and a base metal are capable of highly diastereoselective hydrogenation reactions, where the base metal adsorbs a heteroatom directing group on the substrate and drives facially-selective hydrogen addition.

Eco-Friendly Innovation: Lead-Free Lindlar Catalyst Evolution.

Shane Chen
Johnson Matthey, West Deptford, NJ

The selective semi-hydrogenation of alkynes plays a vital role in industrial applications, but the use of conventional Pb-containing Lindlar catalysts raises significant environmental concerns. This research focuses on developing Pb-free alternatives through innovative approaches in catalyst design, characterization, and kinetic analysis, offering sustainable solutions to these challenges.

Production of Biorenewable, Enantiopure (S)-3-Hydroxy-γ-Butyrolactone for Pharmaceutical Applications.

Justin Waters[1], Elnaz Jamalzade[2], Hussein T. Abdulrazzaq[3], Nathaniel Kuch[4], Sampath Gunukula[1], James A. Dumesic[5], Philip Kersten[4], and ***Thomas Schwartz***[3]
(1)University of Maine, Orono, ME, (2)Chemistry, University of Maine, orono, ME, (3)Chemical and Biomedical Engineering, University of Maine, Orono, ME, (4)Forest Products Laboratory, Madison, WI, (5)Department of Chemical and Biological Engineering, University of Wisconsin-Madison, Madison, WI

This presentation describes recent efforts at synthesizing (S)-HBL from biomass at mild conditions, showing quantitative yield of enantiopure (S)-HBL can be obtained from glucose at 298K, using a combination of biological and chemical catalysis. Enzyme catalysis converts glucose to an intermediate that is converted to (S)-HBL by homogeneous chemical catalysis.

OTHER EVENTS

MONDAY POSTER SESSION

Monday, June 9, 2025 6:00 PM - 8:00 PM
Grand Hall

The Role of Zinc in Fe-Co-Zn Trimetallic Catalysts for CO_2 Conversion to Light Olefins.

James Carter*, Haaris Razzaq, Jared Lugo, and Cheng Zhang*
Long Island University Post, Brookville, NY

Fe_1Co_2 was identified as the optimal ratio for Fe-Co bimetallic catalysts, and the role of Zn as a promoter in Fe-Co-Zn trimetallic catalysts ($Fe_1Co_2Zn_1$) was investigated. The novelty of this work lies in the use of Fe, Co, and Zn organometallic complexes to synthesize highly magnetic Fe-Co-Zn trimetallic catalysts.

Microkinetic Modelling of Ethylene Oligomerization on H-BEA Zeolites.

Sai Praneet Batchu[1]*, Boen Cao[2], Rajamani Gounder[2], and Linda Broadbelt*[1]
(1)Department of Chemical and Biological Engineering, Northwestern University, Evanston, IL, (2)Charles D. Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN

We perform microkinetic modelling of ethylene oligomerization to form linear and cyclic alkanes, alkenes, dienes, and aromatics on H-BEA. Such complex mechanistic models for this chemistry are handful in literature, and specifically none on H-BEA. Network generation techniques, kinetic and thermodynamic formalisms, and experiments are synchronized to make this model.

Bimetallic SSZ-13 Catalyst for Partial Methane Oxidation to Methanol.

Motunrayo Ogunleye *and Daniel Shantz*
Tulane University, New Orleans, LA

Secondary transition metals (Co, Zn, Ni, Fe) were doped into Cu-SSZ-13 to improve its catalytic activity for partial methane oxidation to methanol. Cu,Zn-SSZ-13 was the best bimetallic catalyst. DRIFTS spectroscopy showed zinc doping increased methanol production by displacing more copper towards the 8membered ring cage i.e. reaction active site.

Selective Hydrogenation of Acetylene Towards Ethylene over Single-Site Catalysts.

Xin Deng[1] *and Weijie Li*[2]
(1)Georgia Institute of Technology, Atlanta, GA, (2)Nankai University, Tianjin, China

The selective hydrogenation of C≡C to C=C remains essential for polymer and fine chemical industries. Single-metal confined within zeolite (M@zeolite) and single-site metallic catalyst (M/Al) achieve high acetylene conversion and ethylene selectivity. Advanced techniques (XAS, STM, in-situ spectroscopy, DFT) reveal their unique structures, hydrogen activation pathways and distinct hydrogenation mechanisms.

A Novel Approach to Synthesize Fe-Zn Bimetallic Catalysts for CO2 Hydrogenation to Value-Added Chemicals..

Habiba Mosbah, ***Kenly Moran***, *Cheng Zhang, and Jared Lugo*
Long Island University Post, Brookville, NY

The performance of the synthesized Fe-Zn catalyst demonstrates favorable results of enhanced CO_2 conversion and selectivity toward light olefins, which are crucial in the chemical industry and offer a promising solution for reducing greenhouse gas emissions while utilizing renewable energy sources.

Synthesis and Application of Re or Ru-Doped Mg_xAlO_y–SiO_2 Catalysts for Ethanol Conversion to 1,3-Butadiene.

Maynara Santos[1], *Fabio Toniolo*[2], *Michael Lanci*[3], *Trong Pham*[4], *Naveen Agrawal*[4], *and* ***Henrique Pacheco***[1]
(1)Chemical Engineering Program - COPPE - UFRJ, Federal University of Rio de Janeiro, Rio de Janeiro, Brazil, (2)Chemical Engineering Program - COPPE - UFRJ, Federal University of Rio de Janeiro, (3)ExxonMobil Corporation, Annandale, NJ, (4)ExxonMobil Technology and Engineering, Annandale, NJ

Ethanol conversion using Mg-Al-Si oxides with Ru or Re reveals high acetaldehyde selectivity (>40%) due to dehydrogenation promotion. The Re catalyst shows reduced dehydration product selectivity and lower BD yield but higher conversion; it deactivates faster than Ru, with a 15% conversion decline after 70 hours versus 7% for Ru.

Sn Doping of PdAg Catalysts for Acetylene Hydrogenation to Improve Selectivity and Activity Profile.

James Earley
Johnson Matthey, Billignahm, United Kingdom

The addition of Sn to PdAg in the selective reduction of acetylene to ethylene has been shown to greatly improve the selectivity and also the activity profile. DFT and advanced characterisation techniques have been used to elucidate the effect

Alcohol-Water Solvent Systems and Their Effects on Selectivity and Product Distribution for the Conversion of Lactates to Sustainable Acrylates.

Sophie Brauer[1]*, Paul J. Dauenhauer*[1]*, and Christopher Nicholas*[2]
(1)Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN, (2)Lakril Technologies Corporation, Chicago, IL

In the lactate-to-acrylate reaction over zeolites, small amounts of alcohol added to aqueous methyl or ethyl lactate feeds can dramatically improve selectivity to acrylate products. Acrylic acid is preferentially formed even at high alcohol concentrations, and cross-esterification with co-fed alcohol appears rare. This phenomenon is not predicted by literature mechanisms.

One-Step Conversion of Whole Lignocellulosic Biomass Components into Bio-Based Amines.

Wo Bin Bae*, Christopher Acquah, and Jun Hee Jang*
Department of Chemical Engineering, Rowan University, Glassboro, NJ

The results of this study will provide useful guidance for the single-step conversion of whole lignocellulosic biomass components into bio-based amines. This includes interpretations that contribute to a fundamental understanding of the reaction mechanisms including SCMD-HDO and amination.

SAF Synthesis By Olefin Co-Oligomerization in an Oil Cooled Bench Scale Reactor.

Christoph Hauber[1] *and* ***Matthias Stehle***[2]
(1)hte GmbH, Heidelberg, Germany, (2)R&D Solutions, hte GmbH, Heidelberg, Germany

Hte a provider of high throughput and bench scale testing herein demonstrates the production of olefins oligomerization data at industrial relevant conditions. Using an oil heated bench scale reactor co-oligomerization of ethylene and i-butylene has been performed at supercritical conditions covering a wide parameter range producing high SAF yields.

Depolymerization of Pre-Commercial Lignins By Supported Platinum-Based Catalyst.

Hans-Joerg Woelk[1]*, Franziska Heck*[1]*, and Ingo Graef*[2]
(1)HPM Innovation Chemicals, Heraeus Precious Metals GmbH & Co. KG, Hanau, Germany, (2)Heraeus Precious Metals GmbH & Co. KG, Hanau, Germany

The negative impact of greenhouse gas emissions and global warming is widely recognized by society, politics, academia, and industry as a major and complex challenge for this decade and the decades to come. The use of biomass as a renewable feedstock to produce chemicals is taking off the ground.

Investigating the Role of Zeolite Framework in Brønsted Acid Catalysis: A Study Using Hofmann Elimination of Tert-Butylamine.

Ali Mohammed[1] *and Omar Abdelrahman*[2]
(1)University of Houston, houston, TX, (2)William A. Brookshire Department of Chemical and Biomolecular Engineering, University of Houston, Houston, TX

This study links pore cavities of aluminosilicate zeolite to catalytic performance, revealing structure-activity relationships. Catalytic rate of Hofmann elimination shows a non-linear dependence on aluminosilicate zeolite pore cavity. However, similar apparent activation energies across zeolite samples were measured, indicating pore cavity-independent transition state stabilization beyond a critical pore diameter.

Brønsted Acid Catalyst for Fructose Etherification: Experimental and Theoretical Study.

Nidhi Kushwaha[1]*, Arindam Modak*[2]*, Ejaz Ahmad*[3]*, and K. K. Pant*[4]
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The study shows the application of Brønsted acid catalyst for tandem catalytic reaction of fructose to 5-ethoxymethylfurfural, where a thorough analysis of reaction intermediates have been done to develop a fundamental reaction mechanism and the same has been validated from density functional theory.

Understanding CO_2 Assisted Alkane Oxidative Dehydrogenation over Ceria-Supported Ni Catalysts.

Anoop P Pushkar, Gouri Ramadas Nayanar, Jithin John Varghese, Sagar Sourav, and ***Niket Kaisare***
Department of Chemical Engineering, Indian Institute of Technology Madras, Chennai, Tamil Nadu, India

CO_2-assisted Oxidative Dehydrogenation (ODH) of alkanes is an alternative to the existing methods of alkene production. Ceria-supported Ni catalysts is known to be active for both alkane and CO_2- activation. This combined experimental and computational work investigates the mechanism of CO_2-assisted ODH of ethane over ceria-supported Ni catalysts.

Improving the Activity of Cu-Based Catalysts for Ester Hydrogenation.

Damilola Akinneye[1] *and J. Will Medlin*[2]
(1)Chemical & Biological Engineering, University of Colorado, Boulder, Boulder, CO, (2)Chemical and Biological Engineering, University of Colorado Boulder, Boulder, CO

In this work, we demonstrate the activity of copper catalysts made by ammonia evaporation for methyl acetate hydrogenation and propose a strategy for activity improvement by promoting interfacial effects. The catalysts were modified to increase the Cu^{+} content, we observed that coating mesoporous layers of SiO_2 led to improved activity.

Evaluation of Ga/HZSM-5 Catalysts Prepared By Atomic Layer Deposition on the Ethane Dehydroaromatization Reaction.

Heloisa Bortolini[1]*, Rita M. B. Alves*[2]*, Elisabete Assaf*[3]*, and Justin Notestein*[4]
(1)Department of Chemical Engineering, Escola Politécnica da Universidade de São Paulo, São Paulo, Brazil, (2)Chemical engineering, Universidade de São Paulo, São Paulo, Brazil, (3)Instituto de Química de São Carlos/Universidade de São Paulo, São Carlos, Brazil, (4)Department of Chemical & Biological Engineering, Northwestern University, Evanston, IL

A direct process to obtain BTX from ethane is highly desired. This study evaluates Ga catalysts prepared by ALD for ethane conversion to aromatics, exploring how synthesis methods can enhance catalyst performance and stability.

Catalytic Upgrading of Tire Pyrolysis Oil By Hydrotreating over NiMo Catalysts .

Xuan Huy LE[1]*, Manh Tung Nguyen*[1]*, Emma Olsson Månsson*[1]*, Hoang Phuoc Ho*[1]*, Quoc Khanh Tran*[1]*, Olov Öhrman*[2]*, Derek Creaser*[1]*, and Louise Olsson*[1]
(1)Chemical Engineering, Chalmers University of Technology, Gothenburg, Sweden, (2)Preem AB, Gothenburg, Sweden

Tire pyrolysis oil is an alternative source of inexpensive and valuable fuels for replacing fossil oils. A study on upgrading process of tire pyrolysis oil by hydrotreating with nickel-molybdenum bimetallic catalyst was investigated. Appreciable catalytic activity and effects of reaction temperature and catalyst loading on upgrading process were observed.

Automated Cohp Calculations for the Prediction of Stability and Catalytic Activity in Mixed Transition Metal Oxides (poster).

Ruchika Mahajan[1]*, Kirsten Winther*[2]*, and Michal Bajdich*[3]
(1)Chemical Engineering, Stanford University, Palo Alto, CA, (2)SLAC National Accelerator Laboratory, Menlo Park, CA, (3)SUNCAT Center for Interface Science and Catalysis, SLAC National Accelerator Laboratory, Menlo Park, CA

This work focuses on finding affordable, stable and active catalysts for ORR/OER in hydrogen technologies. By leveraging ICOHP-based bulk descriptors and automating high-throughput

DFT calculations with AutoCatLab python library, we efficiently screen ternary oxides. Finally Prediction models like GPR and GNN help predict bulk stability, accelerating discovery of effective catalysts.

Understanding the Mechanisms of Catalyst Deactivation during Hydrothermal Gasification..

John Sackey[1]*, Michael Timko*[2]*, Xinhua Liang*[3]*, and Jesse Bond*[1]
(1)Biomedical and Chemical Engineering, Syracuse University, Syracuse, NY, (2)Chemical Engineering, Worcester Polytechnic Institute, Worcester, MA, (3)Department of Energy, Environmental & Chemical Engineering, Washington University in St. Louis, St. Louis, MO

Hydrothermal gasification converts organic feedstocks into methane using nickel catalysts. However, deactivation from coke formation, sintering, oxidation, and pore collapse limits performance. This study compares Ni/SiO_2 catalysts prepared via Incipient Wetness Impregnation and Atomic Layer Deposition, emphasizing stability challenges and proposing alternative supports to enhance catalyst longevity and efficiency.

Reductive Catalytic Fractionation of Lignocellulose Using Ru/Mg(OH)2 Using Self-Supplied Hydrogen.

Shinjae Lee *and Kwangjin An*
UNIST, Ulsan, Korea, Republic of (South)

Lignocellulose, a green carbon source, can replace fossil fuels. This study presents a $Ru/Mg(OH)_2$ catalyst for self-supplied hydrogen reductive catalytic fractionation (SCF) of lignocellulose, achieving 50.7 wt% yield of lignin-derived monomers with water as solvent. Model studies elucidate the lignin depolymerization pathway, advancing sustainable biorefinery technologies.

Niw Catalysts Supported on Mesostructured Al_2O_3-Nb_2O_5 for Simultaneous Hdo/HDS Co-Processing.

Luis Jorge Rodriguez Castillo[1,2]*, Franklin J. Méndez*[3]*, Jorge García-Macedo*[3]*, Lina A. Calzada*[4]*, Elim Albiter*[4]*, Jose Eduardo Hernandez*[1]*, Felix Cancino*[1]*, Juan A. Alcantara*[1]*, Carlos Eduardo Santolalla-Vargas*[1]*, and Victor Florencio Santes Hernandez*[1]
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NiW catalysts supported γ-Al_2O_3 mixed with Nb_2O_5 were investigated to examine the influence of Nb content in the simultaneous HDO/HDS co-processing. Supports and catalysts were studied through SEM-EDX, N_2 physisorption, powder XRD, UV-vis DRS, Raman spectroscopy, and H_2-TPR. Sulfured catalysts were further characterized by XPS and HRTEM.

Kinetic Effect of Metal Chloride Ions on the Dehydration of Xylose to Furfural.

Faeze Akbari[1] *and Thomas Schwartz*[2]
(1)Chemical Engineering, GT, ATLANTA, GA, (2)Chemical and Biomedical Engineering, University of Maine, Orono, ME

The study is significant because it explores how metal ions leached from reactor materials impact furfural yield, a critical factor in industrial production. Understanding these interactions can help optimize reaction conditions, minimize furfural degradation, and improve the efficiency of the process, ultimately contributing to more sustainable and cost-effective industrial practices.

Catalytic Influence of Magnesium in Sulfite Acid Black Liquor When Co-Pyrolyzed with Sawdust. a Kinetic Study Using Vyazovkin Method..

Nampe Majoe[1,2]*, Bilal Patel Sr.*[1]*, Isaac N. Beas*[3]*, and Joshua Gorimbo*[4]
(1)Civil and chemical engineering, Unisa, Florida, South Africa, (2)Chemical Engineering, Durban University of Technology, Durban, South Africa, (3)Specialty Chemicals, Botswana Institute for Technology Research and Innovation, (4)CSET, Institute for the Development of Energy for African Sustainability, Florida, South Africa

Vyazovkin kinetics investigated catalytic effect of magnisium, in black liqour (BL). The addition of BL to sawdust lowers the activation energy (*Ea*), with best results in terms of BL to sawdust ratio of 0.7: 0.3. *Ea* lowered from 209.20 kJ/mol to 136.15 kJ/mol.

Catalytic Regeneration of Amine Solvents for Less Energy Intensive Direct Air and Point Source Carbon Capture.

Alexander Wiechert[1]*, Michael Cordon*[1]*, Abishek Kasturi*[1]*, Gyoung Gug Jang*[1]*, Diana Stamberga*[2]*, Jong K. Keum*[3]*, Dhruba Jyoti Deka*[4]*, Aye Meyer*[1]*, Radu Custelcean*[2]*, and Costas Tsouris*[1]
(1)Manufacturing Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN, (2)Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN, (3)Center for Nanophase Materials Sciences and Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge, TN, (4)Pacific Northwest National Laboratory, Richland, WA

Solvent regeneration accounts for a considerable portion of the capture costs incurred in amine-based point source and direct air CO_2 capture systems. The results obtained in this work demonstrate that the energy demand of regeneration can be dramatically reduced through the use of certain catalysts.

Methanol from Reactive Carbon Capture – TEA & LCA Comparisons between Direct RCC-to-Methanol Vs. Indirect Via RCC-to-CO Approaches..

Anh To[1], *Daniel A. Ruddy*[1], *Eric Tan*[1], *Jonathan Martin*[2], *Wilson McNeary*[1], *Martha A. Arellano-Treviño*[1], *Chae Jeong-Potter*[1], *and Alexander J. Hill*[1]
(1)Catalytic Carbon Transformation and Scale-Up Center, National Renewable Energy Laboratory, Golden, CO, (2)National Renewable Energy Laboratory, Golden, CO

This poster compares the feasibility of methanol production using 2 RCC approaches developed by our group at NREL: MeOH-selective or CO-selective followed by separate MeOH synthesis by TEA and LCA comparison

The Effect of Surface Chemistry, Particle Size and Humidity on the Performance and Stability of Functionalized Resins in Direct Air Capture.

Peter Flippo[1], *Jeroen van den Reijen Sr.*[2], *and* ***Marlene Fuhrer***[1,2]
(1)RDS, Avantium, Amsterdam, North Holland, Netherlands, (2)RDS, Avantium, Amsterdam, Netherlands

Avantium R&D Solutions developed a platform to test CO2 adsorbents. Four resins were tested through multiple adsorption-desorption cycles and pretreatment conditions. The study found variations in breakthrough curves, initial capacities, and deactivation rates among the resins due to differences in their chemical and physical properties.

Electric & Magnetic Field-Dependent Carbon Dioxide Adsorption on Mixed-Metal Metal-Organic Frameworks.

Hetansha Boricha[1], *Nitharshni R. G.*[1], *Marcello B. Solomon*[2], *Aravind Chandiran*[1], *Deanna D'Alessandro*[2], *and* ***Niket Kaisare***[1]
(1)Department of Chemical Engineering, Indian Institute of Technology Madras, Chennai, India, (2)School of Chemical and Biomolecular Engineering, The University of Sydney, Sydney, NSW, Australia

This study studies the influence of external electric and magnetic fields on CO_2 adsorption in mixed-metal MOFs, because observations have been made that ZIF-67 showing a 6% decrease under electric fields and a 23.5% increase under magnetic fields. These findings highlight a novel, energy-efficient approach for CO_2 capture and release.

Synthesis of a Highly Magnetic Fe-Mn Bimetallic Catalyst for CO_2 Conversion to Value-Added Chemicals.

Jared Lugo*, Tyler Davide, Jayalatha Robinson, and Cheng Zhang*
Long Island University Post, Brookville, NY

Our research focuses on the catalytic hydrogenation of CO_2 to light olefins and other value added chemicals as a means of addressing CO_2 emissions while simultaneously developing novel

methods of light olefin production for industrial use in polymer, plastic, and hydrocarbon-based material production.

High Yield Synthesis of CO from CO_2 Via Reverse Water-Gas Shift Reaction Using Chemical Looping System.

***Shota Manabe**, Risa Sakurai, Haruka Nishiyama, Keisuke Iijima, Noritoshi Yagihashi, and Yuki Nakama*
SEKISUI CHEMICAL CO.,LTD, Tsukuba, Japan

This work reports investigation of oxygen carrier materials for chemical looping reverse water-gas shift reaction (RWGS-CL). Impregnation of Ni on doped CeO_2 improved H_2 conversion and higher than 90% CO yield was achieved.

Impact of the Metal Center (Zr or Hf) of the Cu/Uio-67 on the Catalytic Performance for Alcohols Production Via CO_2 Hydrogenation.

*Luana Paula, **Janaina F. Gomes**, and **Jose Assaf***
Chemical Engineering Department, Federal University of São Carlos, São Carlos, Brazil

This study explores the influence of metal centers (Zr and Hf) in UiO-67 as supports for Cu sites, emphasizing their role in CO_2 hydrogenation under atmospheric pressure with focus on ethanol production. The increased formation of ethanol may be attributed to the higher density of defects in the Cu/UiO-Zr structure.

Influence of Catalyst Support on Fe-Co Bimetallic Catalyst for Carbon Dioxide Conversion.

***Tyler Davide**[1], Jayalatha Robinson[1], Sanjaya D. Senanayake[2], and Cheng Zhang[1]*
(1)Long Island University Post, Brookville, NY, (2)Chemistry Division, Brookhaven National Laboratory, Upton, NY

This study tackles climate change by leveraging CO_2 as a resource. Using CeO_2-supported Fe-Co bimetallic catalysts with varying Fe/Co ratios, researchers achieved efficient CO_2 hydrogenation. A 1:1 Fe/Co ratio demonstrated high selectivity for light olefins, highlighting the potential of advanced catalysts to reduce emissions and enable sustainable energy solutions.

Identifying Mechanistic Differences between Co-Fed CO_2 Hydrogenation and Reactive CO_2 Capture Using Ru Dual Function Materials.

***Chae Jeong-Potter**, Neha Mehra, Carrie A. Farberow, and Daniel A. Ruddy*
Catalytic Carbon Transformation and Scale-Up Center, National Renewable Energy Laboratory, Golden, CO

We report key differences in surface population and intermediate formation during reactive carbon capture (CO_2 capture then conversion) and co-fed hydrogenation (simultaneous CO_2+H_2

flow) on a Ru-based dual function material. As a result, 100% selective methane production is achieved in RCC but not in co-fed hydrogenation.

Enhanced Isoparaffin Selectivity in CO_2 Hydrogenation By Combining Na-Promoted Fe_3O_4 and Pt/WO_3-ZrO_2 Catalysts.

Changhun Hur[1] *and Kwangjin An*[2]
(1)Ulsan National Institute of Science and Technology, Ulsan, Not US or Canada, Korea, Republic of (South), (2)Ulsan National Institute of Science & Technology, Ulsan, Korea, Republic of (South)

The combination of Na-promoted Fe_3O_4 and acidic Pt/WO_3-ZrO_2 (PtWZ) catalysts with dual-bed system in a single reactor enhanced the synthesis of isoparaffin-rich hydrocarbons in CO_2 hydrogenation. Especially, acidic PtWZ catalyst showed superior isoparaffin production in liquid hydrocarbons and greater coke resistance compared to other acid zeolites (ZSM-5 and MCM-22).

Indium Oxide/Zirconia Catalyst for Carbon Dioxide Hydrogenation to Methanol.

Kun Yang*, An Zhang, and Weijian Diao*
Chemical Engineering, Villanova University, Villanova, PA

This work prepared In_2O_3/ZrO_2 catalysts in wet impregnation (WI) method at different calcination temperature from 300℃ to 600℃ to control In_2O_3 particle size and investigated its influence on catalytic performance over In_2O_3/ZrO_2 catalysts.

Impact of Temperature-Induced Restructuring on Rh/CeO_2 Catalysts in CO_2 Hydrogenation.

Maria Isabella Soares[1]*, Ananda V. Paladino Lino*[2]*, Jose Assaf*[3]*, Elisabete Assaf*[4]*, and Luiz Vieira*[5]
(1)University of São Paulo, São Carlos, Brazil, (2)Universidade Federal de São Carlos, São Carlos, Brazil, (3)Chemical Engineering Department, Federal University of São Carlos, São Carlos, Brazil, (4)Instituto de Química de São Carlos/Universidade de São Paulo, São Carlos, Brazil, (5)Sao Carlos Institute of Chemistry (IQSC), University of Sao Paulo (USP)

High-temperature treatment of Rh/CeO_2 catalysts influences CO_2 valorization via the reverse water-gas shift reaction. At 0.1% Rh, redispersion forms a solid solution with ~100% CO selectivity. Higher Rh loadings (0.5%-1.0%) retain nanoparticles, promoting H_2 spillover and undesired CH_4 formation. Thermal treatment stabilizes active sites, affecting selectivity and activity.

Study of Cu,Zn-Based Methanol Synthesis Catalysts.

Cheonwoo Jeong *and Joonwoo Kim*
Research Institute of Industrial Science & Technology, Gwangyang, Korea, Republic of (South)

In this study, methanol synthesis was investigated using a bench-scale reactor system, achieving a liquid methanol production rate of approximately 534 g/day.

Synthesis of a Novel Magnetic Fe-Co-Zn Trimetallic Catalyst for Carbon Dioxide Conversion to Light Olefins.

Haaris Razzaq**, James Carter, Jared Lugo, and **Cheng Zhang
Long Island University Post, Brookville, NY

We incorporated Zn as a promoter to Fe-Co, forming Fe-Co-Zn trimetallic catalysts for CO_2 hydrogenation. The novelty of this work lies in the use of Fe, Co, and Zn organometallic complexes with varying ratios as precursors.

Synthesis of a Novel Magnetic Fe-Mg Bimetallic Catalyst for CO_2 Conversion to Light Olefins.

***Jawad Mahmud**[1], Cheng Zhang[2], Jared Lugo[2], and Jayalatha Robinson[2]*
(1)Long Island University, Brookville, NY, (2)Long Island University Post, Brookville, NY

In this study, a novel Fe-Mg based catalyst was synthesized, and its performance regarding light olefin yield was recorded and discussed.

Synthesis of a Highly Magnetic Fe-Zr Bimetallic Catalyst for CO_2 Conversion to Light Olefins.

***Laine Leonard**, Laura Pena Marin, Jared Lugo, and Cheng Zhang*
Long Island University Post, Brookville, NY

A synthesized bimetallic catalyst composed of Fe-Zr was evaluated for CO_2 hydrogenation to light olefins. A trend was observed where CO_2 conversion and light olefin production increased with rising temperatures.

A Novel Approach to Synthesize Magnetic FeCo Bimetallic Catalysts for Carbon Dioxide Hydrogenation.

***Jayalatha Robinson**[1], Tyler Davide[1], Sanjaya D. Senanayake[2], and Cheng Zhang[1]*
(1)Long Island University Post, Brookville, NY, (2)Chemistry Division, Brookhaven National Laboratory, Upton, NY

We aim to catalytically transform CO_2 into valuable chemicals, contributing to solutions for global warming and advancements in green energy science. This combination of iron and cobalt results in a robust catalytic system that balances high CO_2 conversion efficiency with excellent selectivity for light olefins.

Zeolite-Metal Nanoparticle Catalysts for Methane Partial Oxidation.

Hannah Even[1]*, Cole Hullfish*[2]*, and Michele Sarazen*[2]
(1)Department of Mechanical and Aerospace Engineering, Princeton University, Princeton, NJ, (2)Department of Chemical and Biological Engineering, Princeton University, Princeton, NJ

Bifunctional palladium nanoparticles supported on or encapsulated in zeolites show promise for methane partial oxidation (MPO) to methanol as investigated by H_2O_2 decomposition reactions. The effect of metal-acid site proximity on H_2O_2 utilization is probed through the physical mixtures of catalysts with acidic supports and addition of aqueous acid.

The Effect of Metal Promoters in an Mo-Supported HZSM-5 Catalyst for the Microwave-Assisted Methane Dehydroaromatization to Aromatics.

Duy Hien Mai[1]*,* ***Swarom Kanitkar***[1]*,* ***Evgeniy M. Myshakin***[2]*, Xinwei Bai*[1]*, Wissam A. Saidi*[3]*, Biswanath Dutta*[1]*, and Daniel Haynes*[4]
(1)NETL Support Contractor, Morgantown, WV, (2)NETL Support Contractor, Pittsburgh, PA, (3)National Energy Technology Laboratory, Pittsburgh, PA, (4)National Energy Technology Laboratory, Morgantown, WV

This study helps to understand the effect of promoting metals on modifying the localized environment in Mo-supported HZSM-5 that is responsible for enhancing MDA performance.

Modeling the Catalytic Activity of Doped Molten Bismuth and Bismuth Trichloride Systems.

Aditya Goyal[1]*, Horia Metiu*[2]*, and* ***Vishal Agarwal***[1]
(1)Department of Chemical Engineering, Indian Institute of Technology Kanpur, Kanpur, India, (2)Department of Chemistry and Biochemistry, University of California, Santa Barbara, CA

In this work, we have modeled various doped molten salt ($BiCl_3$) and metal (Bi) systems to investigate the catalytic activity of methane activation as it is envisaged that doping molten $BiCl_3$ with Bi metal produces sub-halides, which may be active for catalysis.

Palladium ZSM-5 Catalysts Selective to C2 Products in Continuous Flow Methane to Oxygenates Reaction.

Dominik Wierzbicki[1]*, Davide Ferri*[2]*, Anna Wach*[3]*, and Maarten Nachtegaal*[2]
(1)Brookhaven National Laboratory, Upton, NY, (2)Paul Scherrer Institute, Villigen, Switzerland, (3)SOLARIS National Synchrotron Radiation Centre, Jagiellonian University, Cracow, Malopolska, Poland

Our research focused on evaluating catalytic activity of Pd/ZSM-5 materials in the reaction of methane oxidation using hydrogen peroxide using a continous liquid flow setup. Palladium supported over ZSM-5 with lower Si/Al exhibited notably higher selectivity towards ethanol compared to Pd/ZSM-5 with higher Si/Al where ethanol traces were undetectable.

When Free Radicals Meet Solids, Ions, and Gases in Photocatalytic Methane Oxidation.

Gang Wan[1] *and Arun Majumdar*[2]
(1)School of Engineering, Stanford University, Stanford, CA, (2)Stanford University, Stanford, CA

This presentation focuses on the free-radical pathways that underpin photochemical methane oxidation.

We will introduce how a combination of kinetic studies and in-situ spectroscopic investigation can shed light into the free-radical mechanism that can accelerate selective methane oxidation and guide the rational design of catalysts and reaction pathways.

Exploring Synthesis of Thin-Film Catalysis Concept for Enhanced Fischer-Tropsch Synthesis.

Avela Kunene
SE-IP, Helmholtz Zentrum Berlin (HZB), Berlin, Germany

0.07wt-%Co-SiO_x/Al thin-film catalyst, synthesized through sputtering, was evaluated for Fischer-Tropsch synthesis activity at WHSV of 842, 3368, and 6736 hr^{-1}. The relatively low X_{CO} levels are ascribed to low Co loading. Nonetheless, the $-r_{CO}$ indicates that thin-film catalysts can perform comparably to or better than powder catalyst systems.

Cascade Gas Process Linking Oxidative Coupling of Methane and Hydroformylation into C3 Commodities..

Alvaro Amieiro Fonseca
Johnson Matthey, Reading, United Kingdom

To valorize and reduce emissions from unexploited methane, European Project C123 partners, validated an efficient and selective transformation to C3 hydrocarbons focusing in propylene, avoiding energy intensive cracking . Methane is selectively converted into C3 commodities, by a novel combination of Oxidative Conversion of Methane (OCoM) and hydroformylation (HF).

Mechanistic Modeling of Dechlorination for a Room-Temperature Upcycling Method of Mixed PVC and Polyolefin Waste.

Benjamin Jackson[1]*, Wei Zhang*[1]*, Boda Yang*[1]*, Mal Soon Lee*[1]*, Sungmin Kim*[1]*, Huamin Wang*[1]*, Janos Szanyi*[1]*, and Johannes Lercher*[1,2]
(1)Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA, (2)Technical University of Munich, Garching b. München, Germany

Polyvinyl chloride (PVC) is a ubiquitous plastic product; however, recycling of these products pose significant economic and technical challenges. Here, we introduce a single-stage process

utilizing $AlCl_3$-based chloroaluminate ionic liquids to catalyze the room-temperature upcycling of PVC waste into liquid iso-alkanes.

Improvement of Polyethylene Hydrogenolysis Performance on Ru/Al_2O_3 Catalysts through Ru Size Control.

Jueun Kim *and Kwangjin An*
UNIST, Ulsan, Korea, Republic of (South)

This study observed the variation in polyethylene hydrogenolysis reactivity with Ru size. On nanosheet-assembled Al_2O_3 (NA-Al_2O_3), Ru formed Ru–Al bonds, resulting in high dispersion and small size. The 1Ru/NA-Al_2O_3 catalyst achieved optimal Ru structure, showing the highest PE conversion rate and liquid/wax production.

Bimetallic Moru/TiO_2 Catalyst for Selective Hydrogenolysis of Polyethylene Terephthalate (PET) Wastes into BTX.

Devita Salsabillah and ***Chunjae Yoo***
Clean Energy Research Center, Korea Institute of Science and Technology, Seoul, Korea, Republic of (South)

This study investigates PET hydrogenolysis using monometallic (Ru/TiO2) and bimetallic (RuMo/TiO2) catalysts. RuMo/TiO2 selectively converts PET into xylene with over 90% selectivity by enhancing redox properties and reducing Lewis acidity. Mechanistic insights, supported by DFT, reveal synergistic effects enabling efficient, recyclable PET conversion to BTX for sustainable waste valorization.

Investigating the Effects of Modified Zeolite Y on the Degradation of Polypropylene: A Systematic Study.

Claudia Fabris[1]*, Elio Sarotto*[2]*, Tomás Cordero-Lanzac*[3]*, Izar Capel Berdiell*[1]*, Sebastian Prodinger*[4]*, Andrea Jouve*[2]*, Valentina Brunella*[2]*, Silvia Bordiga*[2]*, and Stian Svelle*[1]
(1)Department of Chemistry, University of Oslo, Oslo, Oslo, Norway, (2)Department of Chemistry, University of Turin, Turin, Turin, Italy, (3)Department of Chemical Engineering, University of the Basque Country (UPV/EHU), Bilbao, Spain, (4)Topsøe A/S, Kgs. Lyngby, Kgs. Lyngby, Denmark

This systematic study demonstrates the effectiveness of modified zeolite Y catalysts, highlighting the interplay of mesoporosity, acidity and incorporation of alkaline-earth metal oxide in the catalytic degradation of polypropylene while generating a significant decrease in its degradation temperature and tuning the catalyst selectivity towards specific gas phase products.

Characterization of Polyolefin Hydrocracking Catalysts with X-Ray Absorption Spectroscopy.

Ozge Bozkurt[1]*, Anna Brenner*[2]*, Griffin Drake*[2]*, Jorge Perez-Aguilar*[1]*, Adam Hoffman*[1]*, Yuriy*

Roman[2], and Simon Bare[1]
(1)Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, Menlo Park, CA, (2)Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, MA

We investigated the reduction behavior of nickel oxide nanoparticles to metallic nickel in bifunctional hydrocracking catalysts by in-situ X-ray absorption spectroscopy by varying the acidic support (silica, zeolite Y, zeolite ZSM-5), varying the hydrogen pressure (1 to 20 bar), and adding a hydrocarbon (dodecane) to the reaction environment.

Tuning Activity and Stability of Bifunctional Ni Catalysts for Polyolefin Waste Hydrocracking.

Jessie Sun[1]*, Dionisios Vlachos[2], and Esun Selvam[3]*
(1)Chemical Engineering, University of Delaware, Newark, DE, (2)Delaware Energy Institute, University of Delaware, Newark, DE, (3)Chemical and Biomolecular Engineering, University of Delaware, Newark, DE

In this work, we demonstrate the high performance of Ce-promoted Ni/BEA for naphtha production. The presence of ceria directly influences the catalytic activity by regulating the metal morphology, reducibility and stability. We reveal the effect of ceria on reaction pressure requirements and metal hydrogenation ability for PO hydrocracking.

Turning Waste into Value: Microwave-Assisted Depolymerization of PET Using Industrial Ecat Catalyst.

Daniela Campos[1]*, **Luis F. Bordini**[1], Giullia Bertrand Marçano[1], Pedro Romano[2], and **João Monnerat**[3]*
(1)School of Chemistry, Federal University of Rio de Janeiro, Rio de janeiro, Rio de janeiro, Brazil, (2)Campus D. de Caxias, Federal University of Rio de Janeiro, Rio de Janeiro, Brazil, (3)Chemistry Institute, Federal University of Rio de Janeiro, Rio de Janeiro, Rio de Janeiro, Brazil

This study highlights ECAT, an FCC byproduct, as an effective catalyst for PET depolymerization. Using microwave-assisted heating, this sustainable method operates at lower temperatures, enhancing energy efficiency. It surpasses conventional acidic hydrolysis by reducing environmental impacts, operational costs, and promoting higher-value applications for ECAT.

Turning Waste into Value: Simultaneous Upcycling of PVC and FCC Catalyst Rejuvenation.

Giullia Bertrand Marçano[1,2]*, Leandro Alves de Sousa[2], Nilson de Paula[3], Pedro Romano[4], Donato Aranda[5], and **João Monnerat**[6]*
(1)School of Chemistry, Federal University of Rio de Janeiro, Rio de janeiro, Rio de janeiro, Brazil, (2)WASTECRAFT, Rio de Janeiro, Brazil, (3)Federal University of Rio de Janeiro, Rio

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This study transforms PVC plastic and deactivated FCC catalysts (ECAT) into valuable resources. Leveraging PVC's chlorine rejuvenates ECAT for reuse in refining while producing chlorine-reduced residue. This scalable upcycling minimizes environmental impact, reduces disposal costs, and advances waste management and catalyst reuse, supporting a circular economy in refining.

Mechanocatalytic Oxidative Cracking of Polyethylene Via a Heterogeneous Fenton Process.

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This work utilizes mechanocatalytic oxidative cracking reaction to overcome poly(ethylene)(PE) chemical inertness and processing challenges. An Fe2O3-based Fenton system with hydrogen peroxide introduces oxygen-based functional groups to the PE backbone, enabling chain cleavage and cracking. The byproducts are CO, CO2, O2, and H2O, with fragments used for fuels and chemicals.

Mechanocatalytic Depolymerization of Poly(styrene).

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We report a physical transition of poly(styrene) from a dispersed powder to an agglomerated, highly-reactive state during ball mill grinding, which causes a significant increase in its rate of mechanochemical depolymerization that exhibits characteristics of autocatalysis.

Selective Hydrogenolysis of Post-Consumer PET into p-Xylene over Pt-Sn Bimetallic Catalyst.

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$PtSn/Al_2O_3$ catalyst enables highly efficient solvent-free hydrogenolysis of waste PET to BTX, achieving 86.8% yield with 10 wt.% catalyst and 99.1% with 30 wt.%. Mechanistic investigations reveal synergistic PtSn alloy interactions that promote selective C=O hydrogenation, precisely facilitating C–O bond cleavage in PET esters for optimized catalytic performance.

Electrified Chemical Upcycling of Waste Plastics.

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Common plastics, such as polypropylene, are inert and require high temperature for conversion. Here, we have developed the electrified catalytic conversion process that breaks down plastic in water at an ambient temperature, producing valuable small organic compounds for fuels and chemicals.

Effects of Plastic Additives on Bifunctional Metal-Acid Catalysts for Alkane Reactions.

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The selective adsorption of triphenylphosphite, an antioxidant plastic additive, on the Brønsted acid sites of the bifunctional catalyst Pt/BEA is demonstrated through the limitation of the metal-Brønsted acid catalyzed hydroconversion of melt-phase hexatriacontane as probe molecules of polyethylene and gas-phase n-heptane.

Advancing Closed-Loop Recycling of Nylon 6 Waste through an Ammonia-Assisted Depolymerization.

Xianyuan Wu[1], Rahul Prasad Bangalore Ashok[2], Matthew Webber[1], ***Xiao Wang***[1]*, Anna Brenner[1], Griffin Drake[1], Joel Miscall[3], Clarissa L. Lincoln[3], Shannon S. Stahl[4], Jason DesVeaux[2], Taylor Uekert[5], Elisabeth Van Roijen[5], Yang Shao-Horn[6], Gregg T. Beckham[3], and Yuriy Roman[1]*
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We developed an ammonia-assisted approach to efficiently depolymerize post-consumer nylon 6 waste to its monomer – ε-caprolactam (>85% yield) with the aid of a Brønsted acid catalyst.

Techno-economic analysis and life cycle assessment revealed that the approach is cost-effective and environmentally benign to close the loop for nylon 6 recycling.

Upcycling of Plastic Waste into Carbon Nanotubes As Efficient Battery Additives.

Kwangjin An
Ulsan National Institute of Science & Technology, Ulsan, Korea, Republic of (South)

This article introduces a technology for converting waste plastics into CNTs for battery applications. CNTs have recently been highly evaluated as conductive additives for a lithium-ion battery. This research presents a new possibility of utilizing waste plastic in the advanced battery industry by increasing the cell capacity.

Influence of Cr Accumulation on Catalyst Structure and Activity during Polyolefins Cracking with Polyoxometalates.

Hongda Zhu[1]*, Justin T. Douglas*[2]*, and Bala Subramaniam*[3]
(1)Center for Environmentally Beneficial Catalysis, University of Kansas, Lawrence, KS,
(2)Nuclear Magnetic Resonance Core Laboratory, University of Kansas, Lawrence, KS,
(3)Center for Environmentally Beneficial Catalysis, The University of Kansas, Lawrence, KS

New fundamental insights into the effects of Cr insertion and reduction on structural stability, the atomic and electronic structures of heteropolytungstates, and thereby their catalytic cracking performance are provided. Such insights are essential to develop durable polyolefin recycling catalysts and sustainable technologies.

Coke Formation Analysis Under Industry-Relevant Conditions.

Teerawit Prasomsri *and Ashten Molley*
Clariant, Louisville, KY

The study investigates coke formation during steam methane reforming (SMR) under industrial conditions. Using nickel-based catalysts, it explores how factors like steam-to-carbon ratios, pressure, and promoter influence coking rates. Results emphasize high-pressure studies for accurate assessment, highlighting promoter's role in mitigating coking for advancing low-carbon hydrogen production technologies.

Nickel Catalysts on High Oxygen Ion Conductivity Supports for Methane Dry Reforming.

Xuan Pham*, Janet Baffoe, and Corey Leclerc*
Department of Chemical Engineering, New Mexico Tech, Socorro, NM

Beside oxygen ion conductivity, nickel particle sizes, metal dispersion and acidity/basicity of supports also contribute to carbon resistance. It is necessary of isolate oxygen ion conductivity with these factors to study its contribution in carbon removal.

Lanthanide Doped Co-Al Catalysts Prepared By Solution Combustion Method in Dry Reforming of Methane.

Svetlana Tungatarova
Chemistry and Chemical Technology faculty, al-Farabi Kazakh National University, Almaty, Kazakhstan; Laboratory of Oxidative Catalysis, D.V. Sokolsky Institute of Fuel, Catalysis and Electrochemistry, Almaty, Kazakhstan

Development of a new efficient catalyst for dry reforming of methane into synthesis gas, which will further promote the organization of a new environmentally friendly energy-saving production.

Scaling and Demonstration of an Integrated LOHC System: Long-Term Catalyst Stability and High Throughput for Efficient Formic Acid Decomposition.

Tanmayi Bathena[1]*, Byun Mi Yeon*[2]*, Alia Cooper*[2]*, Uriah Kilgore*[2]*, S Thomas Autrey*[2]*, and Mark Bowden*[3]
(1)CHEMICAL ENGINEERING, OREGON STATE UNIVERISITY, CORVALLIS, OR, (2)Pacific Northwest National Laboratory, Richland, WA, (3)Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA

This research explores formic acid as a liquid organic hydrogen carrier to overcome challenges in hydrogen storage and transport. A prototype formic acid reformer is developed for efficient hydrogen production, aiming for a scalable solution producing 1 kg H2/hour to enable practical, distributed green hydrogen adoption.

Efficient Dehydrogenation Catalysts for Polystyrene-Derived Liquid Organic Hydrogen Carriers.

Hyeongeon Lee[1] *and Kwangjin An*[2]
(1)Ulsan National Institute of Science and Technology (UNIST), Ulsan, Korea, Republic of (South), (2)Ulsan National Institute of Science & Technology, Ulsan, Korea, Republic of (South)

This study presents an innovative way to upcycle polystyrene waste into liquid organic hydrogen carrier (LOHC) applications and propose an efficient dehydrogenation catalyst for the dehydrogenation of the LOHC system. Pt catalyst supported on nanosheet-assembled alumina with large pore volume and size showed the highest dehydrogenation performance.

Coupling Light and Heat: Synergistic Effects to Improve Catalyst Performance for Decarbonization Applications.

Elise Elkingon *and Emma Lovell*
Chemical Engineering, University of New South Wales, Sydney, NSW, Australia

To date, there have been limited demonstrations in literature of the study of ammonia decomposition (AD) for hydrogen generation under thermo-photo conditions. Furthermore, the

mechanisms associated with light enhancement for AD remain highly contentious. To address this gap, this work examines ceria-supported bimetallic Ni-Co catalysts for thermo-photo AD.

Oxygen Evolution Reaction (OER) on Transition Metal Oxide Surfaces to Optimize the Bronsted-Evans-Polanyi Relationship.

David Ukuku[1] *and Craig Plaisance*[2]
(1)Louisiana State University, Baton Rouge, LA, (2)Cain Department of Chemical Engineering, Louisiana State University, Baton Rouge, LA

This study investigates the Oxygen Evolution Reaction (OER) using Brønsted-Evans-Polanyi (BEP) relationships to optimize transition metal oxide catalysts. Advanced simulations with VASPsol and GGA+U reveal structural sensitivities at active sites, enabling efficient catalyst design for energy applications, bridging gaps in activity, stability, and scalability.

Study on the Water-Gas Shift Reaction of Cu-Based Catalysts Enhanced for High-Temperature Stability and Reusability for Hydrogen Production from Waste.

I-Jeong Jeon[1]*, Chang-Hyeon Kim*[1]*, Eun-Su Yoon*[1]*, Jae-Hak Lim*[1]*, Chae-Min Yoon*[1]*, Kyung-Won Jeon*[2]*, Won-Jun Jang*[3]*, Jung Sang Cho*[4]*, and Jae-Oh Shim*[1]
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The SPCZC catalyst achieved a CO conversion rate of 76% at a relatively high reaction temperature of 400 °C with real waste-derived syngas containing approximately 38% CO and maintained stable catalytic activity for 50 h. Zirconia effectively enhanced the OSCC and the amount of defective oxygen in ceria.

Ni-Based Catalysts for Steam Reforming of Mixed Alkane Hydrocarbons Reaction: Effect of Promoter and Support.

JI-Hyeon Gong*, Min-Ju Kim, Jae-Min Kwon, and Won-Jun Jang*
Ajou University, Suwon-si, Korea, Republic of (South)

Alkane hydrocarbons in pyrolysis gas can produce hydrogen through steam reforming, upgrading pyrolysis oil for waste plastic recycling. However, challenges like carbon deposition, sintering, and cracking occur. This study develops an optimized catalyst, showing that Ni dispersion is critical for CeO_2 supports, while acidity is key for Al_2O_3 supports.

Development of Ni Catalysts Supported on Porous Yolk-Shell Structures with Enhanced Stability and Alkali Resistance.

Hyun-Seog Roh*, Ho-Ryong Park, Jong-Hoon Han, Pil-Jae Kim, and Min-Sang Kwak*
Yonsei University, Wonju, Korea, Republic of (South)

Hydrogen production from biomass faces challenges due to alkali impurities. Ni/Al_2O_3 yolk-shell catalysts, prepared via spray pyrolysis, showed excellent stability and activity in SRM under alkali poisoning. $Ni/pys\text{-}Al_2O_3$ outperformed others with high CH_4 conversion, minimal deactivation, and strong resistance to carbon deposition, attributed to its unique structure and Ni dispersion.

Exploring Electrocatalytic Hydrogenation of p-Nitrophenol Using Nitrogen-Doped Carbon Nanostructures (CN_x).

Anant Sohale[1]*, Niharika Vennala*[1]*, Snehal Patil*[1]*, James N. Gyamfi*[1]*, Seval Gunduz*[1]*, Anne Co*[2]*, and Umit Ozkan*[1]
(1)William G. Lowrie Department of Chemical & Biomolecular Engineering, The Ohio State University, Columbus, OH, (2)Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH

Electrocatalytic hydrogenation of organic compounds is a safer alternative to conventional catalytic hydrogenation as it avoids the use of strong reducing agents like $NaBH_4$ or high-pressure hydrogen gas. This study explores the use of nitrogen-doped carbon nanostructures (CN_x) for treatment of toxic contaminant p-Nitrophenol by electrocatalytic hydrogenation.

Identifying the Bulk and Surface Characteristics of Ni-Doped LaFeO3 Under Environmental Conditions.

Neelesh Kumar[1]*, Bar Mosevitzky Lis*[2]*, Musa Najimu*[3]*, Yoon Jin Cho*[4]*, Kandis Leslie Gilliard-Abdulaziz*[3]*, Eranda Nikolla*[5]*, and Israel Wachs*[6]
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Operando spectroscopic methods are employed to elucidate the surface and bulk chemistry of La-based perovskite oxides as cathode catalysts in SOCs using optical (Raman, IR), and ion (HS-LEIS) probes and interrogated the nature of surface sites with methanol as a “smart” chemical probe.

Direct Evidence of Redox Coupling By Electrochemical Polarization in Bimetallic Aerobic Oxidation Reaction..

Bohyeon Kim[1]*, James Spragg*[2]*, Isaac Daniel*[2]*, Graham J. Hutchings*[2]*, Samuel Pattisson*[2]*, and Steven McIntosh*[1]
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This study demonstrates compelling evidence of redox reaction coupling between two physically mixed bimetallic catalysts during the aerobic oxidation of 1,2-butanediol. By capturing electron transfer between the catalysts under identical conditions, it reveals that the catalytic activity is predominantly governed by the quantity of transferred electrons.

Probing Solvation Effects within the Electrochemical Double Layer during Alcohol Oxidation Reactions.

Geoffrey Hopping, *Selma Kadric, Richa Ghosh, and David Flaherty*
School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA

This work utilizes kinetic measurements of electrocatalytic alcohol oxidations with varying supporting electrolyte concentration, alcohol concentration, and alcohol chain length to manipulate the electrochemical double layer structure and examine the effects of the electric field and solvent reorganization on kinetic barriers influencing observed reaction rates.

Development of Multifunctional Tungsten-Supported Catalysts for Oxygen Evolution and Hydrogen Oxidation Reactions in Unitized Regenerative Fuel Cells.

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Ir/WO_3 catalysts were developed to enhance HOR and OER activities for URFCs. WO_3 supports with varying crystallinity were synthesized to study their impact on performance. Structural and surface properties were analyzed, revealing catalysts optimized for OER also showed excellent HOR activity, advancing efficient catalyst design for URFCs.

Electrochemical Ammonia Decomposition over Nickel and Cobalt Nanostructures on Nickel Foam for Sustainable Hydrogen Production.

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Electrochemical ammonia decomposition (EAD) into hydrogen is a viable pathway for a sustainable energy future. Herein, we investigated the performance of nickel and cobalt nanostructures on nickel foam (NF) for EAD. Additionally, DFT calculations elucidate the underlying reaction mechanisms. Overall, the results highlight the potential of sustainable hydrogen production.

Photocatalytic Degradation of Antibiotics: Nalidixic Acid and Sulfanilamide, a Study Using TiO_2 P25.

***Juan Martin Castro Alonso**, Daniela González-Pereyra, Brenda Zermeño, Elisa Alfaro, Elisa Leyva, and Edgar Moctezuma*
Facultad de Ciencias Químicas, Universidad Autónoma de San Luis Potosí, San Luis Potosí, SL, Mexico

The present work investigates the photocatalytic degradation and analysis of intermediates of antibiotics (nalidixic acid and sulfanilamide) by UV-A light. TiO_2 P25 was used as a catalyst and the interaction between each drug and the catalyst was studied by adsorption experiments. Mineralization of each reagent was monitored by TOC.

Synthesis of Heterojunction Catalysts of Fe^{3+} and Ti^{4+} Oxides Used for the Photocatalytic Degradation of Organic Compounds.

***Daniela González-Pereyra**, Juan Martin Castro Alonso, Ilse Acosta, Brenda Zermeño, and Edgar Moctezuma*
Facultad de Ciencias Químicas, Universidad Autónoma de San Luis Potosí, San Luis Potosí, SL, Mexico

Heterojunctions Fe_2O_3-TiO_2 catalysts were synthesized through a solid-state reaction of ilmenite combined with TiO_2 impregnation to mineralize model organic compounds. The photocatalytic activity was determined by the phenol reaction. The catalyst with 2% of iron oxide showed the highest mineralization percentage, suggesting that Fe_2O_3 obtained by ilmenite enhances photocatalytic reactions.

The Application of TiO2 Thin-Film Coatings for Photocatalytic Chemical Synthesis: The Light-Driven Conversion of Benzyl Alcohol to Benzaldehyde.

***Atsu Kludze** and Shu Hu*
Department of Chemical and Environmental Engineering, Yale University, New Haven, CT

This study demonstrates the use of thin-film coatings to improve the stability and modify the surface kinetics of photocatalysts used in light-driven chemical synthesis. TiO_2-coated CdS particulate panels, decorated with Ni nanoparticle cocatalysts, were used for the photocatalytic conversion of benzyl alcohol to benzaldehyde and H_2.

Understanding Strong Metal Support Interactions for Electrocatalysis.

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Strong metal support interactions (SMSI) are well understood for thermochemical catalysis, however, there exists a significant gap in our understanding of its behaviour in electrocatalysis.

Here, we explore how SMSI overlayers affect reactivity and stability for electrocatalysis. We also explore how stable the overlayers are in harshly oxidizing electrochemical conditions.

Towards Spatial Control of Reaction Selectivity on Photocatalysts Using Area Selective Atomic Layer Deposition on Model Dual Site Electrocatalyst Platform.

Wilson McNeary[1]*, William Stinson*[2]*, Moaz Waqar*[3]*, Wenjie Zang*[3]*, Xiaoqing Pan*[4]*, Daniel Esposito*[5]*, and Katherine Hurst*[6]
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In this work, area selective atomic layer deposition was used to develop oxide interphase layers for site-specific redox selectivity on a model electrocatalyst. This lays the groundwork for increasing solar-to-hydrogen efficiency of Z-scheme water splitting photocatalysts by mitigating undesired diffusional coupling.

Au-Pd Single Atom Alloy Catalysts for Electrochemical CO_2 Reduction.

Jiwon Kim[1] *and Joaquin Resasco*[2]
(1)Mcketta Department of Chemical Engineering, The University of Texas at Austin, Austin, TX, (2)McKetta Department of Chemical Engineering, The University of Texas at Austin, Austin, TX

We have demonstrated that alloying Au with a small amount of more reactive metal Pd accelerates CO_2 activation and suppresses the hydrogen evolution reaction (HER), resulting in enhanced electrocatalytic activity and selectivity for CO_2-to-CO conversion.

Fe-Beta Zeolite for Simultaneous SCR of NOx and N_2o with NH_3: Effect of Chemical Composition and Preparation Method on Catalytic Performance.

Hwajun Lee
Korea Institute of science and technology, Seoul, Korea, Republic of (South)

The effect of chemical composition and preparation method on the catalytic properties of Fe-beta zeolite for simultaneous selective catalytic reduction of NOx and N_2O by NH_3 has been investigated. Our findings revealed optimal conditions for maximizing the performance of Fe-beta considering the Si/Al ratio, Fe sources, and loading method.

Impact of NO_2 on Sulfur Poisoning and Impact of Sulfur on NO_2 Reactions on Cu-SSZ-13 Catalysts.

Afrina Zaman Shoronika[1]*, Poonam Rani*[1]*, Rohil Daya*[2]*, and William Epling*[1]

(1)Chemical Engineering, University of Virginia, Charlottesville, VA, (2)Cummins Inc., Columbus, IN

Sulfur poisoning is known to negatively impact Cu-SSZ-13 SCR catalysis. Here, we show how NO_2 affects sulfation, and that sulfation affects the formation of ammonium nitrate and copper nitrate. Controlling NO_2 exposure time helps manage sulfur species on the catalyst surface, with long NO_2 exposure time being detrimental to desulfation.

Impact of Cu Speciation in Cu/SSZ-13 on Oxidation Reactions.

Kanika Meena[1]*, Rohil Daya*[2]*, Christopher Paolucci*[1]*, and William Epling*[1]
(1)Chemical Engineering, University of Virginia, Charlottesville, VA, (2)Cummins Inc., Columbus, IN

The distribution of active copper species in Cu/SSZ-13 changes with changes in reaction conditions, which can lead to different reactivities toward the various reactions that go on over diesel aftertreatment catalysts. This study investigates how copper loading and distribution in Cu/SSZ catalysts impacts oxidation reactions.

A Global Kinetic Model for Next-Gen Fuels Using Lean NOx Traps.

Benjamin Foulon[1]*, Erin Thomson*[2]*, Ujjal Das*[1]*, and Leo DeRita*[1]
(1)Johnson Matthey, Wayne, PA, (2)Johnson Matthey, Royston, United Kingdom

A model to accurately predict emissions from an LNT-based aftertreatment system for a split-cycle ICE running on CH_4 and CH_4/H_2 blend feedstocks is presented. The model facilitated optimization leading the LNT to successfully drop emission levels below specified CARB targets under optimized engine conditions, with further fuel blend optimizations underway.

Effects of Sulfur Exposure on Cu Speciation and NH_3 Storage in SSZ-13.

Arig-Undram Zolboot[1]*, William Epling*[1]*, Rohil Daya*[2]*, Christopher Paolucci*[1]*, and* ***Asanka Wijerathne***[1]
(1)Chemical Engineering, University of Virginia, Charlottesville, VA, (2)Cummins Inc., Columbus, IN

The fundamental understanding of sulfation effects on Cu speciation and NH_3 interactions can aid in improving selective catalytic reduction (SCR) catalysts used in automotive emissions control. In this study, we investigated sulfur transfer from Cu monomers to dimers and compared NH_3 desorption behaviors of sulfated and non-sulfated Cu dimers.

NO_x-Assisted Mercury Oxidation in the Selective Catalytic Reduction of NO By NH_3 over a V_2O_5-WO_3/TiO_2 Catalyst.

Kang Hun Kim and ***Moon Hyeon Kim***

Department of Environmental Engineering, Daegu University, Gyeongsan, Korea, Republic of (South)

This study proposes a way of converting Hg^0 to its oxidized species under conditions in which not only the oxidation may avoid an inhibitory effect by NH_3 but it may be also probable without highly acidic, corrosive additives, such as hydrogen chloride (HCl).

Characterization of FCC SOx Reduction Additives.

*Mahe Rukh[1], **Karoline Menze**[2], Xunhua Mo[2], Austin Gallagher[2], and Mehdi Allahverdi[2]*
(1)North Carolina State University, Raleigh, NC, (2)Johnson Matthey, Savannah, GA

This work probes the impact of the intrinsic nature of FCC SOx reduction additives on the performance using various characterization techniques. A comprehensive understanding of the impact of the intrinsic properties will provide a fundamental basis for the design and development of more stable and efficient SOx reduction additives.

Lab-Scale Insights into FCC CO Promoter Evaluation for Real-World Applications.

***Juliana Forero Arevalo**, Xunhua Mo, and Mehdi Allahverdi*
Johnson Matthey, Savannah, GA

The purpose of this work is to develop reliable lab scale testing methods to accurately predict the performance of CO promoters in commercial Fluid Catalytic Cracking (FCC) units. Another objective is to investigate how different deactivation conditions and mechanisms impact activities for CO oxidation.

N_2o Formation during Selective Catalytic NO_x Reduction on Cu-Exchanged Zeolite Catalysts.

***Dhruba Jyoti Deka**[1], Garam Lee[1], Kenneth Rappe[1], Janos Szanyi[1], and Yong Wang[1,2]*
(1)Pacific Northwest National Laboratory, Richland, WA, (2)The Gene and Linda Voiland School of Chemical Engineering and Bioengineering, Washington State University, Pullman, WA

This study investigates N_2O formation during low-temperature SCR. Temperature-programmed-desorption and DRIFTS show that Bronsted-acid-catalyzed NH_4NO_3 decomposition produces N_2O when NO_2 is present, and H_2O is absent in the reaction mixture. In the presence of H_2O, however, N_2O seems to originated from intermediates that are less stabile than NH_4NO_3.

Theoretical Investigation of Co and Ni Diffusion and Sintering on CeO_2(111).

***Nusrat Jahan Rifat** and Ye Xu*
Cain Department of Chemical Engineering, Louisiana State University, Baton Rouge, LA

Ceria-supported metals catalyze important reactions, including Fischer-Tropsch and hydrocarbon reforming. Metal particle formation on ceria is, therefore, an important aspect of catalytic

applications. Ni and Co are seen in STM forming numerous nanoparticles on CeO_2(111), but DFT-calculated diffusion barriers are prohibitive at ambient temperature. A possible mechanism is proposed.

Support Effects and Kinetic Analysis of Acetone Hydrogenation over Platinum Catalysts.

Yaqin Tang[1]*, Robson Schuarca*[2]*, and Jesse Bond*[2]
(1)Syracuse University, Syracuse, NY, (2)Biomedical and Chemical Engineering, Syracuse University, Syracuse, NY

Biomass is a key renewable resource, with technologies for energy and chemical production advancing rapidly. Carbonyl hydrogenation on Pt and Pt-Sn catalysts efficiently forms alcohols. Using SiO2 and γ-Al2O3 supports, we synthesized platinum catalysts and conducted active-site titration experiments to investigate catalytic behaviors and the impact of support properties.

Investigating Acetone Hydrogenation over Pt/SiO_2 and $Pt\text{-}Sn/SiO_2$ Catalysts.

Mohammed Tahseen Islam[1]*, Yaqin Tang*[2]*, Robson Schuarca*[3]*, and Jesse Bond*[3]
(1)Biomedical and Chemical Engineering, Syracuse University, SYRACUSE, NY, (2)Syracuse University, Syracuse, NY, (3)Biomedical and Chemical Engineering, Syracuse University, Syracuse, NY

This study investigates acetone hydrogenation using monometallic Pt/SiO_2 and bimetallic $Pt\text{-}Sn/SiO_2$ catalysts. The bimetallic catalysts indicated enhanced activity and selectivity due to Sn's promoting effects in modifying Pt's behavior. These findings will provide critical insights for streamlining catalytic systems which are essential for sustainable biomass conversion and chemical production.

Unraveling Manganese-Promotion of Cobalt-Based CO_2 Hydrogenation Catalysts.

Cherie Hsu[1]*, Luca J. Weigel*[1]*, Robin Gutounig*[1]*, Shabaaz Abdullah*[2]*, Rabia Ilica*[1,3]*, Erisa Saraçi*[1,3]*, Anna Zimina*[1,3]*, Mohamed Fadlalla*[2]*, Jan-Dierk Grunwaldt*[1,3]*, Michael Claeys*[2]*, and Moritz Wolf*[1,4]
(1)Institute of Catalysis Research and Technology (IKFT), Karlsruhe Institute of Technology (KIT), Eggenstein-Leopoldshafen, Germany, (2)Department of Chemical Engineering, Catalysis Institute, University of Cape Town, Cape Town, South Africa, (3)Institute for Chemical Technology and Polymer Chemistry (ITCP), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany, (4)Engler-Bunte-Institut (EBI), Karlsruhe Institute of Technology (KIT), Karslruhe, Germany

Investigation of the supported Co-Mn model catalysts focusing on the interaction of Mn with the active Co phase through XRD, TEM, ICP-OES, TPR, TPD, XAS, and catalytic activity testing in fixed-bed reactors was conducted under CO_2 hydrogenation condition to provide further insights

Effects of Alcohol and Epoxide Chain Lengths on Liquid-Phase Epoxide Alcoholysis over *BEA Zeolites.

Huston Locht[1]*, David S. Potts*[2]*, Zahra Rangoonwala*[1]*, and David Flaherty*[1,2]
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Reactant structure greatly alters the kinetics of liquid-phase Brønsted and Lewis acid zeolite chemistries through coordination with confined solvent molecules, reactive species, and zeolite moieties. Here, we combine kinetic and calorimetric studies to examine and molecularly interpret the consequences of varying the alcohol and epoxide size on epoxide alcoholysis kinetics.

Water-Enhanced Bifunctional Metal-Acid Catalyst for C=C Bond Hydrogenation.

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With DFT and meta-dynamics simulations, we designed a novel model of hydrated H_2O-$B(OH)_3$ acid complex on the Ni(111) surface. This bifunctional metal-acid catalyst can dramatically decrease the reaction barriers and enhance the hydrogenation of C=C bond of cyclohexene in organic solvent with the proton-shuttling mechanism.

Utilizing Site-Dependent NO Reduction to Probe Step Sites on Supported Pt Nanoparticles: A Combined Theoretical and Experimental Study.

Sugandha Verma[1]*, Silvia Marino*[2]*, Asanka Wijerathne*[1]*, Colby Whitcomb*[1]*, William Epling*[1]*, Robert Davis*[1]*, and Christopher Paolucci*[1]
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Conventional supported metal nanoparticles are characterized by site heterogeneity arising from different coordination environments. Undercoordinated sites catalyze several major reactions, thus, quantification of these sites is essential. Here we use the site dependent nature of NO reduction over supported Pt catalysts to quantify stepped sites.

Probing the Role of CO_2 As a Promoter in H_2O_2 Synthesis on Pd Containing Alloy Catalysts.

Adam Senko*, Sucharita Vijayaraghavan, and David W. Flaherty*
School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA

While CO_2 enhances H_2O_2 formation rates and selectivities on monometallic catalysts, it reduces selectivity in some Pd alloys. We investigate the effects of CO_2 on Pd-containing random alloy

and ordered intermetallic catalysts to assess contributions to differences in kinetics from reaction pathways introduced by CO_2 and adsorbate induced restructuring.

Open Circuit Potential Decay Transients Track Chemical Reaction of Electrochemically Formed Surface Intermediates.

Richa Ghosh[1]*, Dingqi Nai*[2]*, Andrew Medford*[1]*, and David Flaherty*[1]
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We correlate transient OCP and *operando* Raman spectroscopy measurements after Au surface polarization to examine the creation of reactive oxygen species (O*) by H_2O electrooxidation and their consumption at open circuit by reaction with CH_3OH. We hypothesize that OCP decay rates will reflect thermochemical reaction rates of CH_3OH with O*.

Atomic-Scale Understanding of Benzaldehyde Hydrogenation Mechanisms at Pd-Water Interfaces.

Alexander von Rueden[1]*, Julia de Barros Dias Moreira*[1]*, Benjamin Jackson*[2]*, Thuy Le*[1]*, Udishnu Sanyal*[2]*, Simuck Yuk*[3]*, Mal Soon Lee*[1]*, and Johannes Lercher*[4]
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Our work elucidates the impact of varying pH and surface charge conditions on the dynamic structures of Pd-water interfaces, providing *atomic-level* mechanistic insights on benzaldehyde hydrogenation. These findings complement our experimental data and offer a fundamental understanding that will help guide advancements in biomass upgrading.

Density Functional Theory Investigation into Modulating Surface–Adsorbate Interactions with Strain for Ammonia Synthesis on a Pd (111) Surface.

Siddhesh Shirish Borkar *and Manish Shetty*
Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX

Using density functional theory (DFT), strain is shown to be a useful catalyst design tool to potentially overcome theoretical activity limitations. Electronic descriptors have rationalized adsorbate-surface interactions under strain, and using NH_3 synthesis on Pd(111), kinetic analysis has revealed that 4% tensile strain can increase the turnover frequency by ~10×.

Mechanistic Studies of H_2 Reduction of Mononuclear Cu^{2+} Sites to Cu^{+} in Cu-Exchanged Chabazite Zeolites.

Angel Santiago-Colón[1]*, Jose Rebolledo-Oyarce*[2]*, William Schneider*[3]*, and Rajamani Gounder*[4]
(1)Chemical Engineering, Purdue University, West Lafayette, IN, (2)Chemical Engineering, University of Notre Dame, Notre Dame, IN, (3)Chemical and Biomolecular Engineering, University of Notre Dame, Notre Dame, IN, (4)Charles D. Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN

H_2 reduction of Cu-CHA samples with varying mononuclear Cu^{2+} site density reveal two distinct reduction pathways that depend on Cu^{2+} proximity. This experimental and computational approach aids in developing molecular interpretations of H_2 TPR profiles that are used to guide Cu-CHA catalyst design for NOx abatement and partial methane oxidation.

Elucidating the Effect of Chlorine on the Distributions and Reactivity of Surface Oxygen Species on Silver Catalysts for Ethylene Epoxidation.

Eric Sarbacker *and David W. Flaherty*
School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA

The selectivity of the oxidation of ethylene to ethylene oxide can be promoted by the addition of chlorine to the catalyst surface. This study uses Raman spectroscopy to evaluate how the presence of chlorine affects the distribution of oxygen species in order to elucidate their individual promotional effects.

Doping of Pd/CeO_2 Single Atom Catalysts Alters the Reaction Mechanism of CO Oxidation.

Saba Rahman[1]*, Alireza Javanmard*[1]*, Kayla Eudy*[1]*, Michael Janik*[1]*, and Robert Rioux*[2,3]
(1)Chemical Engineering, The Pennsylvania State University, University Park, PA, (2)Department of Chemistry, The Pennsylvania State University, University Park, PA, (3)Department of Chemical Engineering, The Pennsylvania State University, University Park, PA

The impact of CeO_2 support modification by doping with Zr was investigated over single-atom Pd catalysts. The addition of Zr to Pd/CeO_2 strengthens CO binding to Pd by inhibiting the formation of PdO_2. Zr impacts the reaction mechanism for CO oxidation leading to enhanced rates per Pd atom.

La Doping of Ceria Controls Accessible Pd Oxidation States in Single Atom Catalysts during CO Oxidation.

Alireza Javanmard[1]*, Kayla Eudy*[1]*, Michael Janik*[1]*, and Robert Rioux*[2,3]
(1)Chemical Engineering, The Pennsylvania State University, University Park, PA, (2)Department of Chemistry, The Pennsylvania State University, University Park, PA, (3)Department of Chemical Engineering, The Pennsylvania State University, University Park, PA

Doping of metal oxide supports can provide additional control over the catalytic properties of a single-atom catalyst (SAC). Doping Pd/CeO_2 SACs with La enhances the formation of oxygen vacancies, and tunability of oxidation states of the metal, offering valuable insights for optimizing the catalytic performance in redox-sensitive reactions.

Machine Learning Force Field Applied to Studying the Effects of Oxygen and Chlorine on Silver Catalysts Reconstruction in Ethylene Epoxidation.

Maria Victoria Zuniga Rodriguez[1]*, Eric Sarbacker*[2]*, David W. Flaherty*[3]*, and Christopher Paolucci*[1]
(1)Chemical Engineering, University of Virginia, Charlottesville, VA, (2)School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA, (3)Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA

A machine-learned force field was developed using sparse Gaussian process active learning to simulate Ag-O-Cl surface reconstruction dynamically. Key findings reveal size and coverage-dependent trends, including subsurface oxygen diffusion and molecular oxygen formation, illustrating how these factors drive silver catalysts reconstruction in ethylene epoxidation.

Aldol Condensation of Mixed Oxygenates on Phosphate Modified TiO_2 Catalysts.

Brandon Oliphant*, Laura Paz Herrera, and J. Will Medlin*
Department of Chemical and Biological Engineering, University of Colorado Boulder, Boulder, CO

This work describes the use of phosphate modifiers on TiO_2 catalysts to improve the selectivity of acetaldehyde-acetone cross-aldol condensation reactions. Reaction order, temperature programmed desorption and X-ray photoelectron spectroscopy results suggest that electronic effects from the phosphate groups result in more stable binding of reactants on the catalyst surface.

Ionic Liquid Overlayers Stabilize Highly Selective Single Atom Pd Catalysts on Oxide Supports.

Ayanna Culmer-Gilbert[1] *and Steven Tait*[2]
(1)Chemistry, Indiana University, Bloomington, IN, (2)Indiana University, Bloomington, IN

Organic ligands and ionic liquid overlayers stabilize single atom Pd catalysts that are highly selective for ethylene in the semi-hydrogenation of acetylene. High selectivity and high activity are steady over many hours of reaction.

Degrees of Rate Control in Interconnected Networks.

Ting Lin *and Aditya Bhan*
Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN

Degrees of rate control in interconnected reaction networks evaluated using kinetic resistance decouple contributions from the pathway of interest and branching pathways. We leverage this formalism to further underscore how mechanistic features such as stoichiometric regularity and network symmetry proffer constraints and relationships for the degrees of rate control.

Gd-Doped CeO_2 Aerogels for Degradation of Organophosphorus Chemical Warfare Simulants.

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CeO_2 and Gd-doped CeO_2 aerogels are highly effective sorbent materials against chemical warfare simulants. Gd-doping improves performance against diisopropyl fluorophosphate (DFP) but inhibits performance against dimethyl methylphosphonate (DMMP). DFT analysis and EPR spectroscopy show that reactive oxygen species stabilized on the Gd-doped surface cause this divergence between simulants.

Investigating the Role of Brønsted Acid Sites on the Diffusion of C_6–C_{12} Methylbenzenes in H-MFI Zeolite.

Ayotunde Alabi[1], *Reilly Afflerback*[2], *David Hibbitts*[1], *and Hansel Montalvo-Castro*[2]
(1)Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN, (2)Department of Chemical Engineering, University of Florida, Gainesville, FL

This work employs periodic density functional theory (DFT) to elucidate the role of Brønsted acid sites on diffusion barriers and the diffusivity of aromatics in H-MFI. Here, we model the diffusion of low-critical-diameter aromatics in MFI in the presence of Brønsted acid sites across all 12 crystallographically unique T-sites.

Interzeolite Conversion of FER-Type Zeolite to CHA for NH_3-SCR.

Daniel Gilleland[1], *Logan Spell*[1], *and Alessandro Turrina*[2]
(1)Johnson Matthey Technology Center, Johnson Matthey, Savannah, GA, (2)Johnson Matthey Technology Centre, Johnson Matthey, Billingham, United Kingdom

FER zeolite has been used as a new alumina source for synthesis of CHA type zeolite. The new CHA has a high crystallinity and purity and demonstrates strong NOx conversion activity and hydrothermal stability.

Organo-Template Free Fe-FER for Improved SCR Performance.

Logan Spell[1], *Alessandro Turrina*[2], *Ugursan Aydogan*[2], *Agnes Raj*[2], *and Alexander Green*[2]
(1)Johnson Matthey Technology Center, Johnson Matthey, Savannah, GA, (2)Johnson Matthey Technology Centre, Johnson Matthey, Billingham, United Kingdom

Organo-template free Ferrierite (FER) for Fe-SCR was synthesized using several methods and tested for catalytic performance under fast-SCR conditions. This study demonstrates that by carefully controlling the synthesis conditions, specifically the choice of SDA, a higher performing and cost-effective zeolite for Fe-SCR can be achieved.

Catalytic Performance of ZSM-5 Zeolite Modified with Zn and Ga in the Transformation of Methanol to Aromatics (MTA).

Luis Aguilar Gonzalez[1], *Julia Aguilar Pliego*[2], *Misael Garcia Ruiz*[2], *Enrique Sastre de Andrés*[3], *Marisol Grande Casas*[3], *and Carlos Márquez Alvarez*[3]
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In the present work, ZSM-5 zeolite was prepared and subsequently modified by ion exchange with Ga and Zn. Finally, the catalytic evaluation was carried out in the MTA reaction, with ZSM-5/Ga showing the highest activity, while ZSM-5/Zn was the most selective to the BTX fraction (23.1 mol %).

Effect of Ligand Environment for Wacker Oxidation in FAU Zeolites.

Mohan Shankar[1], *Deepak Sonawat*[2], *Siddarth Krishna*[2], *and Christopher Paolucci*[1]
(1)Chemical Engineering, University of Virginia, Charlottesville, VA, (2)Chemical and Biological Engineering, University of Wisconsin-Madison, Madison, WI

The study explores Wacker oxidation using Pd/Cu-exchanged zeolites, focusing on catalyst stability and coke suppression. Density functional theory revealed that increasing NH_3 or H_2O ligands bound to Pd^{2+} reduces ethylene dimerization, enhancing catalyst stability. The findings highlight how ligand environments can mitigate deactivation in heterogeneous Wacker Oxidation.

Activity Improvement for Alkanes Oxidation on Functionalized TS-1.

Zhuoming Feng, *Seyeon Park, Raymond Gorte, and John Vohs*
Department of Chemical and Biomolecular Engineering, University of Pennsylvania, Philadelphia, PA

Synthetic TS-1 is functionalized by organosilane to form a hydrophobic layer on catalyst surface, which enables TS-1 to be fully contact with liquid alkanes during the reaction to increase the reaction rate.

Solvent-Induced Active Site Mobilization and Local Electric Field Effects in Lewis Acid-Containing Zeolites.

*Christopher Paolucci, **Kelsey Levine**, Sugandha Verma, and Asanka Wijerathne*
Chemical Engineering, University of Virginia, Charlottesville, VA

In zeolite-catalyzed reactions with liquid solvents, the solvent plays a key role in controlling catalytic performance and reaction selectivity due to its impact on microenvironments around active sites. This work quantifies the electric field of the solvent and its impact on reaction rate, facilitating optimal selection of solvents and catalysts.

Impact of Ion-Exchange of Brønsted Acid Sites of SAPO-34 with Metal Cations on Olefin Selectivity during CO_2 Hydrogenation.

Fatima Mahnaz[1]*, C D Balaji*[2]*, Jasan Robey Mangalindan*[1]*, Jenna Vito*[1]*, Jithin John Varghese*[3]*, and Manish Shetty*[1]
(1)Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX, (2)Department of Chemical Engineering, Indian Institute of Technology Madras, Chennai, India, (3)Department of Chemical Engineering, Indian Institute of Technology Madras, Chennai, Tamil Nadu, India

The likelihood of solid-state ion exchange (SSIE) of Brønsted acid sites of SAPO-34 with cations from metal-oxides (In_2O_3, ZnZrOx, Cr_2O_3) was estimated by calculating metal-vacancy formation energies using DFT simulations. Our experimental findings confirmed that metal-oxides with low metal-vacancy formation energy facilitated SSIE, significantly affecting olefin selectivity during CO_2 hydrogenation.

Ni and Ru Metallic Nanoparticles Supported on Crystalline and Embryonic HZSM-5 for CO_2 Methanation.

Ana Simões[1]*, Robson De Souza Filho*[1]*, Amanda Guimarães*[2]*, Leandro V. Pontual*[3]*, Joyce R. Oliveira*[4]*, Larissa G. Souza*[4]*, Ludmila P. C. Silva*[5]*, Fabio B. Passos*[6]*, Maria H. Araujo*[1]*, Sara S. Vieira*[4]*, and **Lisiane Veiga Mattos***[3]
(1)Departament of Chemistry, Universidade Federal de Minas Gerais, Belo Horizonte, Brazil, (2)Fluminense Federal University, Niteroi, Brazil, (3)Department of Chemical and Petroleum Engineering, Fluminense Federal University, Niteroi, Brazil, (4)Departament of Inorganic Chemistry, Fluminense Federal University, Niteroi, Brazil, (5)Department of Chemical and Petroleum Engineering, Universidade Federal Fluminense, (6)Department of Chemical and Petroleum Engineering, Universidade Federal Fluminense, Niteroi, Brazil

Ni and Ru metallic nanoparticles supported on crystalline and embryonic HZSM-5 were synthesized and tested for CO_2 methanation. Zeolite supports preserved structural features, however, metals' addition changed supports' textural properties. Catalysts exhibited high CH_4 selectivity, representing a significant advancement in addressing one of the primary challenges in CO_2 utilization.

Atomic Configurations of Dissolved Transition Metal Atoms As Catalytic Active Sites in Liquid Gallium.

Bin Liu
Chemical Engineering, Kansas State University, Manhattan, KS

This work will help us determine the optimal approach to obtain accurate machine learning interatomic potentials for subsequent investigations of liquid Ga's chemical and physical properties during catalytic methane conversions.

Insights into Segregation and Aggregation in Dilute Atom Alloy Catalysts Using DFT and Machine Learning.

Arnold Sison[1], *Keishana Navodye S. a.*[1], *Michael Quaynor*[1], *and Kasun Gunasooriya*[2]
(1)School of Sustainable, Chemical, Biological, and Materials Engineering, University of Oklahoma, Norman, OK, (2)Chemical, Biological & Materials Engineering, University of Oklahoma, Norman, OK

We investigated segregation and aggregation energy of dilute atom alloys by combining high-throughput DFT data with machine learning. We further calculated Bader charges and projected density of states (pDOS) to underscore the electronic structure of solutes at dilute conditions and offer a potential way to tune catalytic performance.

Machine Learning for Catalyst Informatics: Decoding the Role of Data.

Parastoo Semnani[1,2,3], *Florence Vermeire*[4,5], *Hugo da Silva Marques*[6], *Joris Thybaut*[7], *and Pedro Mendes*[5,6]
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Machine learning has emerged as a powerful tool in catalyst discovery, yet its reliability is tightly bound to data quality. This study investigates the effects of dataset characteristics via various ML models, to draw guidlines for a more reliable catalyst design modeling.

Data Science Shows That Entropy Correlates with Accelerated Zeolite Crystallization in Monte Carlo Simulation.

Seungbo Hong[1], *Giovanni Pireddu*[2], *Wei Fan*[1], *Rocio Semino*[2], *and Scott M. Auerbach*[3]
(1)Department of Chemical Engineering, University of Massachusetts Amherst, Amherst, MA, (2)Physico-chimie des Electrolytes et Nanosystèmes Interfaciaux (PHENIX), Sorbonne

Université, CNRS, Paris, France, (3)Department of Chemistry, University of Massachusetts, Amherst, MA

Data science methods revealed that adding a secondary organic structure-directing agent (OSDA) speeds up all-silica LTA zeolite formation by reducing the configurational entropy of the silica network, thus lowering the barrier to crystallization.

Electron Density Based Descriptors for on-the-Fly Machine Learning of Solid-State Materials and Catalytic Interfaces.

Lucas Timmerman[1]*, Andrew Medford*[2]*, and Phanish Suryanarayana*[3]
(1)Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA, (2)School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA, (3)School of Civil and Environmental Engineering, Georgia Institute of Technology, Atlanta, GA

We implement a framework for on-the-fly machine learned force fields that utilizes novel density-based descriptors. We demonstrate the flexibility and effectiveness of this approach by considering bulk alloys with up to 6 elements. We present preliminary results showing the scheme is extensible to surfaces with adsorbates relevant to carbon catalysis.

Understanding the Binary Interactions between CO_2 and Water for Direct Air Capture Using ML Modelling.

Romalya Ranasinghe[1]*, Navya Tyagi*[2]*, Sonika Tyagi*[2]*, Paul Webley*[1]*, and* ***Akshat Tanksale***[1]
(1)Chemical and Biological Engineering, Monash University, Clayton, VIC, Australia, (2)School of Computing Technologies, Royal Melbourne Institute of Technology, Melbourne, VIC, Australia

Direct air capture (DAC) using solid amine adsorbents shows promise for CO_2 removal, but challenges arise from the competitive adsorption of water. Using experimental data, a machine learning model is developed to analyze physicochemical properties, which reveals moisture-CO_2 correlations. The model will aid tailored adsorbent design and be open-sourced post-validation.

Fast and Domain-Accurate Graph Neural Network for Pt Single Atom Systems Via Transfer Learning.

Jeong Woo Han and ***Seokhyun Choung***
Department of Materials Science and Engineering, Research Institute of Advanced Materials, Seoul National University, Seoul, Korea, Republic of (South)

A data-efficient GNN, fine-tuned with transfer learning on 29 DFT-calculated Pt/CeO2 structures, predicts configurations with high accuracy (MAE: 0.01–0.08 eV). This work provides an efficient computational framework for exploring Pt/CeO_2 catalyst structures (acceleration by 3x) and demonstrates the potential of data-efficient machine learning in accelerating catalyst design.

Machine Learning Prediction of Catalysts Performance for Dry Reforming of Methane.

*Yago M. Benites[1], Andressa Andrade Alves da Silva[1], **Héctor Napoleão Cozendey da Silva**[2,3], João Felipe Mitre[1], and **Lisiane Veiga Mattos**[1]*
(1)Fluminense Federal University, Niteroi, Brazil, (2)SENAI CETIQT, Rio de Janeiro, Brazil, (3)University of the State of Rio de Janeiro, Rio de Janeiro, Brazil

Biogas, a renewable energy, can be converted into synthesis gas through DRM to produce hydrogen. Developing efficient catalysts for this process is costly, and Machine Learning aids in catalyst optimization. This study employs Exploratory Data Analysis and XGBoost modeling, achieving strong accuracy (RMSE: 13.09, R^2: 0.80).

Catbench: Benchmark of Graph Neural Networks for Adsorption Energy Predictions in Heterogeneous Catalysis.

Jinuk Moon[1]*, Uchan Jeon[2], and Jeong Woo Han[1]*
(1)Department of Materials Science and Engineering, Research Institute of Advanced Materials, Seoul National University, Seoul, Korea, Republic of (South), (2)Department of Materials Science and Engineering, Seoul National University, Seoul, Korea, Republic of (South)

We have developed CatBench, a comprehensive library dedicated for consistent benchmarking of GNN models on various datasets. CatBench facilitates comparisons between various GNN models, evaluates dataset dependencies, and assesses the effectiveness of transfer learning. It offers a robust framework for a wide range of applications in GNN research and development.

Bayesian Optimization Based Discovery of Optimal Condition for Highly Active Ceria Exsolution Catalyst.

Yunkyung Kim[1]*, Dongjae Shin[1], and Jeong Woo Han[2]*
(1)Department of Materials Science and Engineering, Seoul National University, Seoul, Korea, Republic of (South), (2)Department of Materials Science and Engineering, Research Institute of Advanced Materials, Seoul National University, Seoul, Korea, Republic of (South)

Strong Metal-Support Interaction (SMSI) enhances catalyst stability by embedding exsolved nanoparticles on ceria. Bayesian Optimization (BO) efficiently identifies optimal exsolution conditions, revealing temperature's key role. The analysis reveals distinct mechanisms governing the exsolution behavior of Co-EC and Pt-EC catalysts, with structural and mechanistic validation of catalytic high-performance.

AI-Driven Catalyst Design for Biomass Valorization.

*Xiaoyang Liu and **Hua Song***
Chemical and Petroleum Engineering, University of Calgary, Calgary, AB, Canada

An AI-driven machine learning framework that integrates Large Language Models (LLMs) and machine learning (ML) techniques has been successfully developed in this study to facilitate catalyst discovery for better triggering methane assisted biomass valorization.

Surface Acoustic Wave Energy Driven Degradation of Aqueous-Based Model Contaminants.

***Xieqi Gu**, Yuqi Huang, John Kuhn, and Venkat Bhethanabotla*
Chemical, Biological, & Materials Engineering, University of South Florida, Tampa, FL

Surface acoustic waves (SAWs) generate free radicals to degrade methylene blue (MB) through water hydrolysis. We investigated the impact of SAW frequency, RF power, and hydrogen peroxide concentration on degradation efficiency for potential environmental contaminant dissociation.

A Novel Electrified Reactor with Radial Current and Flow for the Intensification of Endothermic Catalytic Processes.

***Luca Cozzarolo**[1], Federica Romanelli[1], Claudio Ferroni[1], Matteo Ambrosetti[1], Bruna Mello Gabbrielleschi[2], Mauro Bracconi[1], Alessandra Beretta[1], Gianpiero Groppi[1], Bryce Williams[2], and Enrico Tronconi[1]*
(1)Laboratory of Catalysis and Catalytic Processes - Dipartimento di Energia, Politecnico di Milano, Milano, Italy, (2)Air Liquide Forschung und Entwicklung GmbH, Frankfurt, Germany

We present a Joule-heated packed foam reactor with radial current and centrifugal gas flow for methane steam reforming. This configuration allows to match locally the reaction heat demand and the electric power generation, minimizing the cold spot, enhancing catalyst activity, and reducing pressure drops.

Low-Carbon Hydrogen Via Biogas Steam Reforming Using Thermally- Conductive Structured Supports with Embedded Heating Elements.

***Matteo Ambrosetti**[1], Giulia Ferri[2], Alessandra Beretta[1], Gianpiero Groppi[1], and Enrico Tronconi[1]*
(1)Laboratory of Catalysis and Catalytic Processes - Dipartimento di Energia, Politecnico di Milano, Milano, Italy, (2)Snam Decarbonization unit, San Donato Milanese, Italy

We report experimental testing and numerical modelling of a new reactor configuration based on the use of thermally conductive structured supports with embedded heating elements for biogas reforming. Thanks to improved heat transfer, it is possible to run the process in intensified condition by reducing the specific H_2 power demand

Radiofrequency Impact on Reaction Pathway in Propane Dehydrogenation.

***Ben Ko**[1], Kian Kwa[1], Han Wang[1], Carlos L. Pueyo[2], Jianping Chen[3], Roel Sanchez-Carrera[4], and Erdem Sasmaz[1]*

(1)Chemical and Biomolecular Engineering, University of California, Irvine, Irvine, CA, (2)BASF, Ludwigshafen am Rhein, Germany, (3)BASF, Beachwood, OH, (4)BASF, Iselin, NY

Inductive heating (IH) shows no significant difference in propane conversion compared to conventional heating (CFH) but enhances propylene selectivity and suppresses ethylene formation over Pt-based catalyst. This work investigates IH's influence on electron transfer in the dehydrogenation mechanism, altering catalytic activity and product distribution rather than thermal effects.

Radio Frequency Heating for Catalytic Propane Dehydrogenation.

Somtochukwu Lambert[1]*, Ankush Rout*[1]*, Debalina Sengupta*[2]*, Micah Green*[1]*, Benjamin Wilhite*[3]*, and Mark Barteau*[1]
(1)Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX, (2)Texas A&M University, (3)Chemical Engineering, Texas A & M University, College Station, TX

This study explores RF heating with RF-responsive Pt-based catalysts for PDH and compares the results to conventional oven heating. RF heating provides comparable performance to conventional heating while offering the advantages of faster heating and reduced reliance on fossil fuels, aligning with sustainable manufacturing goals.

Electrified Reactor Design for Sustainable Methane Reforming: Converting Greenhouse Gases into Syngas.

Ashwin Kishor Hatwar[1]*, Akshat Tanksale*[1]*, and Hamza Asmat*[2]
(1)Chemical Engineering, Monash University, Clayton, VIC, Australia, (2)Chemical and Biological Engineering, Monash University

Dry reforming of methane (DRM) is an energy-intensive process for converting CO_2 into syngas. Emerging additive manufacturing enables complex reactor geometries for improved heat and mass transfer. We demonstrated inductively heated 3D-printed Inconel monoliths. Joule heating integration with such substrates and perovskite catalysts warrants further investigation for scalability and efficiency.

Electrified Reformer for Syngas Production – Additive Manufacturing of Coated Microchannel Monolithic Reactor.

Hamza Asmat[1]*, Puja Paul*[2]*, Fergus McLaren*[3]*, Lee Djumas*[3,4]*, James Bott*[3,4]*, Matthew R. Hill*[5,6]*, and Akshat Tanksale*[2]
(1)Department of Chemical Engineering, Monash University, Clayton, VIC, Australia, (2)Department of Chemical and Biological Engineering, Monash University, Melbourne, VIC, Australia, (3)Department of Material Science and Engineering, Monash University, Melbourne, VIC, Australia, (4)Woodside FutureLab, Monash University, Melbourne, VIC, Australia, (5)Department of Materials Science and Engineering, Monash University, Clayton, VIC,

Australia, (6)Department of Material Science and Engineering, Monash University, Clayton, VIC, Australia

We present an electrified reformer with 3D-printed catalyst-coated monoliths (Gyroid, Octet, Voronoi) powered by highly efficient induction heating for clean sustainable energy. The Gyroid reactor achieved >99 % CO_2/CH_4 conversion at 900 °C, demonstrating excellent catalytic performance with negligible pressure drop, extended time on stream activity, and no coke formation.

Exploring Metastable Surface Contributions to the Mechanochemical Reduction of Molybdenum Oxide.

Neung-Kyung Yu[1]*, Letícia Rasteiro*[1]*, Van Son Nguyen*[1]*, Kinga Golabek*[1]*, Carsten Sievers*[2]*, and Andrew Medford*[1]
(1)School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA, (2)School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA

This study demonstrates the progressive mechanochemical reduction of MoO_3 during milling, employs DFT calculations to establish an atomistic framework for identifying reactive metastable surfaces, and highlights their importance in mechanocatalytic processes.

Phase Sensitive Detection Analysis of Modulation Excitation Spectra: Such a Thing As a Free Lunch?.

Eleonora Vottero *and Arnaud Travert*
Université de Caen Normandie, Caen, France

Phase Sensitive Detection is examined in the framework of multivariate curve resolution (MCR) models. It is shown that PSD should be used with caution, as noise reduction is also accompanied by a loss of information on active species. Alternative processing and analysis of modulation excitation spectra are proposed.

Quantification of Silanol Groups on Silica Supports By Solid-State NMR in Comparison with Other Analytical Techniques.

Cíntia Salomão Pinto Zarth[1]*,* ***Li Li***[2]*, Antonio Marchi Netto*[2]*, and Diogo Lima Marques da Silva*[1]
(1)Braskem S.A., Triunfo, Brazil, (2)Braskem America Inc, Pittsburgh, PA

This study presents a novel, efficient ^1H MAS-NMR method for silanol group quantification on silica supports, comparing it to other techniques like TGA and DRIFTS. The method differentiates silanol species and provides guidelines for selecting appropriate characterization tools based on laboratory resources and research goals.

Integrating Air-Controlled and Cryogenic Electron Microscopy Workflows for Catalyst Development.

Jae Jin Kim
Shell International Exploration and Production Inc., Houston, TX

This study demonstrates the integration of air-controlled and cryogenic electron microscopy workflows for the development of advanced catalytic systems. By preserving air-sensitive catalysts' native states, these workflows enable precise characterization of structures, interfaces, and mechanisms, advancing the design of high-performance, efficient, and sustainable catalysts for industrial and energy applications.

Investigating the Activation of Fe-Based Catalyst for CO_2 Hydrogenation Using the *in-Situ* mass Analyzer..

Mei Ju Goemans[1]*, Pio Gramazio*[1]*, Björn Frederik Baumgarten*[1]*, Rune Myrstad*[2]*, Jia Yang*[3]*, and Edd Blekkan*[1]
(1)Department of Chemical Engineering, Norwegian University of Science and Technology, Trondheim, Norway, (2)SINTEF Industry, Kinetics and Catalysis Research Group, Trondheim, Norway, (3)College of Smart Energy, Shanghai Jiao Tong University, Shangai, China

We introduce the *In-Situ* Mass Analyzer for advanced characterization of Fe-based CO_2 hydrogenation catalysts. Vibrational frequency of a quartz fixed-bed reactor relates to mass changes of the iron-phases, making real time monitoring of the catalyst at reaction conditions while measuring activity and selectivity with an online GC and MS possible.

Assessing Critical Dose for Beam-Sensitive MOFs Using Low-Dose *in-Situ* Video.

Benjamin Miller *and Cory Czarnik*
Gatan, Pleasanton, CA

This study focuses on low-dose transmission electron microscopy (TEM) characterization of metal-organic frameworks (MOFs). It demonstrates how recent advancements in TEM electron counting camera technology enable the preservation of pristine MOF structures during extended electron irradiation. This allows for accurate characterization of nano-scale structures, enhancing understanding of structure-property relationships.

Chromatographic Dynamic Chemisorption.

Abeer Abuothman[1]*, Atharva Burte*[2]*, and Omar Abdelrahman*[2]
(1)Chemical and Biomolecular Engineering, University of Houston, Houston, TX, (2)William A. Brookshire Department of Chemical and Biomolecular Engineering, University of Houston, Houston, TX

This work goal is to develop a reliable technique for measuring the dispersion of supported metal catalysts, using equipment readily available in a catalysis focused research laboratory. Given the ubiquity of chromatography-based analysis, a simple technique to measure the dispersion using a gas chromatograph via isothermal dynamic CO chemisorption.

Surface Area Determination with a Laboratory Scale and Room Humidity from Single-Point BET Analysis of Physisorbed Water.

Ismail Paykar[1]*, Simon Friedrich*[2]*, John Regalbuto*[3]*, and Christopher Williams*[3]
(1)Chemical Engineering Department, University of South Carolina, Columbia, SC, (2)Virginia Commonwealth University, Richmond, VA, (3)Chemical Engineering, University of South Carolina, Columbia, SC

Single point BET analysis using physisorbed water from atmospheric humidity as the adsorbate on a series of activated alumina is validated using TGA. The effective cross-sectional area of water is calculated and applied to determine surface area via a laboratory scale, incorporating humidity dependent weights of the supports.

In Situ Synchrotron Radiation XPS Studies of Core-Shell Niga@GaO_x Catalysts for Propane Dehydrogenation.

Yiyi Xu[1] *and Andrew Beale*[2]
(1)UCL, London, London, United Kingdom, (2)Finden Ltd, Didcot, United Kingdom

In Situ Synchroron radiation XPS validate the formation of NiGa@GaO_x core-shell structure due to strong interaction between Ni and GaO_x and further separate the functional role of partially-reduced GaO_x overlayer as reactive sites and subsurface metallic Ni site as electronic promoter, enhancing Ga-H species and promoting C-H activation of propane.

Frequency Screening in Modulation Excitation Spectroscopy Forassessment of Reaction Intermediates during Ethanol Oxidation Ongold Catalysts.

Bhagyesha Patil[1]*, Alejandra Torres Velasco*[2]*, and Juan Bravo-Suarez*[3]
(1)Chemical & Petroleum Engineering, The University of Kansas, Lawrence, KS, (2)Center for Environmentally Beneficial Catalysis, The University of Kansas, Lawrence, KS, (3)Chemical Science Divison, ORNL, oak ridge, TN

This study expands a frequency screening methodology in modulation excitation spectroscopy for the simultaneous study of reaction intermediates and spectator species. Application to ethanol oxidation on gold catalysts further emphasizes the role of support adsorption in determining product selectivities in catalyzed reactions.

Time-Resolved and Multimodal X-Ray Studies of Inverse Ceria-Copper Catalysts for CO_2 Hydrogenation.

Jorge Moncada[1]*, Evan Jahrman*[2]*, Eli Stavitski*[3]*, and Jose Rodriguez*[4]
(1)Theiss Research, La Jolla, CA, (2)Department of Chemical and Biomolecular Engineering, University of Delaware, Newark, DE, (3)National Synchrotron Light Source II, Brookhaven National Laboratory, Upton, NY, (4)Chemistry, SUNY Stony Brook

This study demonstrates the power of time-resolved synchrotron X-ray techniques in uncovering the structure-reactivity relationships in inverse CeOx/Cu catalysts. The insights gained here provide a foundation for optimizing catalyst design and reaction conditions very fast and dynamic processes.

Oxidative Dehydrogenation of Ethane (ODHE) to Ethylene By the Bulk Movnbte (M1 Phase) Mixed Oxide Catalyst: Surface and Bulk Properties.

Dang Nguyen[1], *Bar Mosevitzky Lis*[1,2], *Agustin De Arriba*[3], *Jose Manuel Lopez-Nieto Sr.*[3], *and Israel Wachs*[4]
(1)Department of chemical and biomolecular engineering, Lehigh University, Bethlehem, PA, (2)Department of Chemical Sciences and Bernal Institute, University of Limerick, Limerick, Ireland, (3)Instituto de Tecnología Química, Universitat Politècnica de València, Valencia, Spain, (4)Department of Chemical and Biomolecular Engineering, Lehigh University, Bethlehem, PA

This project employs multiple bulk-sensitive (Raman and XRD) and surface-sensitive (NAP-XPS and HS-LEIS) techniques to characterize the M1 phase of the bulk $MoVNbTeO_x$ catalyst under oxidative and ethane-reducing conditions. The surface of the bulk M1 phase was shown to be dynamic and a strong function of experimental conditions.

New Insights on Deactivation Mechanism of the Crox/Al_2O_3 Dehydrogenation Catalyst..

Vladimir Fridman[1], *Renqin Zhang*[2], *and Rong Xing*[3]
(1)Research and Development, Clariant Corporation, Louisville, KY 40210, USA, KY, (2)Clariant, Louisville, KY, (3)Research and Development, Clariant Corporation, Louisville, KY

This paper describes TEM and XRD study of the CrOx/Al2O3 catalyst aged for different degrees and model mixtures of gama-Al2O3 and Cr2O3, and alpha Cr2O3 and Al2O3. These study provided additional insight to the CrOx/Al2O3 catalyst deactivation model.

Development of a Novel Reactor for the Production of Sustainable Aviation Fuel.

Jay Clarkson[1], *Andrew Coe*[2], *James Paterson*[3], *and* ***Virginie Viseur***[2]
(1)Johnson Matthey, Stockton on Tees, United Kingdom, (2)Johnson Matthey, London, No State, United Kingdom, (3)Fischer-Tropsch, bp, Kingston upon Hull, United Kingdom

Here we present a unique reactor enhancement device (CANS^{tm}), which can be used at both large and small scale, to meet the targets of reduction in greenhouse gases emissions. This device contains submm catalyst particles, resulting in an increase of the productivity per unit volume of reactor.

Electrochemical H_2 Pumping Enhances the Activity of Selective Semi-Hydrogenation Catalysts.

Michael Lemelin[1] *and* ***Ezra L. Clark***[2]

(1)Chemical Engineering, The Pennsylvania State University, University Park, PA, (2)Chemical Engineering, Penn State, University Park, PA

The rate of selective acetylene semi-hydrogenation over Cu is enhanced by a factor of ~1000 by supplying H* via electrochemical H_2 pumping since the overall rate of reaction is limited by H_2 activation in conventional thermal reactors.

Hierarchical Zeolite-Based Catalysts for Tandem One-Step Renewable Diesel Production Via Fischer-Tropsch Synthesis.

Binchao Zhao[1]*, Chunxiang Zhu*[1,2]*, Fangyuan Liu*[3]*, and Pu-Xian Gao*[2,4]
(1)Materials Science and Engineering, University of Connecticut, Storrs, CT, (2)3D Array Technology LLC, Storrs, CT, (3)Institute of Materials Science, University of Connecticut, Storrs, CT, (4)Department of Materials Science and Engineering, University of Connecticut, Storrs, CT

In this work, through rational materials design and manipulation, we have formulated a multi-layer hierarchical monolithic catalyst which can integrate the syngas-to-wax hydrocarbons and wax hydrocarbons-to-diesel fuel conversions in a tandem one-step catalysis process for sustainable drop-in renewable diesel production via Fischer tropsch synthesis.

Twin Fixed Bed Reactors for Accelerated Deactivation Testing Protocols Via Mixed Steady-State/Transient Pulsing.

Greg Barber[1]*, Christopher Lieb*[1]*, and Robert Rioux*[2,3]
(1)Chemical Engineering, The Pennsylvania State University, University Park, PA, (2)Department of Chemistry, The Pennsylvania State University, University Park, PA, (3)Department of Chemical Engineering, The Pennsylvania State University, University Park, PA

Catalyst lifetime, or productivity is rarely the focus of academic research, yet it represents a critical piece of knowledge needed by industry. We have developed a mirrored reactor to develop accelerated catalyst aging protocols to produce data to aid in the development of ML models for catalyst degradation predictions.

Predicting Lifetime Performance and Deactivation of CrO_x/Al_2O_3 As a Catalyst for Propane Dehydrogenation through Multiscale Characterization and Model Development.

Nicholas Thornburg[1]*, **Adam Yonge***[2]*, Meagan Crowley*[2]*, Hariswaran Sitaraman*[2]*, Dingqi Nai*[3]*, Jason Malizia*[4]*, Stephen Kristy*[4]*, Rong Xing*[5]*, Mingyong Sun*[6]*, Lars Grabow*[7]*, Rebecca Fushimi*[4]*, Andrew Medford*[3]*, and Peter Ciesielski*[2]
(1)Center for Energy Conversion & Storage Systems, National Renewable Energy Laboratory, Golden, CO, (2)National Renewable Energy Laboratory, Golden, CO, (3)School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA, (4)Idaho National Laboratory, Idaho Falls, ID, (5)Research and Development, Clariant Corporation, Louisville, KY, (6)Clariant, Louisville, KY, (7)William A. Brookshire Department of Chemical and Biomolecular Engineering, University of Houston, Houston, TX

This presentation leverages outputs of dynamic catalyst science experiments and informatics-based mechanism determination to develop transient multiscale models that predict and inform on supported CrO_x/Al_2O_3 catalyst deactivation phenomena for industrial propane dehydrogenation. These findings provide actionable physicochemical insights into catalyst evolution that may guide practical improvements for commercial reactor operation.

Podcat: Stories and Strategies from the Catalysis Community.

*Thomas P. Senftle[1], Ezra L. Clark[2], and **Marc Porosoff**[3]*
(1)Smalley-Curl Institute, RICE University, Houston, TX, (2)Chemical Engineering, Penn State, University Park, PA, (3)Department of Chemical Engineering, University of Rochester, Rochester, NY

The poster is to advertise our podcast targeted toward early-career researchers, featuring career advice and interviews with top catalysis experts from industry and academia. Guests include Eranda Nikolla, Susannah Scott, Charlie Campbell, and Cathy Tway.

Comparative Hydrogenation of Ortho- and Para-Nitrophenol Using Palladium on Aryl-Bridged Polysilsesquioxanes: Kinetic Insights and Solvent Effects.

***James Nana Gyamfi**[1], Snehal Patil[1], Luke Gillespie[1], Chidimma Maryjane Nwankwaor[1], Anant Sohale[1], Seval Gunduz[1], Paul Edmiston[2], and Umit Ozkan[1]*
(1)William G. Lowrie Department of Chemical & Biomolecular Engineering, The Ohio State University, Columbus, OH, (2)The College of Wooster, Wooster, OH

Pd supported on aryl-bridged polysilsesquioxanes (ABPS) exhibited excellent catalytic activity and stability in hydrogenating toxic nitrophenols (ONP, PNP). Results revealed solvent-dependent reaction kinetics and substrate-support polarity interactions, highlighting Pd/ABPS as a promising eco-friendly catalyst for water remediation under mild conditions.

Silica Supported Sub-2 Nm CeO_x Nanoislands for CO Oxidation.

***Ying Zheng**[1], Bailey Holmes[2], Asuka Firdaus[3], and Jingyue Liu[1]*
(1)Department of Physics, Arizona State University, Tempe, AZ, (2)School of Molecular Sciences, Arizona State University, Tempe, AZ, (3)Ira A. Fulton Schools of Engineering, Arizona State University, Tempe, AZ

Experimental results demonstrated the tuning of catalytic properties of silica supported CeO_x nanoislands by gas phase treatment, leading to significantly enhanced activity for CO oxidation

Plasma-Assisted Oxidative Coupling of Methane over Sodium-Promoted Gold Catalysts.

Yiteng Zheng
Chemical and Biological Engineering, Princeton University, Princeton, NJ

Oxidative coupling of methane is a promising processes that convert methane into C_2 hydrocarbons. We coupled non-thermal plasma and catalysts to produce C_2 products from methane at room temperature. A reactor was developed to enable in-situ/operando Raman spectroscopy with plasma. Kinetic measurements were collected for plasma-assisted oxidative coupling of methane.

Electrochemical CO2 Reduction: Data-Driven Prediction of the Selectivity.

Michael Albrechtsen[1] *and Alexander Bagger*[2]
(1)DTU Physics, Technical University of Denmark, Kongens Lyngby, Denmark, (2)Chemistry, University of Copenhagen

Electrochemical CO_2 reduction needs highly selective catalysts. We pair a high-dimensional DFT-derived descriptor fingerprint with tree-based machine learning to map catalysts to experimental product distributions. The model predicts Faradaic efficiencies within ~4 % and reveals key descriptors, enabling mechanism-agnostic, data-driven screening of selective electrocatalysts.

Brønsted and Lewis Acidity Characterization of ZSM-5 with Varying Si/Al Ratios Via Temperature-Programmed Desorption.

Urim Pearl Kim
Micromeritics, Norcross, GA

Ammonia TPD is widely used to characterize the overall acidity of a zeolite.

Impact of Pre-Ion Plasma Treatment on Catalyst Efficacy in Plasma-Assisted Dry Reforming of Methane.

Md Monir Hossain *and Ruigang Wang*
Chemical Engineering and Materials Science, Michigan State University, East Lansing, MI

A dual-plasma approach combining high-energy ion plasma pre-treatment and dielectric barrier discharge (DBD) plasma is used to enhance catalyst performance in dry reforming of methane (DRM). CeO_2 nanorod-supported Ni/Ru catalysts are modified with ion plasma, and changes in surface properties are analyzed using various techniques, including in-situ DRIFTS and chemisorption.

Potential-Dependent Metal Dissolution Behavior Using Online ICP-MS and Design Implications for Durable Pt-M Alloy Catalysts in Pemfcs.

Kyounghee Kim[1]*, Seongmin Yuk*[1]*, Jinseong Choi*[1]*, Jaejun Ko*[1]*, and Chang Hyuck Choi*[2]
(1)Hyundai Motor Company, Yongin-Si, Korea, Republic of (South), (2)Department of Chemistry, Pohang University of Science and Technology (POSTECH), Pohang, Korea, Republic of (South)

This study identifies potential-dependent metal dissolution in Pt-alloy catalysts and highlights how mesoporous carbon supports enhance durability, providing insights for designing stable, high-performance PEMFC catalysts through alloy surface control and structural optimization.

Dissolution Phenomena of Transition Metal Alloy Catalysts and Their Effects on Fuel Cell Performance.

Seongmin Yuk[1]*, Kyounghee Kim*[1]*, Jinseong Choi*[1]*, Jaejun Ko*[1]*, and Chang Hyuck Choi*[2]
(1)Hyundai Motor Company, Yongin-Si, Korea, Republic of (South), (2)Department of Chemistry, Pohang University of Science and Technology (POSTECH), Pohang, Korea, Republic of (South)

We investigated the dissolution behavior of transition metals from Pt-alloy catalysts and its impact on fuel cell. The dissolution profiles, cumulative dissolution of metal ions and its detrimental effects were elucidated using an online ICP-MS, XRF and EIS, respectively.

Unraveling Serial Degradation Pathways of Supported Catalysts through Reliable Electrochemical Liquid-Cell TEM Analysis.

Young-Jung Heo
Advanced Fuel Cell Technology Development Team 1, Hyundai Motor Group, Yongin-Si, Gyeonggi-do, Korea, Republic of (South)

We developed an advanced electrochemical liquid-cell TEM technique to reliably track the real-time degradation of Pt/C catalysts under polarization. High-resolution Imaging reveals that catalyst degradation is predominantly driven by nanoparticle migration, leading to sequential coalescence and detachment, offering new insights into size-dependent durability mechanisms for supported catalysts.

PLENARY LECTURES

2025 PAUL H. EMMETT AWARD PLENARY LECTURE BY PHILLIP CHRISTOPHER

Tuesday, June 10, 2025 8:00 AM - 9:00 AM
Centennial Ballroom

Chair: Suljo Linic, University of Michigan, Ann Arbor

Atomically Dispersed Pt-Group Metal Catalysts: Active Site Structure, Function and Design.

Phillip Christopher
Department of Chemical Engineering, University of California, Santa Barbara, Santa Barbara, CA

I will highlight efforts focused on: (1) the synthesis and characterization of uniform atomically dispersed Pt active sites, (2) the development of structure-function relationships, (3) the local

restructuring of these active sites due to changes in environmental conditions and (4) atomically dispersed Rh based catalysts for alkene hydroformylation.

AI - AI-DRIVEN CATALYSIS

AI - APPLICATION-DRIVEN AI CATALYST DESIGN

Tuesday, June 10, 2025 9:30 AM - 11:30 AM
Regency Ballroom VII

Chair: Long Qi, Ames Laboratory

Co-Chair: Nancy M. Washton, Pacific Northwest National Laboratory

Catalyst Discovery for Ammonia Synthesis Using Active Learning.

Jochen Lauterbach[1] *and Withana A R Jayarathna*[2]
(1)Department of Chemical Engineering, University of South Carolina, Columbia, SC, (2)University of South Carolina, Columbia, SC

Literature data for heterogeneous catalysts make it a great source for AI searches, and selectively adding experimental data via Active Learning allows for the efficient discovery of novel catalysts. We employ this framework for heterogeneous catalyst development for ammonia synthesis, reporting previously unknown formulations.

Autonomous AI-Driven Discovery of Multicomponent Oxides for CO_2 Utilization in Chemical Looping.

Anders Hellman
Competence Centre for Catalysis, Chalmers University of Technology, Göteborg, Sweden

Utilizing a self-learning cycle, we discover several new multi-component oxygen carriers for CO_2 splitting in chemical looping. The study demonstrates the self-learning cycle's scalability and effectiveness in accelerating material discovery while contributing to advancements in carbon utilization and hydrogen production processes.

Accelerated Discovery of Heterogeneous Catalysts Using Machine Learning Approach.

Ken-ichi Shimizu[1] *and* ***Takashi Toyao***[2]
(1)Institute for Catalysis, Hokkaido university, Sapporo, Japan, (2)Hokkaido University, Sapporo, Japan

We demonstrate a ML approach to develop new multi-elemental reverse water-gas shift catalysts. By performing 44 cycles of the closed loop discovery system (ML prediction + experiment), we experimentally tested 300 catalysts and identified more than 100 catalysts with superior activity compared to those of the previously reported high-performance catalysts.

Atomistic Evolution of Active Sites in Multi-Component Heterogeneous Catalysts.

Cameron Owen[1], *Lorenzo Russotto*[1], *Christopher O'Connor*[2], *Nicholas Marcella*[3], *Anders Johansson*[1], ***Albert Musaelian***[1], *Ralph G. Nuzzo*[3], *Anatoly I. Frenkel*[4,5], *Christian Reece*[1], *and Boris Kozinsky*[1,6]
(1)Harvard University, Cambridge, MA, (2)Rowland Institute at Harvard, Harvard University, Cambridge, MA, (3)University of Illinois Urbana-Champaign, Urbana, IL, (4)Stony Brook University, Stony Brook, NY, (5)Brookhaven National Laboratory, Upton, NY, (6)Robert Bosch LLC Research and Technology Center, Watertown, MA

This work studies PdAu metal nanoparticle catalysts using machine learning force field techniques to conduct simultaneously accurate and scalable atomic-scale simulations. Among other results, we provide direct atomistic evidence that verifies existing experimental hypotheses for bimetallic catalyst deactivation under reaction conditions, namely that Pd preferentially segregates into the Au bulk.

Accelerating Material Discovery in Syngas Hydrogenation Via Open-Access Feature Engineering and Semantic Standardization.

Mohammad Khatamirad[1], *Tiago Goncalves*[2], *Edvin Fako*[2], *Sandip De*[2], *Raoul Naumann d'Alnoncourt*[1], *Michael Geske*[1], *Stephan A. Schunk*[2,3], *Sonja Schimmler*[4], *and Frank Rosowski*[1,2]
(1)BasCat - UniCat BASF JointLab, Berlin, Germany, (2)Group Research, BASF SE, Ludwigshafen, Germany, (3)hte GmbH, Heidelberg, Germany, (4)Open Communication Systems, Fraunhofer FOKUS, Berlin, Germany

This work presents a data-driven approach to accelerate multi-component catalyst discovery for the syngas-to-ethanol reaction. By leveraging open-access descriptors, predictive modeling, and semantic standardization, this study identifies novel catalyst compositions, enhancing ethanol yield without time-intensive computations, and establishes a reusable framework for machine-actionable catalytic data.

Development of Improved Promoted Pt Catalysts for Propane Dehydrogenation through Bayesian Optimization with Uncertainty Quantification.

Harsh Darji[1], *Unni Kurumbail*[1], *Matias Alvear*[2], *Siying Chen*[2], *and Ive Hermans*[1,2,3]
(1)Department of Chemical & Biological Engineering, University of Wisconsin-Madison, Madison, WI, (2)Department of Chemistry, University of Wisconsin - Madison, Madison, WI, (3)Wisconsin Energy Institute, University of Wisconsin - Madison, Madison, WI

This study presents a Bayesian optimization strategy to identify highly active and stable multi-metallic heterogeneous catalysts within a large design space of ~1.4MM possible formulations of Pt/γ-Al_2O_3 catalysts for propane dehydrogenation. The approach employs a two-tiered optimization process, incorporating finer variations in metal loadings and integrating uncertainty into surrogate models.

BIOMASS - BIOMASS AND WASTE VALORIZATION CATALYSIS

BIOMASS - BIOMASS CONVERSION

Tuesday, June 10, 2025 9:30 AM - 11:30 AM
Regency Ballroom VI

Chair: Yomaira Pagan Torres, University of Puerto Rico at Mayaguez

Co-Chair: Mike Griffin, National Renewable Energy Laboratory

An Electrobiomanufacturing Strategy for the Production of Renewable Adipic Acid.

Prathamesh T. Prabhu[1,2], Deep M. Patel[1,2], Marco Nazareno Dell'Anna[1,2], Devanshi Mistry[1,2], Luke T. Roling[1,2], and ***Jean-Philippe Tessonnier***[1,2]
(1)Center for Biorenewable Chemicals (CBiRC), Ames, IA, (2)Department of Chemical and Biological Engineering, Iowa State University, Ames, IA

Biobased *cis,cis*-muconic acid is converted to adipic acid, a Nylon monomer, using an electrobiomanufacturing approach that leverages biomass as renewable carbon feedstock, water as a hydrogen source, and green electricity to drive the transformation. Outer-sphere and surface-mediated electrohydrogenation pathways are controlled by the nature of the metal catalyst and pH.

Developing Nanoscale Catalysts for Biomass Electro-Valorization through Structure-Property Relationships.

Nicholas Bedford[1] *and Yuwei Yang*[2]
(1)Colorado School of Mines, Golden, CO, (2)University of New South Wales, Sydney, Australia

This contribution summarizes our group's recent work in implementing electrocatalytic approaches toward the valorization of biomass-derived substrates. This will include electrooxidation and electrocoupling reactions and will showcase the importance of understanding structure-property relationships to help elucidate catalytic properties.

Characterization of Catalyst Performance for Conversion of Bio-Derived Oxygenates Using Dual-Column GC.

Christopher P. Nicholas*, Benjamin R. Hoekstra, and Lyle Monson*
Lakril Technologies Corporation, Chicago, IL

The dual-column GC method uses a single injection to analyze samples containing high levels of water, organic acids, oxygenates, and permanent gases (CO, CO2, and C2H4) using a single injection. This method has been utilized to investigate reaction pathways during lactate dehydration and the impact of feedstock impurities on catalysis.

Role of Phosphorous in Transition Metal Phosphides for Selective Hydrogenolysis of Hindered C–O Bonds.

Conor Waldt[1,2]*, Hansel Montalvo-Castro[1], Justin Atlas[1], Angela Aguirre[1,2,3], Alvaro Loaiza[4], Craig Plaisance[4], and David Hibbitts*[1,2]
(1)Department of Chemical Engineering, University of Florida, Gainesville, FL, (2)Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN, (3)Chemical

Engineering, University at Buffalo, Buffalo, NY, (4)Cain Department of Chemical Engineering, Louisiana State University, Baton Rouge, LA

Adding P to Ni and other transition metals generally leads to an increase in selectivity for cleaving hindered C–O bonds. These shifts in selectivity are resultant of electronic modifications of the M atoms by P and to a lesser degree changes in the size of the continuous M atom ensembles.

Selective Production of Biobased Primary Amines By Reductive Amination over Atomically Dispersed Pt_1/S-C.

***Yangming Ding**, Guanna Li, Tomas Haasterecht, van, and Johannes Hendrik Bitter*
Wageningen University, Wageningen, Netherlands

Reductive amination of furfural is a sustainable strategy towards primary amine synthesis. The electronic effect of Pt has a significant influence on the selectivity. Pt single atom and nanoparticles supported on carbon doped S was prepared for proof of concept. The highest yield to furfural amine was achieved over Pt_1/S-C.

Catalytic Lactide Production from Renewable Alkyl Lactates over Ti MWW-Type Zeolite Catalysts.

*Haerin Lee, **Seung Hyeok Cha**, and Dong Won Hwang*
Korea Research Institute of Chemical Technology (KRICT), Daejeon, Korea, Republic of (South)

Ti-MWW catalysts demonstrate superior lactide productivity in the gas-phase conversion of methyl lactate, outperforming TiO_2/MCM-41 and TS-1. Accessible tetrahedral TiO_4 active sites on 12-ring cup-shaped external surfaces enhance catalytic activity, doubling the turnover frequency compared to other catalysts, highlighting Ti-MWW's efficiency and selectivity for lactide production.

C2+ - CATALYSIS OF C2+ CHEMISTRY

C2+ | ETHANE DEHYDROGENATION AND AMMOXIDATION REACTIONS

Tuesday, June 10, 2025 9:30 AM - 11:30 AM
Hanover Hall CDE

Chair: Nathaniel Eagan, Tufts University

Co-Chair: Stephen Purdy, Oak Ridge National Laboratory

Kinetic Consequences of Oxygen Vacancies in Cobalt-Molybdenum Oxides on C−H Activation of Ethane.

***Guangming Cai**[1], Gregory Novotny[2], Alyssa Hensley[3], Prashant Deshlahra[2], and Ya-Huei (Cathy) Chin[1]*
(1)Department of Chemical Engineering and Applied Chemistry, University of Toronto, Toronto, ON, Canada, (2)Department of Chemical and Biological Engineering, Tufts University,

Medford, MA, (3)Chemical Engineering and Materials Science, Stevens Institute of Technology, Hoboken, NJ

This work highlights the kinetic consequences of O-vacancies in ethane C−H bond activation, emphasizing the necessity of considering in situ defect dynamics to accurately establish structure-reactivity relationships.

Modeling Particle Size Effect for Ethane Dehydrogenation over Pt Catalysts.

Mubarak Bello[1]*, Bhawana Rayamajhi*[1]*, Olajide Bamidele*[1]*, Wenqiang Yang*[1]*, and Andreas Heyden*[2]
(1)Chemical Engineering, University of South Carolina, Columbia, SC, (2)Department of Chemical Engineering, University of South Carolina, Columbia, SC

A new particle-based microkinetic modeling approach was used to investigate the effect of Pt particle size on ethane dehydrogenation (EDH) kinetics and mechanism. Better kinetic agreement with experiment was achieved and new insights into the EDH mechanism uncovered.

Unlocking Superior Ethylamine Electro-Oxidation and Nitrile-like Intermediates Poisoning Resistance on Pt Enabled By Electronic and Geometric Modulation.

Yanlin Zhu*, Jinyao Tang, and Zhenmeng Peng*
Chemical Engineering, University of South Carolina, Columbia, SC

Platinum (Pt) is active for ethylamine electro-oxidation but deactivates quickly. We developed a Pt_3Ni_1@Au catalyst, utilizing electronic effects from Pt-Ni alloying and geometric modulation via Au deposition, achieving enhanced stability. After 100 CV cycles, its activity retention is 5 times higher than pure Pt, showcasing its potential for hydrogen storage.

Subtle Changes to the Active Sites of Zeolite-Supported Metals during Reaction: Understanding the Promotional Effect of Parallel CO_2 Reduction on Ethane Dehydrogenation.

Wenqi Zhou, Ron Runnebaum, and ***Coleman Kronawitter***
Chemical Engineering, University of California, Davis, CA

Co-feeding CO_2 has a promotional effect on the rate of ethane dehydrogenation for many catalyst material systems, but the mechanism is not understood. This work leverages a zeolite-based catalyst with well-defined active sites, combined with operando X-ray absorption spectroscopy, to understand the impact of parallel CO_2 reduction on ethane dehydrogenation.

CO_2 Oxidative Ethane Dehydrogenation on CeO_2/SiO_2 Supported $NiFe_3$ Catalysts.

Rachel Spurlock[1,2]*, Ezgi Erdem*[1,2]*, Sang-Won Lee*[1,2]*, Junjie Chen*[1,2]*, Alessandro Gallo*[1,2]*, Adam Nielander*[2]*, and Thomas Jaramillo*[1,2]

(1)Chemical Engineering, Stanford University, Stanford, CA, (2)SUNCAT Center for Interface Science and Catalysis, SLAC National Accelerator Laboratory, Menlo Park, CA

Supporting $NiFe_3$ on a mixed CeO_2 on SiO_2 support system allows the creation of a solid solution of Fe-doped CeO_2 crystals. The solid solution results in high ethylene production rate, as well as high ethylene selectivity; a marked improvement over a CeO_2-only supported $NiFe_3$, which shows poor ethylene selectivity.

Influence of Metal Identity on Acetonitrile Selectivity in Ethane Ammoxidation.

Jieun Lee[1]*, Yongwoo Kim*[1]*, Jing Luo*[2]*, Ida (xue) Chen*[3]*, and David W. Flaherty*[1]
(1)Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA, (2)Engineering and Process Science, The Dow Chemical Company, Midland, MI, (3)Dow, Inc., Manvel, TX, 77578, TX

We synthesize, characterize, and kinetically examine catalysts formed by ion exchange of metal cations (M-BEA) to beta zeolites for ethane ammoxidation to acetonitrile. Co and Ni-BEA show higher acetonitrile selectivity, likely because Co and Ni bind with NH_3 to form a stable metal-amine complex required for acetonitrile formation.

ELECTRO PHOTO - ELECTROCATALYSIS AND PHOTOCATALYSIS

ELECTRO PHOTO - ORGANIC ELECTROCHEMICAL TRANSFORMATIONS 2

Tuesday, June 10, 2025 9:30 AM - 11:30 AM
Centennial Ballroom I

Chair: Jason Bates, University of Virginia

Co-Chair: Robert Warburton, Case Western Reserve University

Elucidating the Influence of Potassium Addition in Ru/TiO_2 on Charge-Carrier Dynamics for Photocatalytically Enhanced Ammonia Synthesis.

Carissa Yim[1]*, Anna Klinger*[2]*, Hannah R. Faustyn*[3]*, Alondra M. Ortiz-Ortiz*[4]*, Daniel Penley*[4]*, Daniel O. Delgado Cornejo*[4]*, Sijun Seong*[1]*, Xiwen Gong*[1]*, Neil P. Dasgupta*[5]*, Galen Fisher*[1]*, Johann Schwank*[1]*, and Andrej Lenert*[1]
(1)Chemical Engineering, University of Michigan, Ann Arbor, MI, (2)Chemical Engineering, University of Michigan, Ann Arbor, Ann Arbor, MI, (3)Mechanical Engineering, University of Michigan, Ann Arbor, Ann Arbor, MI, (4)Mechanical Engineering, University of Michigan, Ann Arbor, MI, (5)Mechanical Engineering and Materials Science, University of Michigan, Ann Arbor, MI

We study the crystallographic structure, Ru nanoparticle (NP) size, and charge-carrier lifetime (τ) in 1 and 4 wt.% Ru/TiO_2 catalysts with 0.2, 4, or 8 wt.% K (y wt.% Ru/ x wt.% K-TiO_2), aiming to inform the design of efficient photocatalysts to help address the demand for distributed NH_3 synthesis.

Selective Formation and Reaction of Surface Oxygen Species to Promote Alkene Epoxidation over Oxygen Evolution on Au Anodes.

***Richa Ghosh**, Jordan W. Lu, Geoffrey Hopping, and David Flaherty*
School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA

Previous attempts to promote epoxidation on electrodes focused on catalyst development. Oscillation of electrode potentials may increase Faradaic efficiencies for alkene epoxidations through O_2 evolution inhibition. Here, we use transient open circuit potential transients and *operando* surface enhanced Raman spectra to develop potential oscillation programs for epoxidation Faradaic efficiency optimization.

Enhancing the Electrooxidation of Furfural with Metal/Oxide Interfaces and Low Loading Catalyst.

***Emma Hollis**, Marc Manye Ibanez, and Adam Holewinski*
Chemical and Biological Engineering, University of Colorado Boulder, Boulder, CO

Metal oxides interfaces and low loading catalyst were explored to enhance reaction efficiency of furfural oxidation in acid. Pt/ATO oxidizes furfural 0.2V lower than Pt/C, leading to sustained current with less decay in rate over time. Further kinetics implies that ATO donates OH to the strongly bound intermediates on Pt.

Complete Electrocatalytic Aqueous Defluorination of PFAS with Nonprecious Materials.

Astrid M Müller
Chemical Engineering, University of Rochester, Rochester, NY

PFAS are persistent pollutants requiring effective remediation strategies. We developed a cost-effective electrocatalytic method using nonprecious nanocatalysts and deep ultraviolet light for complete mineralization of PFOS, PFOA, and GenX. This approach minimizes energy use and prevents anode fouling, demonstrating significant advancements in PFAS destruction technologies.

KEYNOTE: Electrified Olefin Epoxidation Via Water Activation.

Karthish Manthiram
Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, CA

We present methods of epoxidizing olefins using water-derived oxygen atoms at ambient conditions. Water is activated at the anode, generating oxygen-containing intermediates that convert olefins into epoxides, while generating hydrogen at the cathode. Spectroscopy unveils structural features of the most active catalysts, acting as design principles for future work.

ENVIRO AUTO - ENVIRONMENTAL AND AUTOMOTIVE CATALYSIS

ENVIRO AUTO - MECHANISTIC INSIGHTS ON SELECTIVE CATALYTIC REDUCTION (SCR) OVER CU-ZEOLITES

Tuesday, June 10, 2025 9:30 AM - 11:30 AM

Hanover Hall FG

Chair: Rohil Daya, Cummins Inc.

Co-Chair: Isabella Maria Nova, Politecnico di Milano

Fundamental Insight from Decoupling RHC and OHC in the Standard-SCR Redox Mechanism over Cu-CHA Catalysts.

*Andrea Gjetja[1], Nicola Usberti[1], Nicole Daniela Nasello[1], Umberto Iacobone[1], Isabella Maria Nova[1], **Enrico Tronconi**[1], Roberta Villamaina[2], Maria Pia Ruggeri[2], Djamela Bounechada[2], Andrew P.E. York[2], and Jillian Collier[2]*
(1)Dipartimento di Energia, Politecnico di Milano, Milan, Italy, (2)Johnson Matthey Technology Centre, Sonning Common, United Kingdom

Decoupling RHC and OHC of the Standard-SCR redox mechanism by transient response methods provides novel insight into the effects of reaction variables and catalyst parameters on NH_3-SCR over Cu-CHA. Such effects are often opposite for the two redox half cycles: they would remain unclear if focusing just on steady-state data.

H2O-Assisted Oxidation Half-Cycle of Low Temperature NH3-SCR over Cu-CHA.

***Gabriele Contaldo**, Isabella Maria Nova, Matteo Maestri, and Enrico Tronconi*
Laboratory of Catalysis and Catalytic Processes - Dipartimento di Energia, Politecnico di Milano, Milano, Italy

H_2O dissociates over dimeric Cu(I) species to form H_2O_2, a strong oxidant that completes the oxidation of a second pair of Cu(I) moieties in adjacent CHA cages. Such results describe the reaction mechanism of OHC of NH_3-SCR and clarify the active role of H_2O in promoting the kinetically relevant step.

NH_3-SCR Redox Kinetics Monitored By Operando UV Spectroscopy.

*Nicola Usberti[1], Gabriele Contaldo[2], Mauro Bracconi[2], **Chiara Negri**[2], Isabella Maria Nova[2], Matteo Maestri[2], and Enrico Tronconi[3]*
(1)Dipartimento di Energia, Politecnico di Milano, Milan, Italy, (2)Laboratory of Catalysis and Catalytic Processes - Dipartimento di Energia, Politecnico di Milano, Milano, Italy, (3)Politecnico di Milano, Milan, Italy

We demonstrated the possibility to extract kinetic relevant data from operando UV-Vis spectroscopy to monitor Cu redox chemistry, during NH3-SCR. By combining a packed bed reactor with a high temperature UV-Vis probe we monitored the evolution of Cu oxidation state, extracting kinetic relevant data aligned with gas phase quantification data.

Insights into NH_3 Inhibition of SCR on Cu-CHA Catalysts.

Dhruba Jyoti Deka[1], *Mingyu Wan*[2], *Garam Lee*[1], *Eric D. Walter*[1], *Fanglin Che*[2], *Kenneth Rappe*[1], *Janos Szanyi*[1], *and Yong Wang*[1,3]
(1)Pacific Northwest National Laboratory, Richland, WA, (2)Chemical Engineering, University of Massachusetts Lowell, Lowell, MA, (3)Washington State University, Pullman, WA

Excess NH_3 in selective catalytic reduction on Cu-CHA hinders NO_x conversion by reducing Cu ion mobility, impacting low-temperature performance. This study provide fundamental insights into NH_3 inhibition mechanism and suggests optimizing Si/Al ratios, Cu loading, and NH_3-to-NO_x ratios to enhance SCR efficiency and guide better urea dosing in diesel engines.

Collective Effects and Aluminum Distribution Control Diffusion and Pairing of $[Cu(NH_3)_2]^+$ Complexes in Cu-CHA.

Joachim Bjerregaard[1], *Martin Votsmeier*[2], *and Henrik Grönbeck*[1]
(1)Department of Physics and Competence Centre for Catalysis, Chalmers University of Technology, Göteborg, Sweden, (2)Umicore, Hanau-Wolfgang, Germany

Copper exchanged chabazite (Cu-CHA) is state-of-the-art catalyst for removal of NO_x from lean burn engines. The pairing of mobile $[Cu(NH_3)_2]^+$ complexes is crucial for sustaining a high activity. Here we utilize machine learning forcefield to investigate the influence of diffusion mechanisms and zeolite compositions on the pairing of $[Cu(NH_3)_2]^+$ complexes.

Role of HTA and Cu Speciation in NH_3-SCR Reactions over Cu-SSZ-13 Catalysts.

Andrea Gjetja[1], *Nicola Usberti*[1], *Isabella Maria Nova*[1], *Enrico Tronconi*[2], *Rohil Daya*[3], *Lai Wei*[3], *Hongmei An*[3], *and Krishna Kamasamudram*[3]
(1)Dipartimento di Energia, Politecnico di Milano, Milan, Italy, (2)Politecnico di Milano, Milan, Italy, (3)Cummins Inc., Columbus, IN

Mild Hydrothermal Aging (HTA) of Cu-SSZ-13 catalysts causes a DeNOx performance loss in NH_3-SCR. A clear effect over the mechanism of the different SCR reactions is still not understood. This work delves into these aspects, understanding the role of the different Cu species.

FUNDAMENTALS - FUNDAMENTALS OF CATALYSIS AND SURFACE SCIENCE

FUNDAMENTALS - CATALYST DESIGN AND SURFACE SCIENCE

Tuesday, June 10, 2025 9:30 AM - 11:30 AM
Centennial Ballroom II

Chair: Benjamin Jackson, Pacific Northwest National Laboratory

Co-Chair: Konstantin Khivantsev, Pacific Northwest National Laboratory

Structure-Activity Relationship of Transition Metal Carbide Catalyst for Hydrodeoxygenation Reaction.

*Raghavendra Meena[1], Johannes Hendrik Bitter[2], and **Guanna Li**[2]*
(1)Wageningen University and Research, Wageningen, Netherlands, (2)Wageningen University, Wageningen, Netherlands

The reaction mechanism and structure-activity relationship of Mo_2C towards hydrodeoxygenation reaction was rationalized by integrating multiple modeling approaches of DFT, molecular dynamics, microkinetic modeling, and machine learning method. The key descriptors correlating to the barrier of the rate-determining step were identified. The in-situ-generated molybdenum oxycarbide is the most active catalyst.

Impacts of Titania Phase on H_2 Adsorption and Spillover on Au/TiO_2 Catalysts.

***Audrey Battiste**[1] and Bert Chandler[2]*
(1)Chemistry, Pennsylvania State Univerisity, State College, PA, (2)Chemical Engineering, Pennsylvania State Univerisity, State College, PA

H_2 adsorption and spillover on Au/TiO_2 catalysts is strongly dependent on TiO_2 phase. Au/rutile exhibits adsorption quantities more than an order of magnitude higher than Au/anatase catalysts. Adsorption thermodynamics also change dramatically with TiO_2 phase and metal identity (e.g. replacing Au with Pt).

Diverse Active Sites on CuO_x Nanoparticles and Their Catalytic Consequences in Oxidation Catalysis.

*William Broomhead[1], Maarten Nachtegaal[2], Peng Zhang[1], Yuechang Wei[3], and **Ya-Huei (Cathy) Chin**[1]*
(1)Department of Chemical Engineering and Applied Chemistry, University of Toronto, Toronto, ON, Canada, (2)Paul Scherrer Institute, Villigen, Switzerland, (3)College of Science, China University of Petroleum, Beijing, China

This study highlights the diverse catalytic roles of Cu in alkanol (oxidative) dehydrogenation and CO oxidation. Cu speciation and its immediate microenvironment (with reactive oxygen species) mediate the stability of the kinetically relevant transition states as well as their ability to bind to the hydroxyl species, thus affecting catalyst stabilities.

Designing the Cu-ZnO Interfacial Structure By Atomic Layer Deposition for Methanol Synthesis from CO_2 Hydrogenation.

***Junjie Chen**[1,2], Nadine Humphrey[1,2], Anshuman Goswami[1,2], Ezgi Erdem[1,2], Rachel Spurlock[1,2], Andrzej Rogala[1,2], Alessandro Gallo[1,2], Frank Abild-Pedersen[1,2], Stacey F. Bent[1,2], and Thomas Jaramillo[1,2]*
(1)Department of Chemical Engineering, Stanford University, Stanford, CA, (2)SUNCAT Center for Interface Science and Catalysis, SLAC National Accelerator Laboratory, Menlo Park, CA

In this work, we utilized model catalysts (Cu/SiO_2, $Cu/ZnO/SiO_2$, $ZnO/Cu/SiO_2$) with uniform Cu nanoparticles synthesized by colloidal chemistry and controllable ZnO overlayer prepared *via* atomic layer deposition to investigate the impact of the original structure of Cu-ZnO interface and ZnO overlayer thickness on CO_2 hydrogenation performance.

Selective Hydrogenation of Aromatic Hydrocarbons over Noble Metal Catalysts.

Yue Qi, Ziyu Tang, and ***Simon Podkolzin***
Department of Chemical Engineering and Materials Science, Stevens Institute of Technology, Hoboken, NJ

Reaction mechanisms for selective hydrogenation of aromatic hydrocarbons to cycloolefins and cycloalkanes over noble metal catalysts were studied at the molecular level. Reactive intermediates were identified by combining experimental IR and Raman spectroscopic measurements with DFT calculations and related to catalytic activity and selectivity differences. Improved catalyst formulations were developed.

Adsorption of Alcohols Allows Defining Hydrophilic and Hydrophobic Interactions in Tectosilicates.

Ruixue Zhao[1]*, Sungmin Kim*[2]*, Mal Soon Lee*[2]*, Fuli Deng*[1]*, Xiaomai Chen*[1]*, Yue Liu*[1]*, and Johannes Lercher*[1,2]
(1)Technical University of Munich, Garching b. München, Germany, (2)Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA

Investigating the interaction of water and alcohols with zeolite pores provides a fundamental insight into molecular interactions and differentiates these from macroscopic properties such as “hydrophilicity” and “hydrophobicity”. This understanding will be critical for using intermolecular forces, surface interactions, and confinement effects, to aid sorption and catalysis.

REACTOR - REACTION ENGINEERING AND REACTOR DESIGN

REACTOR - MODELING AND SCALE-UP OF REACTORS FOR INDUSTRIAL APPLICATIONS

Tuesday, June 10, 2025 9:30 AM - 11:30 AM
Centennial Ballroom III

Chair: Nicholas Thornburg, National Renewable Energy Laboratory

Co-Chair: Weijian Diao, Villanova University

Catalytic Depolymerization of Polyethylene By Induction Heating: A Continuous Flow Reactor System.

Bernard Whajah*, Sharonda Angelle, James Dorman, and Kerry Dooley*
Cain Department of Chemical Engineering, Louisiana State University, Baton Rouge, LA

Our system combining induction heating, metal-exchanged zeolites and in particular those with BEA morphology offers a good chance of long-term catalyst operation for polyolefin depolymerization to gasoline-range products without added H_2. These results underscore the importance of both catalyst selection and operating conditions for the continuous depolymerization of LDPE.

Model-Based Reactor Design and Process Optimization for Scaling up Direct CO_2 Hydrogenation to Dimethyl Ether Production.

Canan Karakaya[1]*, Dylan Weber*[1]*, Aye (pimphan) Meyer*[1]*, and Hai-Ying Chen*[2]
(1)Manufacturing Science Division, Oak Ridge National Laboratory, Oak Ridge, TN, (2)National Transportation Research Center, Oak Ridge National Laboratory, Knoxville, TN

This study uniquely combines a multi-scale reactor model with TEA and LCA analyses to assess the viability of the CO_2-to-DME process. The results underscore the importance of process optimization to enhance reactor design, maximizing yield, catalyst lifespan, and energy efficiency.

Imposing Atom Conservation on Physics-Informed Neural Networks for Catalytic Reactor Model Surrogates.

Felix Döppel*, Mauro Bracconi, and Matteo Maestri*
Laboratory of Catalysis and Catalytic Processes - Dipartimento di Energia, Politecnico di Milano, Milano, Italy

Physics-informed neural networks (PINNs) leverage *a priori* physical knowledge to provide highly performant, yet physically plausible surrogates of catalytic reactors or derive kinetic models from integral reactor data. However, most works on PINNs ignore the fundamental law of atom conservation. Here, we develop atom conserving PINNs to guarantee physical consistency.

Accelerating Catalyst Discovery Utilizing Nanoparticle Mega Libraries & Compositionally Controlled Thin Films: Development of a Spatially Resolved Scanning Probe Reactor.

Muntaseer Bunian[1]*, Neil Schweitzer*[2]*, and Selim Alayoglu*[3]
(1)Paula M. Trienens Institute for Sustainability and Energy, Northwestern University, Evanston, IL, (2)Department of Chemical and Biological Engineering, Northwestern University, Evanston, IL, (3)Department of Chemical & Biological Engineering, Northwestern University, Evanston, IL

In the space of continuous and parallel catalyst discovery, a scanning probe reactor system was developed to spatially detect and analyze local catalytic activity across domains ranging from thin films to nanoparticles with the goal of achieving detection at the single particle level.

Effects of POCS design on the intensification of heat transfer in FT structured reactors: a pilot plant experimental study.

*Martino Panzeri[1], Carlo Giorgio Visconti[2], **Gianpiero Groppi**[2], and Enrico Tronconi[1]*
(1)Politecnico di Milano, Milan, Italy, (2)Dipartimento di Energia, Politecnico di Milano, Milan, Italy

We have studied experimentally the effect of the geometry of conductive POCS with skin for heat management of the FT synthesis. Our data identify the relative density RD as the most important parameter. This work shows that structured internals are a promising solution for the intensification of FT reactors.

Scaleup of Additively Manufactured Microchannel Reactor for Single-Step Conversion of Ethanol into n-Butene-Rich Olefins for Alcohol-to-Jet Application.

***Austin Winkelman**[1], Johnny Saavedra-Lopez[1], Matthew Coblyn[2], Patrick Mcneff[4], Michael Hubbard[1], Kwangtae Son[2], Goran Jovanovic[2], Brian Vincente[3], Ralph Gillespie[3], Brian Paul[4], and Robert A. Dagle[1]*
(1)Pacific Northwest National Laboratory, Richland, WA, (2)School of Chemical, Biological and Environmental Engineering, Oregon State University, Corvallis, OR, (3)LanzaTech, Skokie, IL, (4)School of Mechanical, Industrial & Manufacturing Engineering, Oregon State University, Corvallis, OR

Sustainable aviation fuel production pathways from renewable ethanol that can be deployed at scale are of substantial interest. This work leverages microchannel technology to enable a 400x scaleup of our catalytic ethanol to n-butene system, demonstrating potential to reduce capital and operating expenditures compared to the current state-of-the-art alcohol-to-jet process.

SYNTHESIS - CATALYST SYNTHESIS AND MANUFACTURING

SYNTHESIS - INNOVATIVE CATALYST MATERIALS AND SYNTHESIS ROUTES

Tuesday, June 10, 2025 9:30 AM - 11:30 AM
Centennial Ballroom IV

Chair: Gianni Caravaggio, Natural Resources Canada (NRCan)

Co-Chair: Jason Wu, Honeywell UOP

KEYNOTE: Development of Soluble and Reusable Polymer-Based Catalysts with Brønsted and Lewis Acidity.

*Ibeh S. Omodolor[1], Subhash Kalidindi[1], Nkem O. Ofole[1], Sarah A. Walz[1], Maria R. Coleman[1], Sridhar Viamajala[1], Ravikumar Gogar[1], Manuel López Granados[2], Francielle Candian Firmino Marcos[3], and **Ana C. Alba-Rubio**[1,3]*
(1)Department of Chemical Engineering, The University of Toledo, Toledo, OH, (2)Institute of Catalysis and Petrochemistry (ICP-CSIC), Cantoblanco, Madrid, Spain, (3)Department of Chemical and Biomolecular Engineering, Clemson University, Clemson, SC

We developed a series of soluble and reusable polymer-based catalysts with Brønsted and Lewis acidity. These catalysts were studied in the one-pot synthesis of hydroxymethylfurfural from

glucose and potato starch. The best catalyst presented similar catalytic activity as a combination of H_2SO_4 and $AlCl_3$ with the advantage of being reusable.

SiC with High Specific Surface Area for Use in Catalysis.

*Adrian Ortega[1], Mario Caccia[2], and **Javier Narciso**[1]*
(1)University of Alicante, Alicante, Spain, (2)Alfred University, Alfred, Spain

In this work, a new synthetic route for SiC is presented. Hierarchical SiC with a surface area of 200 m^2/g has been obtained. This SiC has been used as a support for Pt, and the Pt-SiC interaction has been studied and how it affects the reaction for obtaining crotyl alcohol.

Rapid Crystallization of Zeolites with Controllable Defects: Disentangling Fluoride Concentration and pH Using Ammonium Fluoride.

***Muhammad Shah**[1], Taras Nagornyy[1], Success Aiwekhoe[1], Seungbo Hong[1,2], Nhan Huu Huy Tran[1], Song Luo[1], Zhu Chen[1], Scott M. Auerbach[1,2], and Wei Fan[1]*
(1)Department of Chemical Engineering, University of Massachusetts Amherst, Amherst, MA, (2)Department of Chemistry, University of Massachusetts Amherst, Amherst, MA

Zeolite synthesis in neutral fluoride-media produces fewer defects, however, this often requires significantly longer crystallization times and involves handling dangerous HF. In the present study, by disentangling fluoride concentration and pH using NH_4F as a safer alternative, we found that the crystallization rate can be significantly improved with fewer defects.

SSZ-43 Zeolites: A Comparative Study of Synthesis Routes and Catalytic Applications.

***Taekyung Ryu**[1], Jesús Pascual[1], Marat Orazov[1], Joel Schmidt[1], C.Y. Chen[2], and Stacey I. Zones[1]*
(1)Chevron, Richmond, CA, (2)Chevron Energy Technical Center, Richmond, CA

Here, we provide an overview of the synthesis and post-synthetic treatment of borosilicate SSZ-43 (B-SSZ-43) zeolites crystallized via different synthesis routes: direct, seed-assisted, and interzeolite conversion. The physicochemical and catalytic characterization of these SSZ-43 materials will be discussed.

Raspberry-Colloid-Templating As a Model Thermocatalytic Platform.

***Kang Rui Garrick Lim**[1] and Joanna Aizenberg[2]*
(1)Chemistry and chemical biology, Harvard University, Cambridge, MA, (2)John A. Paulson School of Engineering and Applied Sciences, Harvard University, Cambridge, MA

The performance of heterogeneous catalysts depend on descriptors related to the nanoparticles, support, and their interactions. However, current methods do not permit independent changes to these parameters. To unequivocally derive structure-property relationships, we developed a raspberry-colloid-templating strategy that enables independent combinatorial variations of the material's building blocks and their organization.

AI - AI-DRIVEN CATALYSIS

AI - USING AI TO NAVIGATE LARGE CATALYST DESIGN SPACES

Tuesday, June 10, 2025 1:00 PM - 3:20 PM
Regency Ballroom VII

Chair: Tibor Szilvasi, The University of Alabama

Co-Chair: Tej Choksi, Nanyang Technological University

Digital Catalysis: Accelerated Discovery through Human in the Loop.

Charles Pare[1]*, Aybike Terzi*[2]*, Christian Kunkel*[1]*, Frederik Rüther*[2]*, Frederic Felsen*[1]*, Raoul Naumann D'Alnoncourt*[2]*, Christoph Scheurer*[1]*, Karsten Reuter*[1]*, and Frank Rosowski*[2]
(1)Fritz Haber Institute of the Max Planck Society, Berlin, Germany, (2)BasCat - UniCat BASF Joint Lab, Technische Universität Berlin, Berlin, Germany

Promoters are indispensable for the optimized performance and lifetime of industrial catalysts, with modern catalysts mostly benefiting from only a small number of promoters. Here we present an accelerated discovery approach that globally explores a high-dimensional multi-promoter design space with only a few experiments and identify promising new catalyst chemistries.

Expanding the Synthesis Window of Zeolites Containing *Lta* Cavities through Rational Design of Structure-Directing Agents and Ionic Environment.

Soonhyoung Kwon[1] *and Yuriy Roman*[2]
(1)Charles D. Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN, (2)Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, MA

We employed high-throughput simulations to design optimal organic structure-directing agents and ionic environments for synthesizing high-silica small-pore zeolites with *lta* cavities. This approach achieved unprecedented Si/Al ratios, superior hydrothermal stability, and phase selectivity in **LTA**, **UFI**, **RHO**, and **KFI** frameworks, expanding the synthesis window for tailored zeolitic materials.

Understanding Metal-Support Interactions By Interpretable Machine Learning.

Chenggong Jiang[1]*, Bryan Goldsmith*[2]*, and Suljo Linic*[1]
(1)Department of Chemical Engineering, University of Michigan, Ann Arbor, MI, (2)Chemical Engineering, University of Michigan, Ann Arbor, MI

Using physics-informed machine learning and molecular dynamics simulations, we identified key oxide support features governing metal-support interactions in Pt nanocatalysts. Surface energy, oxygen bond order, dipole, and work function predict Pt-oxide interaction strength. This enables screening of 10,000+ oxide surfaces for sinter-resistant supports, accelerating stable nanocatalyst discovery.

Micro-Kinetic Modeling of Temporal Analysis of Products Data Via Kinetics-Informed Neural Networks.

Dingqi Nai[1]*, Gabriel Gusmão*[2]*, Zachary Kilwein*[1]*, Fani Boukouvala*[3]*, and Andrew Medford*[2]
(1)Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA, (2)School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA, (3)School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA

We utilize kinetics-informed neural networks to efficiently model TAP data. KINNs can fit transient data, retrieve kinetic parameters, and interpolate unseen pulse behavior even when thin-zone information is unavailable. KINNs outperform traditional methods in noise tolerance and computational efficiency, offering a promising alternates for interpreting transient kinetics in catalysis research.

Advantages in the Use of AI-Based Regressions for the Kinetic Modelling of Industrial Catalysts.

Hugo Pétremand[1]*, Andrea Pappagallo*[1]*, and Emanuele Moioli*[2]
(1)Paul Scherrer Institute, Villigen, None, Switzerland, (2)Politecnico di Milano, Milano, None, Italy

This papers shows the potential of using AI-based regressions (artificial neural networks, random forests) for kinetic models of industrial catalysts, comparing them with standard LHHW-based approaches

Representation Learning for Predicting Shape Selectivity in Nanoporous Zeolites.

Yachan Liu[1]*, Ping Yang*[1]*, Aaron Sun*[2]*, Zezhou Cheng*[2]*, Gustavo Perez*[2]*, Wei Fan*[1]*, Subhransu Maji*[2]*, and* ***Peng Bai***[1]
(1)Department of Chemical Engineering, University of Massachusetts Amherst, Amherst, MA, (2)College of Information and Computer Sciences, University of Massachusetts Amherst, Amherst, MA

ZeoNet, a representation learning framework based on 3D convolutional neural networks and a new volumetric representation, was developed for capturing shape selectivity in zeolites. ZeoNet was found to significantly outperform other popular materials representations including graph networks, vision transformers, and point clouds in predicting Henry's constants of long-chain hydrocarbon isomers.

Investigating the Sulfur Poisoning Characteristics of High-Entropy Alloys Using a Multi-Property Graph Neural Network.

Gaurav Deshmukh[1]*, Madison Bird*[2]*, and Jeffrey Greeley*[3]
(1)Chemical and Biological Engineering, Northwestern University, Evanston, IL, (2)Charles D.

Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN, (3)Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN

Sulfidation stability of high-entropy alloy catalysts was explored using a multi-property graph neural network (SlabGCN) trained on a Pt-Pd-Rh-Cu quaternary alloy dataset. Sulfur coverage as a function of reaction conditions was visualized using surface phase diagrams. An optimal quaternary alloy composition was discovered using a Monte Carlo-inspired optimization scheme.

BIOMASS - BIOMASS AND WASTE VALORIZATION CATALYSIS

BIOMASS - FURANS

Tuesday, June 10, 2025 1:00 PM - 3:20 PM
Regency Ballroom VI

Chair: Silvia Morales de la Rosa, Instituto de Catálisis y Petroleoquímica, Spanish National Research Council (CSIC)

Co-Chair: Thomas Schwartz, University of Maine

Reductive Amination of Acetal-Protected 2,5-Diformylfuran to 2,5-Bis(aminomethyl)Furan Using Co_2P Nanorod (NR) Catalyst.

Nirupama Sheet[1], Ryota Osuga[1], Satoshi Suganuma[1], Takato Mitsudome[2], and ***Kiyotaka Nakajima***[1]
(1)Institute for Catalysis, Hokkaido University, Sapporo, Japan, (2)Graduate School of Engineering Science, Department of Materials Engineering Science, Osaka University, Toyonaka, Osaka, Japan

A stepwise reaction system was designed to synthesize 2,5-bis(aminomethyl)furan (BAMF) by the reductive amination of acetal-protected 2,5-diformylfuran (DFF) with 1,3-propanediol (PD) using a state-of-the-art Co_2P nanorod (NR) catalyst. The current system realized the production of BAMF in high yields (> 90%) even using concentrated solutions (10-20 wt%).

Catalytic Upgrading of Furfural Using Hierarchical ZSM-5 Zeolite.

Sancler C. Vasconcelos[1], Thiago Lima[1], and ***Fabio B. Passos***[2]
(1)Institute of Chemistry, Universidade Federal Fluminense, Niteroi, Brazil, (2)Department of Chemical and Petroleum Engineering, Universidade Federal Fluminense, Niteroi, Brazil

This work presents the use of hierarchical ZSM-5 zeolites for lignocellulosic biomass upgrading in liquid phase catalysis, in particular the conversion of furfural . Furfural conversion increased along with materials acidity, and the alkaline treatment lead to higher conversion.

Synthesis of a Jet Fuel Precursor By Hydroxyalkylation-Alkylation of 2-Methylfuran with Furfural Using Hierarchical H-Y Zeolites.

Odiri Siakpebru[1,2], *Lakshmiprasad Gurrala[1,2], Anoop Uchagawkar[1,3], Oliver Norris[1,2], Jared Bartlett[1,2], and Ana Colaco Morais[1,2]*

(1)Chemical and petroleum Engineering, University of Kansas, Lawrence, KS, (2)Wonderful Institute for Sustainable Engineering, Department of Chemical and Petroleum Engineering, The University of Kansas, Lawrence, KS, (3)Center for Environmentally Beneficial Catalysis, University of Kansas, Lawrence, KS

We described the production of jet fuel precursor through the hydroxyalkylation-alkylation of 2-methylfuran with furfural using hierarchical H-Y zeolites synthesized from Na-Y (Si/Al = 2.6) via surfactant templating technique. Hierarchical H-Y-mod-1 zeolite demonstrated high reactant conversion and jet fuel precursor yield due to its strong Brønsted acidity and improved mesoporosity.

Modification of Gold Catalysts for the Selective Oxidation of 5-Hydroxymethyl Furfural to 2,5-Furandicarboxylic Acid.

Hidde Nolten[1] *and Petra E. de Jongh*[2]
(1)Utrecht University, Utrecht, Netherlands, (2)Inorganic Chemistry and Catalysis, Utrecht University, Utrecht, Netherlands

Oxidation of 5-hydroxymethylfurfural facilitates plastics production from biomass. We improve this important reaction by tuning the particle size and composition of a Au/TiO_2 catalyst, visualized with atomic-resolution electron microscopy. Our results show that adding Ag or increasing the particle size to 4 nm massively increases the desired product yield.

Hydrodeoxygenation of Tetrahydrofuran 2,5-Dicarboxylic Acid to Adipic Acid Driven By Pt-MoO_x Interfacial Sites.

Samir Castilla Acevedo Sr.[1]*, Ben Auer*[1]*, John Styers*[1]*, Sebastian Amaya-Roncancio*[1]*, and Alan Allgeier*[2]
(1)Chemical and Petroleum Engineering, University of Kansas, Lawrence, KS, (2)Center for Environmentally Beneficial Catalysis (CEBC), University of Kansas, Lawrence, KS

The proximity of Pt and Mo is a critical factor for AA selectivity since it ensures the optimal degree of reduction of the oxyphilic metal and activate pathways where catalytic bifunctionalities are essential.

Sustainable Cu-Fe/Al_2O_3 Bimetallic Catalyst Synthesis Using Extract of Aged *Rosa Chinensis Jacq* Petals and Its Use in Furfural Hydrogenation..

Barbara Lino Galarza[1,2]*, Javier Rivera De la Rosa*[1]*, Carlos Enrique Escarcega González*[1]*, Carlos Javier Lucio Ortíz*[1]*, Ladislao Sandoval*[3]*, Diana Bustos Martínez*[1]*, and Antonia Infantes-Molina*[2]
(1)Facultad de Ciencias Químicas, Universidad Autónoma de Nuevo León, Monterrey, NL, Mexico, (2)Química Inorgánica, Cristalografía y Mineralogía, Universidad de Malaga, Malaga, Malaga, Spain, (3)Escuela De Ingeniería y Ciencias, Instituto Tecnológico y de Estudios Superiores de Monterrey, Monterrey, NL, Mexico

Aged *Rosa Chinensis Jacq* petals, extracted with green solvents, were used to synthesize Cu-Fe/Al_2O_3 catalysts at low temperature. These catalysts, particularly contained the Cu_4Fe phase, showed high efficiency in the hydrogenation of furfural, a key step in biorefinery processes.

Selective Hydrogenation of Biomass-Derived Furans over Cu Catalysts: Experiments and Theory.

***Evangelos Smith**, Michael Rebarchik, Hochan Chang, James A. Dumesic, and Manos Mavrikakis*
Department of Chemical and Biological Engineering, University of Wisconsin-Madison, Madison, WI

Herein, we combine reaction kinetics experiments with density functional theory (DFT) calculations to investigate the selective hydrogenation of HAH, a biomass-derived platform molecule, over copper catalysts. These findings may assist in the rational design of transition metal catalysts for the hydrogenation of compounds containing both aliphatic and aromatic double bonds

CO2 - CO2 CAPTURE AND UPGRADING

CO2 - CO_2 CONVERSION TO METHANE

Tuesday, June 10, 2025 1:00 PM - 3:20 PM
Centennial Ballroom IV

Chair: Haruka Nishiyama, SEKISUI CHEMICAL CO.,LTD

Co-Chair: Matteo Monai, Utrecht University

Elucidating the Crucial Role of Ta Dopant in Enhanced Selectivity of CO_2 Methanation Reaction over Ru/CeO_2 Catalyst at Lower Temperature.

*Jose Rodriguez and **Deboshree Mukherjee***
Chemistry, Brookhaven National Laboratory, Upton, NY

Ru/CeO_2 catalyst prepared with varying wt.% of Ta (0, 2.5, 11, and 18 wt.%) dopant, and applied for CO_2 Methanation reaction. At lower temperature, a consistent increase in methane selectivity was observerved with increasing Ta wt.%. In-situ DRIFTS and EXAFS were perfomed to explain the findings.

Deciphering Effects of Nanoparticles Shape and Size on the Structure Sensitivity of CO_2 Methanation Reaction on Ni.

***Gabriele Spanò**[1], Matteo Ferri[1], Raffaele Cheula[1], Matteo Monai[2], Bert M. Weckhuysen[2], and **Matteo Maestri**[1]*
(1)Laboratory of Catalysis and Catalytic Processes - Dipartimento di Energia, Politecnico di Milano, Milano, Italy, (2)Inorganic Chemistry and Catalysis, Institute for Sustainable and Circular Chemistry, Utrecht University, Utrecht, Netherlands

Nickel nanoparticle shape critically influences turnover frequency (TOF) in CO2 methanation, but conflicting trends in TOF are reported. In this study we reveal that shape, not just size, governs the overall catalytic activity. Therefore, we offer a framework that reconciles highly debated discrepancies in the experimental literature

Mechanistic Insights and Selectivity Control in CO_2 Hydrogenation on Dispersed Ru, Co, and Ni Nanoparticles.

Wenshuo Hu[1]*, Gregory Tate*[2]*, and Enrique Iglesia*[3]
(1)Chemical Engineering, Texas Tech University, Lubbock, TX, (2)Chemical Engineering, University of California, Berkeley, Berkeley, CA, (3)University of California at Berkeley, Berkeley, CA

This study elucidates mechanistic elementary steps mediating CO_2-H_2 reactions on dispersed Ru, Co, and Ni nanoparticles, which are similar in identity and kinetic relevance. These mechanism and kinetic formalisms demonstrate that the presence of CO at specific inlet pressures enables the exclusive formation of CH_4 from CO_2-H_2 reactants.

Promoting Ni-Catalyzed CO_2 Methanation Via Gd Doping.

Majed Alam Abir[1] *and* ***Madelyn Ball***[2]
(1)Chemical and Biomedical Engineering, West Virginia University, Morgantown, WV, (2)Chemical Engineering and Materials Science, Michigan State University, East Lansing, MI

We have demonstrated enhanced performance for CO_2 methanation by doping Ni/SiO_2 catalysts with Gd at varied ratios. The addition of Gd impacts performance by changing the nature of the surface species under reaction conditions, enabling development of structure-performance relationships.

Advanced Biogas Methanation Catalysts for Generating Renewable Natural Gas.

Mathew Rasmussen[1]*, Sawyer Halingstad*[2]*, Dipesh Adhikari*[3]*, Weijie Zhang*[4]*, Robert Davis*[5]*, Sen Zhang*[6]*, and Matthew M. Yung*[7]
(1)Bioenergy Science and Technology Department, National Renewable Energy Laboratory, Golden, CO, (2)National Renewable Energy Laboratory, Golden, CO, (3)university of virginia, charlottesville, VA, (4)Chemical Engineering, chemistry, university of Virginia, Charlottesville, VA, (5)Chemical Engineering, University of Virginia, Charlottesville, VA, (6)Chemistry, University of Virginia, Charlottesville, VA, (7)National Bioenergy Center, National Renewable Energy Laboratory, Golden, CO

In this work, we have compared the performance of Ni-based catalysts for converting biogas, a 50:50 mixture of CO_2 and CH_4, into renewable natural gas (RNG). We have demonstrated the feasibility of this technology by converting raw biogas from a wastewater treatment facility into pipeline-compliant RNG continuously for 100 hours.

Catalytic Methanation of CO_2 over Ni Nanoparticles for Production of Renewable Natural Gas from Biogas.

Dipesh Adhikari[1]*, Robert Davis*[2]*, Colby Whitcomb*[2]*, Weijie Zhang*[3]*, Matthew M. Yung*[4]*, Mathew Rasmussen*[5]*, Sen Zhang*[6]*, Sawyer Halingstad*[7]*, Bryan Schmerber*[8]*, and Lisa M. Colosi*[9]
(1)university of virginia, charlottesville, VA, (2)Chemical Engineering, University of Virginia, Charlottesville, VA, (3)Chemical Engineering, chemistry, university of Virginia, Charlottesville, VA, (4)National Bioenergy Center, National Renewable Energy Laboratory, Golden, CO, (5)Bioenergy Science and Technology Department, National Renewable Energy Laboratory, Golden, CO, (6)Chemistry, University of Virginia, Charlottesville, VA, (7)National Renewable Energy Laboratory, Golden, CO, (8)South Platte Renew, Englewood, CO, (9)Civil and Environmental Engineering, University of Virginia, Charlottesville, VA

This work investigates the roles of Ni particle size and support composition in the catalytic CO_2 methanation reaction for biogas upgrading to renewable natural gas. Life cycle analysis and techno-economic assessment of catalytic methanation utilizing renewable H_2 compared to conventional pressure swing adsorption reveal improvements in environmental and economic outcomes.

Reaction Pathways and Site Requirements for H-Assisted CO_2 Activation at Ni-Ce Interfaces.

Suchetana Samanta*, Jeffrey D. Rimer, and Praveen Bollini*
William A. Brookshire Department of Chemical and Biomolecular Engineering, University of Houston, Houston, TX

This work elucidates the reaction pathways and intermediates mediating methanation turnovers at the Ni-Ce interface. Kinetic, in-situ spectroscopic, and isotopic measurements provide evidence for hydrogen-assisted CO_2 activation routes at these interfaces, with hydrogen-assisted C-O bond scission of bidentate carbonates being the rate-determining step and bidentate formates acting as spectators.

ENVIRO AUTO - ENVIRONMENTAL AND AUTOMOTIVE CATALYSIS

ENVIRO AUTO - SUPPORTED METAL-OXIDES FOR EMISSION CONTROL CATALYSIS

Tuesday, June 10, 2025 1:00 PM - 3:20 PM
Hanover Hall FG

Chair: Krishna Gunugunuri, Cummins Inc.

Co-Chair: Sreshtha Sinha Majumdar, Oak Ridge National Laboratory

Developing the Science of Self-Healing Catalysts.

Abhaya Datye[1]*, Hien N. Pham*[1]*, Andrew T. DeLaRiva*[1]*, Chase Thompson*[1]*, Stephen Porter*[1]*, Hao Xu*[2]*, Konstantin Khivantsev*[3]*, Yipeng Sun*[4]*, Holmes Ahari*[5]*, and Yong Wang*[6]
(1)Department of Chemical and Biological Engineering and Center for Micro-Engineered

Materials, University of New Mexico, Albuquerque, NM, (2)Chemical and Bio Engineering, Washington State University, Pullman, WA, (3)Physical and Computational Sciences Directorate and Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA, (4)BASF, Iselin, NJ, (5)Fiat Chrysler Automobile US, Auburn Hills, MI, (6)The Gene and Linda Voiland School of Chemical Engineering and Bioengineering, Washington State University, Pullman, WA

Emission control catalysts are subjected to accelerated aging at temperatures ~1000 C where the catalytically active metals (Pt, Pd and Rh) are emitted to the vapor phase. Here we describe how catalyst supports allow these catalysts to function over their full useful life, a process we describe as self-healing.

Tuning Support Lattice Oxygen Activity for Emission Control Catalysts.

Hao Xu[1]*, Weixin Huang*[2]*, Hien N. Pham*[3]*, Andrew T. DeLaRiva*[3]*, Abhaya Datye*[3]*, and Yong Wang*[4]
(1)Chemical and Bio Engineering, Washington State University, Pullman, WA, (2)Department of Chemical Engineering, Washington State University, Pullman, WA, (3)Department of Chemical and Biological Engineering and Center for Micro-Engineered Materials, University of New Mexico, Albuquerque, NM, (4)Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA

Here, we develop strategies for synthesizing catalyst supports and demonstrate that the modulation of support lattice oxygen greatly benefits catalyst efficiency for emission control purposes.

The Reducibility of Ce, Pr and Tb Containing Mixed Oxides Have Been Studied and Trends with Composition Determined and the Effect on Twc Transient Catalytic Activity Shown..

David Thompsett*, Amy Kolpin, and Janet Fisher*
Johnson Matthey Technology Centre, Sonning Common, United Kingdom

Ce and Pr fast and total reducibility have been determined as a function of CeZr and PrZr mixed oxide composition. Ce oxides show limited reduction which improve with Zr content while Pr oxides show opposite trends. These differences in redox behaviour show benefit during TWC transients.

Influence of Nanoparticle Structure in Bimetallic PtPd/Al_2O_3 Catalysts on Activity and Stability during Emission Control Applications.

Joachim Czechowsky[1]*, Paolo Dolcet*[1]*, Carina B. Maliakkal*[2]*, Silke Behrens*[3]*, Michael Türk*[4]*, Moritz Wolf*[3]*, Jan-Dierk Grunwaldt*[1,3]*, and Maria Casapu*[1]
(1)Institute for Chemical Technology and Polymer Chemistry (ITCP), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany, (2)Institute of Nanotechnology (INT), Karlsruhe Institute of Technology (KIT), Eggenstein-Leopoldshafen, Germany, (3)Institute of Catalysis

Research and Technology (IKFT), Karlsruhe Institute of Technology (KIT), Eggenstein-Leopoldshafen, Germany, (4)Institute for Technical Thermodynamics and Refrigeration (ITTK), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

By using various synthesis methods, different initial states of $PtPd/Al_2O_3$ catalysts were obtained, which allowed to derive robust structure-activity correlations during lean CO-/NO-oxidation. Hydrothermal aging and extensive characterization were used to identify the factors responsible for structural changes and deactivation such as size effects, alloying and particle segregation during use.

Enhanced NH_3-SCO Performance through Synergistic Effects of PtCu Intermetallics and $PtCuO_x$ Clusters.

***Jiaxing Li**, Yue Peng, and Junhua Li*
State Key Joint Laboratory of Environment Simulation and Pollution Control, Tsinghua University, Beijing, China

This work highlights the electron-rich effect of PtCu intermetallic compounds in lowering NH_3 activation temperature and the tandem role of CuOx clusters in enhancing N_2 selectivity, achieving efficient NH_3-SCO catalysis.

Decomposition and Hydrolysis of Sulfonamides on CeO_2(111).

*Timm McNeese, Nusrat Jahan Rifat, and **Ye Xu***
Cain Department of Chemical Engineering, Louisiana State University, Baton Rouge, LA

Sulfonamides are widely used to treat bacterial and fungal infections in humans and livestock. They accumulate in the environment resulting in antibiotic resistance in bacteria. DFT calculations are performed to investigate the ability of ceria to catalyze the hydrolysis of sulfonamides and shed light on factors that affect its efficacy.

Controlling Rh-CeO_2 Interaction Enhances N_2o Decomposition.

***Yi Liu**[1,2], Hao Xu[2], Wenda Hu[3], Chia-Yu Chang[4], Bing Joe Hwang[4], and Yong Wang[5]*
(1)CHEMICAL ENGINNERING, Washington State University, pullman, WA, (2)Chemical and Bio Engineering, Washington State University, Pullman, WA, (3)The Gene and Linda Voiland School of Chemical Engineering and Bioengineering, Washington State University, Pullman, WA, (4)Chemical Engineering, National Taiwan University of Science and Technology, Taipei, Taiwan, (5)Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA

By tuning the Rh coordination environment through calcination temperature, a signficant self-promotion effect is observed for 0.5 wt.%Rh/CeO_2-1000 sample after reaction with N_2O, attributed to abundant active oxygen species and higher Rh-O coordination number. It provides crucial insights into optimizing Rh/CeO_2 interaction for more effective N_2O abatement technology.

FUNDAMENTALS - FUNDAMENTALS OF CATALYSIS AND SURFACE SCIENCE

FUNDAMENTALS - CHARACTERIZATION TECHNIQUE FOCUSED

Tuesday, June 10, 2025 1:00 PM - 3:20 PM
Centennial Ballroom II

Chair: Steven Chavez, University of California, Los Angeles

Co-Chair: Andrew Palermo, Johnson Matthey

Revealing Kinetics of Pt Exsolution Phenomenon and High Reactivity: Combining Operando X-Ray Absorption Spectroscopy and Graph Neural Network.

Yunkyung Kim[1]*, Wonjun Lee*[1]*, and Jeong Woo Han*[2]
(1)Department of Materials Science and Engineering, Seoul National University, Seoul, Korea, Republic of (South), (2)Department of Materials Science and Engineering, Research Institute of Advanced Materials, Seoul National University, Seoul, Korea, Republic of (South)

Operando XAS was employed to study the exsolution dynamics of Pt, providing real-time insights into Pt coordination and identifying optimal conditions to minimize sintering while enhancing stability. The resulting Pt-exsolved catalysts demonstrated superior reactivity and durability, with GNN-DFT modeling and DRIFTS highlighting the role of strain effects near interfaces.

Quantifying Ambient Pressure Charge Transfer: NH_3 on Ru.

Jesse Canavan[1]*, Rajat Daga*[1]*, Justin Hopkins*[1]*, Ulrick Gaillard*[1]*, Matthew Neurock*[1]*, Alon McCormick*[1]*, Omar Abdelrahman*[2]*, and Paul J. Dauenhauer*[1]
(1)Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN, (2)William A. Brookshire Department of Chemical and Biomolecular Engineering, University of Houston, Houston, TX

The extent of charge transfer due to NH_3 adsorption on a Ru thin film has been measured and quantified at temperatures and pressures typical of heterogeneous catalysis. This technique can be used to study trends in the affinity of adsorbates to different metal surfaces at reaction conditions.

Dynamic Transformations of Heterogeneous Catalysts Under Operando Conditions.

Umberto Raucci[1]*, Axel tosello Gardini*[2]*, Manyi Yang*[3]*, Francesco Mambretti*[2]*, and Michele Parrinello*[2]
(1)Italian Institute of Technology, Genova, Italy, (2)Atomistic Simulations, Italian Institute of Technology, Genova, Italy, (3)Nanjing University, Nanjing, China

Traditionally considered static entities, catalysts were mainly thought to maintain fixed active sites during reactions. However, our work challenges this view, demonstrating that catalysts

undergo profound structural transformations when exposed to industrial reaction conditions, such as high temperatures, pressures, and reactant flows.

Effects of Microwave Heating on Atomically Dispersed Fe-N-C Catalysts.

Takatoshi Murakami[1], Yusaku Yamazaki[1], Shin R. Mukai[2], and ***Isao Ogino***[2]
(1)Graduate School of Chemical Sciences and Engineering, Hokkaido University, Sapporo, Japan, (2)Faculty of Engineering, Hokkaido University, Sapporo, Japan

Despite significant advances in the activity of Fe-N-C catalysts for the electrochemical oxygen reduction reaction (ORR), rapid deactivation persists as a challenge. Brief microwave heating enhances their $4e^-$ ORR selectivity and reduces H_2O_2formation, a key deactivation factor. We report how microwave heating modifies catalyst properties, enabling improved selectivity.

In-Situ Characterization of Pt-Cu Single-Atom Alloy Catalysts: Pt Mobility Under Reaction Conditions.

Francisco Zaera
Chemistry, University of California-Riverside, Riverside, CA

Bimetallic $CuPt_x$/SBA-15 catalysts were tested for the selective hydrogenation of unsaturated aldehydes. Catalysts with x = 0.001 to 0.05 proved quite selective toward the desired unsaturated alcohol. However, *in situ* spectroscopy experiments found the Pt atoms embedded at the metal/silica interface. The role of Pt is remote and indirect.

Measuring Dispersion of Zr-SiO_2 with *in Situ* Titration.

Emily Chase[1] *and Justin Notestein*[2]
(1)Northwestern University, Evanston, IL, (2)Department of Chemical & Biological Engineering, Northwestern University, Evanston, IL

In situ titration with methylphosphonic acid was used to quantify and describe kinetically relevant Zr species on Zr-SiO_2 materials for the MPV reduction of cyclohexanone. Two distinct active species were identified: titratable, isolated Zr with higher intrinsic activity and non-titratable Zr with lower intrinsic activity.

In Situ Measurement of Nanoparticle-Support Interactions in Supported Bimetallic Catalysts.

Andrew Baker[1], Sai Vishnubohtla[1], Sanjana Karpe[2], Yahui Yang[2], Tevis Jacobs[1], and ***Götz Veser***[2,3]
(1)Materials Science, University of Pittsburgh, Pittsburgh, PA, (2)Department of Chemical and Petroleum Engineering, University of Pittsburgh, Pittsburgh, PA, (3)Mascaro Center for Sustainable Innovation, University of Pittsburgh, Pittsburgh, PA

Adhesion of nanoparticles critically impacts their performance and stability. However, scientific advances are currently hampered by a lack of experimental accessibility. We present a novel in situ technique for the direct measurement of adhesion of individual nanoparticles, which enables first insight into the impact of alloying for bimetallic systems.

MICRO MESO - MICROPOROUS AND MESOPOROUS MATERIALS

MICRO MESO - HYDROCARBON REACTIONS ON ZEOLITIC MATERIALS

Tuesday, June 10, 2025 1:00 PM - 3:20 PM
Hanover Hall CDE

Chair: Michele Sarazen, Princeton University

Co-Chair: Stephen Schuyten, Johnson Matthey Inc.

Toluene Alkylation with Ethylene on Acidic Mordenite Zeolite: The Role of Proton Location in Catalysis.

***Kemakorn Ithisuphalap**, Michelle Nolen, and Stephanie Kwon*
Colorado School of Mines, Golden, CO

This study demonstrates that protons in the small 8-membered ring (8-MR) pores of Mordenite (MOR) zeolites can facilitate alkylation reactions of toluene (C_7H_8) with ethylene (C_2H_4), despite steric restrictions. This challenges conventional assumptions about zeolite catalysis and introducing a new perspective on "pore mouth" catalysis.

Quantifying Deactivation Phenomena during Low-Temperature Toluene Methylation on Brønsted Acid Zeolite Catalysts.

***Sopuruchukwu Ezenwa**[1], Andrew Norfleet[2], David Hibbitts[2,3], and Rajamani Gounder[2]*
(1)Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN, (2)Charles D. Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN, (3)Department of Chemical Engineering, University of Florida, Gainesville, FL

We investigate the deactivation mechanism and influences of zeolite properties and reaction conditions on deactivation rate during low-temperature toluene methylation. We show that deactivation rates predominantly reflect the rate of accumulation of bulky polymethylated aromatics within intracrystalline domains, which depend on their rates of formation and diffusion within zeolite crystallites.

Atypical Reactivity of Mesoporous Silicalite-1 in Alkene Oligomerization.

***Nibras Hijazi**[1], Alla Dikhtiarenko[2], Rushana Khairova[1], Jose Cerrillo[1], and Jorge Gascon[1]*
(1)KAUST Catalysis Center, King Abdullah University of Science and Technology, Thuwal, Saudi Arabia, (2)KAUST Core Labs, King Abdullah University of Science and Technology, Thuwal, Saudi Arabia

This work demonstrates that accessible H-bonded silanol groups are highly reactive towards propene oligomerization, which leads to a reconsideration of the origins of reactivity in zeolites in the context of alkene oligomerization.

KEYNOTE: Conversion of Short-Chain Alcohols over Hierarchical Zeolites and the Dependence of Their Porosity and Composition on the Formed Coke Species.

Leandro Martins
State University of Sao Paulo, Araraquara, Brazil

The study shows how structural and chemical modifications of zeolite catalysts and the associated operational conditions impact coke speciation and, consequently, the distribution of compounds from converting short-chain alcohols, methanol, ethanol, and glycerol.

Impact of Al Distribution on Methane Activation over FER-Type Aluminosilicate Zeolite.

Peipei Xiao, Kengo Nakamura, Hiroto Toyoda, Yong Wang, and ***Toshiyuki Yokoi***
Institute of Integrated Research, Institute of Science Tokyo, Yokohama, Kanagawa, Japan

FER zeolites with different Al distributions were prepared using 1,4-dioxane as the pore-filling agent or pyrrolidine as the OSDA. We have found the significance of the distribution and arrangement of Al atoms in FER zeolite for methane oxidation over FER-type aluminosilicate zeolite.

Process Intensification at the Nanoscale: Embedding SiC in Zeolites for Energy-Efficient Catalysis.

Alexandre Young[1]*, Julia de Souza*[2]*, Antonio Mario Leal Martins Costa*[1]*, Pedro Romano*[3]*, Javier García-Martínez*[4]*, and* ***João Monnerat***[5]
(1)LIPCAT (UFRJ), Rio de Janeiro, Rio de Janeiro, Brazil, (2)LIPCAT, Rio de Janeiro, Brazil, (3)Campus D. de Caxias, Federal University of Rio de Janeiro, Rio de Janeiro, Brazil, (4)Molecular Nanotechnology Lab, Department of Inorganic Chemistry, University of Alicante, Alicante, Spain, (5)Chemistry Institute, Federal University of Rio de Janeiro, Rio de Janeiro, Rio de Janeiro, Brazil

Incorporating SiC nanoparticles into FER zeolite during synthesis enhanced catalytic activity by 2.5 times for Friedel-Crafts alkylation under microwave heating, with over 40% energy savings compared to the physical FER/SiC mixture. This novel synergy, optimizing SiC-FER interaction for sustainable catalysis, represents a previously unreported advancement in microwave-assisted catalysis.

NITRO CHEM - NITROGEN CHEMISTRY

NITRO CHEM - SUSTAINABLE AMMONIA SYNTHESIS

Tuesday, June 10, 2025 1:00 PM - 3:20 PM
Centennial Ballroom I

Chair: Nirala Singh, University of Michigan

Co-Chair: Andrew Medford, Georgia Institute of Technology

Recent Findings and Open Questions on the Fundamental Chemistry and Practical Realization of Photocatalytic Nitrogen Fixation.

Andrew Medford[1]*, Po-Wei Huang*[1]*, Nianhan Tian*[2]*, and Marta Hatzell*[3]
(1)School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA, (2)School of Chemical & Biomolecular Engineering, Georgia Tech, Atlanta, GA, (3)George W. Woodruff School of Mechanical Engineering, Georgia Institute of Technology, Atlanta, GA

Ammonia is important for producing synthetic fertilizers to sustain the growing global population, and photocatalytic ammonia synthesis is a promising strategy for sustainable ammoina. Although widely reported, there are open debates on the detailed molecular mechanism of photocatalytic ammonia synthesis, and conflicting reports on the reliability of measured rates.

Electrochemical Nitrate Reduction to Ammonia on Cu(111): Potential Dependent DFT Study.

Adyasa Priyadarsini[1] *and Shyam Kattel*[2]
(1)Physics, Florida A&M University, Tallahassee, FL, (2)Department of Physics, University of Central Florida, Orlando, FL

Our work provides an atomistic insight into the stability of Cu catalysts at experimental conditions and importantly, can be extended to study other catalytic surfaces. Furthermore, the reaction pathways, reaction energetics and kinetics of NO_3RR on Cu(111) will provide key insight into the design of selective catalysts.

Ru/PrO_x Catalysts for Mild Ammonia Synthesis.

Samuel Drummond*, Jennifer Naglic, Alexis Allegro, Thossaporn Onsree, and Jochen Lauterbach*
Department of Chemical Engineering, University of South Carolina, Columbia, SC

Here we have produced multiple new, more efficient, promoted ruthenium-based catalysts to reduce emissions from ammonia synthesis. After screening and optimization, the new catalyst produced more than three times the best previous catalysts on a per-ruthenium basis. Further, in situ spectroscopy led to determination of the mechanism of these catalysts.

Earth-Abundant Manganese Nitride Catalysts for Mild-Condition Ammonia Synthesis.

Weiye Qu*, Pranav Roy, Brandon C. Bukowski, and Chao Wang*
Department of Chemical and Biomolecular Engineering, Johns Hopkins University, Baltimore, MD

We developed a ζ-phase $MnN_{0.43}$ catalyst for low-temperature NH_3 synthesis. This catalyst exhibits high NH_3 synthesis activity at 250-350 °C, surpassing the conventional noble metal-based Ru/MgO catalyst. Our work offers fundamental insights into the NH_3 synthesis mechanisms on earth-abundant transition metal nitrides, highlighting their significant potential for NH_3 synthesis.

Metal Hydride/Carbon-Based Nanocomposites As Catalysts for Ammonia Synthesis at Moderate Conditions.

Juliette Verschoor[1]*, Petra E. de Jongh*[1,2]*, and Peter Ngene*[1]
(1)Materials Chemistry and Catalysis, Utrecht University, Utrecht, Netherlands, (2)Inorganic Chemistry and Catalysis, Utrecht University, Utrecht, Netherlands

Alkali hydride–graphite nanocomposites were prepared via mechanochemical synthesis, i.e. ball milling (BM), and tested for thermal ammonia synthesis. Both potassium and sodium based catalysts are active without the presence of transition metals and adding small amounts of iron to these catalysts resulted in a significant increase in catalytic activity.

Mechanochemical Ammonia Synthesis over Transition Metal Nitrides.

Jacob A. Dewitt[1]*, Erin V. Phillips*[2]*, Karoline L. Hebisch*[1]*, Andrew W. Tricker*[3]*, and Carsten Sievers*[4]
(1)School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA, (2)Chemistry & Biochemistry, Georgia Institute of Technology, Atlanta, GA, (3)AAAS/NSF, Washington, DC, (4)School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA

In an effort to reduce the environmental cost of modern ammonia production, ambient-conditioned mechanochemical ammonia synthesis represents a promising pathway for improving sustainability. This work investigates the catalytic activity of transition metal nitride catalysts titanium, molybdenum, zirconium, vanadium, and niobium, by demonstrating catalytic performance and analysis of phase behavior.

Fundamental Chemistry in Lithium-Mediated Nitrogen Reduction Reaction Revealed By First-Principles Simulations.

Chengyu Zhou[1] *and Qing Zhao*[2]
(1)Northeastern University, Boston, MA, (2)Department of Chemical Engineering, Northeastern University, Boston, MA

Lithium-mediated nitrogen reduction reaction (Li-NRR) is a sustainable and feasible approach for ammonia electrosynthesis. We apply advanced computational tools based on electronic structure theory to elucidate fundamental chemistry in Li-NRR, including elementary reaction mechanisms of N_2 activation and reduction and microenvironments of the active solid-electrolyte interface layer.

REACTOR - REACTION ENGINEERING AND REACTOR DESIGN

REACTOR - REACTOR DESIGN FOR EMERGING APPLICATIONS
Tuesday, June 10, 2025 1:00 PM - 3:20 PM
Centennial Ballroom III

Chair: Ali Hussain Motagamwala, Shell

Co-Chair: Sungmin Kim, Pacific Northwest National Laboratory

Inductively Heated Structured E-Reactors for Dry Reforming of Methane.

*Mohammad Raihan Arfin, **Akshat Tanksale**, and Hamza Asmat*
Chemical and Biological Engineering, Monash University, Clayton, VIC, Australia

The double pancake coil improves magnetic flux density, enhancing current and temperature distribution. Gyroid monoliths achieve higher temperatures than octet monoliths due to efficient heat propagation through interconnected channels. These findings highlight the critical role of coil configuration and lattice geometry in understanding strucutred e-reactor design for chemical processes.

Catalyst Discovery and Bench-Scale Reactor Design for Ammonia Autothermal Reforming As a Route to Net-Zero-Carbon Hydrogen.

*Kathleen D. Brown[1], Gabrielle Kliegle[1], Jacob H. Miller[1], Adam Yonge[1], Carrie A. Farberow[1], Justin M. Bracci[1], Alexander J. Hill[1], Matthew Yung[1], and **Nicholas Thornburg**[2]*
(1)National Renewable Energy Laboratory, Golden, CO, (2)Center for Energy Conversion & Storage Systems, National Renewable Energy Laboratory, Golden, CO

This presentation encompasses several years of efforts by NREL reaction engineers to develop multifunctional supported ruthenium catalysts and to establish a unique fixed bed reactor capability leveraged to investigate an underappreciated autothermal strategy for ammonia conversion to hydrogen. These insights enable advantaged catalyst formulation and commercially relevant reformer design strategies.

Kinetic Study for CO_x Methanation Based on in-Situ Spatially Resolved Measurements in a Catalytic Plate Reactor..

*Pakpong Roongruangsree, Varun Surendran, and **Jan Kopyscinski***
Catalytic & Plasma Process Engineering, Department of Chemical Engineering, McGill University, Montreal, QC, Canada

With our novel catalytic plate reactor, a significantly larger set of data for the kinetic parameter estimation can collected than by use of a typical steady-state reactor with concentration measurements at the outlet only, which makes this setup very suitable for studying the kinetics of heterogeneous catalyzed reactions.

Enabling syngas production with negative CO_2 emissions via intensified and electrified Reverse Water Gas Shift: an experimental study..

Federico Nicolini[1], *Francesca Zaio*[1], *Matteo Ambrosetti*[2], *Alessanda Beretta*[1], *Gianpiero Groppi*[1], *Enrico Tronconi*[3], *Mariasole Cipolletta*[4], *and Alessia Marini*[4]
(1)Dipartimento di Energia, Politecnico di Milano, Milan, Italy, (2)Decarbonization unit, SNAM, San Donato Milanese, Italy, (3)Politecnico di Milano, Milan, Italy, (4)Rosetti Marino SpA, Ravenna, Italy

Syngas production is the building block of several chemical processes, but its production heavily contributes to the emission of green-house gases. In this work we present an innovative concept of electrified reactor aimed at the production of green syngas via Reverse Water Gas Shift.

Enabling High-Pressure Ammonia Reforming: Reactor Design,Validation, and Kinetic Insights.

Ceyhun Ege Köseoglu[1], *Michael Geske*[1], *Grigorios Kolios*[2], *Jan Pottbacker*[2], *Sophie Hund*[3], *Martin Lerch*[3], *Michael Kraemer*[2], *and Frank Rosowski*[2]
(1)BasCat - UniCat BASF Joint Lab, Technische Universität Berlin, Berlin, Germany, (2)Group Research, BASF SE, Ludwigshafen, Germany, (3)Anorganische Chemie/Festkörperchemie, Technische Universität Berlin, Berlin, Germany

A novel reactor for high-pressure ammonia reforming enables precise thermal control up to 50 bar and 750°C. Initial tests with Ni/Al_2O_3 and Fe_3Mo_3N catalysts demonstrate high hydrogen productivity and provide kinetic insights, advancing sustainable hydrogen production and supporting techno-economic evaluations of small-scale reforming plants.

KEYNOTE: Sustainable Catalysts with Membranes or Plasma for Energy and Environmental Applications.

Sibudjing Kawi
Department of Chemical and Biomolecular Engineering, National University of Singapore, Singapore, Singapore

In this presentation, I will address how our research group has avoided catalyst issues by systematically developing efficient non-noble metal catalysts to tackle CO_2, CH_4 and H_2 challenges (such as for CO_2 methane reforming, biomass tar reforming, water gas shift, CO_2 methanation, CO_2 hydrogenation to methanol, methane pyrolysis, methane coupling).

ADV CHARAC - NEW AND ADVANCED METHODS IN CATALYST CHARACTERIZATION

ADV CHARAC - MECHANISTIC INSIGHTS FROM ADVANCED CHARACTERIZATION TOOLS

Tuesday, June 10, 2025 3:40 PM - 5:40 PM
Hanover Hall FG

Chair: Yuanyuan Li, Oak Ridge National Laboratory (ORNL)

Co-Chair: Amrit Venkatesh, University of Virginia

Learning from Failure: Advanced Characterizations on SPA Catalysts.

***Renqin Zhang**, Seif Yusuf, and Greg Korynta*
Clariant, Louisville, KY

In the journey of understanding the characteristics of catalyst performance, we learned from failure. To predict the performance of solid phosphoric acids catalysts, in-situ characterization on catalysts under practical condition is necessary due to its dynamic nature, as well as the fact that it has hygroscopic property.

N_2o and CH_4 Utilization Via a Site-Specific Fe^{2+}/Fe^{3+} Redox Couple in Fe-Exchanged Zeolites.

***Daniel Camilo Cano Blanco**[1,2], Jörg W.A. Fischer[3], Daniele Bonavia[1,4], Gabriela-Teodora Dutca[1,2], Gunnar Jeschke[3], Oliver Kröcher[1,2], and Davide Ferri[1]*
(1)Paul Scherrer Institute, Villigen, Switzerland, (2)EPFL, Lausanne, Switzerland, (3)ETH Zurich, Zurich, Switzerland, (4)ESRF, Grenoble, France

We employed advanced operando techniques with modulated-excitation to determine the nature of active Fe sites in Fe-SSZ-13 during N_2O activation and CH_4 hydroxylation. Site-specific monomeric Fe undergoes reversible Fe^{2+}/Fe^{3+} redox, with temperature-dependent contributions from species. We highlight the advantage of combining multiple spectroscopic techniques to interrogate complex catalysts

Surface Anchoring Requirements for Vanadia Clusters on Titanium Oxide Surface and Their Impact on Activity for Oxidative Dehydrogenation of Ethanol..

***Dongmin Yun**[1], Jose Herrera[2], Nicholas Jaegers[3], Jian Zhi Hu[4], Adrian Hucal[2], and Yong Wang[5]*
(1)SK Innovation, San Francisco, CA, (2)Department of Chemical and Biochemical Engineering, Western University, London, ON, Canada, (3)University of California at Berkeley, Berkeley, CA, (4)Pacific Northwest National Laboratory, Richland, WA, (5)The Gene and Linda Voiland School of Chemical Engineering and Bioengineering, Washington State University, Pullman, WA

By using oxygen doped TiN as support for vanadia clusters, we carry a detailed study of the relationship between support oxygen content, vanadia dispersion, and catalytic performance for ethanol partial oxidation. Lattice oxygen from the titania support play a critical role in the catalytic activity of the vanadia species.

Advancing Spectrokinetics in Heterogeneous Catalysis: From Bulk to Surface Species and Beyond.

***Juan Bravo-Suarez**[1], Alejandra Torres Velasco[1,2], Hashim Alzahrani[1,2,3], Bhagyesha Patil[1,2], Yue Qi[4], Simon Podkolzin[4], and Hongda Zhu[2]*

(1)Chemical & Petroleum Engineering, The University of Kansas, Lawrence, KS, (2)Center for Environmentally Beneficial Catalysis, The University of Kansas, Lawrence, KS, (3)Chemical and Materials Engineering Department, King Abdulaziz University, Jeddah, Saudi Arabia, (4)Department of Chemical Engineering and Materials Science, Stevens Institute of Technology, Hoboken, NJ

This work proves the feasibility of utilizing steady state and transient in situ/operando spectroscopy to extract mechanistic information that reduces and leads to robust kinetic models. It also opens new avenues to explore kinetics and mechanisms with charge transfer data in heterogeneous catalysis.

Good Practices for Pulse Chemisorption.

Benjamin Le Monnier *and Katie A. Cychosz-Struckhoff*
Anton Paar Quantatec, Boynton Beach, FL

This presentation discusses optimizing pulse chemisorption parameters for accurate catalyst characterization. Key factors like carrier gas flow, temperature, and detector settings are explored using examples from propane dehydrogenation and carbon capture. These optimizations enhance repeatability and accuracy, providing practical guidance for researchers in applied catalysis.

Elucidating the Origin of Electrocatalytic Phenomena Using Steady State Isotopic Transient Kinetic Analysis.

Abigail Circelli[1] *and Ezra L. Clark*[2]
(1)Chemical Engineering, The Pennsylvania State University, University Park, PA, (2)Chemical Engineering, Penn State, University Park, PA

This presentation will demonstrate electrochemical SSITKA for the first time using DEMS and methanol oxidation over Pt as a test reaction to understand the rise and decline of the methanol oxidation activity in the low overpotential regime. This general analytical method will accelerate understanding of a variety of electrocatalytic phenomena.

AI - AI-DRIVEN CATALYSIS

AI - DEVELOPMENT OF NEW AI-DRIVEN METHODOLOGIES

Tuesday, June 10, 2025 3:40 PM - 5:40 PM
Regency Ballroom VII

Chair: Siddharth Deshpande, University of Rochester

Co-Chair: Christian Sandoval Pauker, RICE University

Text Mining Experimental Heterogeneous Catalysis Literature with Large Language Models.

Benjamin Walls[1] *and Suljo Linic*[2]

(1)Department of Chemical Engineering, University of Michigan, Ann Arbor, Ann Arbor, MI, (2)Chemical Engineering, University of Michigan, Ann Arbor, MI

We programmed a computational workflow to extract catalyst names, properties, and operating conditions from heterogeneous catalysis research papers using large language models. We identified model choices and prompting strategies that maximized performance and then used the workflow to extract 2773 measurements from 423 papers on the oxidative coupling of methane.

Hybrid Generative AI – Quantum Chemistry Feedback for Catalyst Discovery.

Mariefel Olarte
Pacific Northwest National Laboratory, Richland, WA

This work reports the first chemical descriptor-driven search algorithm for catalyst discovery that incorporates LLM knowledge space with quantum-chemical feedback. We will present experimental and DFT validation results for carbon monoxide conversion to methanol as use case.

Agentic Artificial Intelligence (AI) for Accelerating Catalytic Materials Research.

Hongliang Xin
Department of Chemical Engineering, Virginia Tech, Blacksburg, VA

Agentic AI accelerates catalysis research by autonomously tackling tasks like knowledge queries and active site optimization. Using multimodal large language models, it identifies metallic nanostructures for nitrate reduction, addressing pollution and enabling net-zero ammonia synthesis. This scalable framework advances reproducibility and sustainability in energy and environmental science.

AI-Driven Analysis of Solvation Thermodynamics of Adsorbates at Catalyst Surfaces and Liquid Water Interfaces.

Jiexin Shi[1] *and Rachel Getman*[2]
(1)William G. Lowrie Department of Chemical and Biomolecular Engineering, The Ohio State University, Columbus, OH, (2)Department of Chemical and Biomolecular Engineering, The Ohio State University, Columbus, OH

This study uses machine learning (ML) models to predict solvation thermodynamic properties of adsorbates at catalytic surfaces, achieving high accuracy while reducing computational costs compared to DFT. By using advanced data representations, these models show strong potential for automating high-throughput catalyst screening and analyzing diverse catalytic environments.

Metric Robustness in Catalysis Reproducibility and Machine Learning Model Development.

Selin Bac[1]*, Seunghwa Hong*[1]*, Emily K. Schroeder*[1]*, Adam Hoffman*[2]*, Jake A. Heinlein*[3]*, Greg*

Barber[4], Simon Bare[2], Robert Rioux[4], Matteo Cargnello[5], and Phillip Christopher[1]
(1)Department of Chemical Engineering, University of California, Santa Barbara, Santa Barbara, CA, (2)Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, Menlo Park, CA, (3)Department of Chemical Engineering, Stanford University, Stanford, CA, (4)Department of Chemical Engineering, The Pennsylvania State University, University Park, PA, (5)Chemical Engineering, Stanford University, Stanford, CA

This study examines the importance of mitigating intra- and inter-lab variability in catalysis, especially when multiple institutions contribute data for machine learning models. We highlight challenges in using common metrics and propose a robust approach that distinguishes experimental errors from variations in catalytic parameters like metal loading.

Generation of Catalysis Testing Data Via Uncertainty Sampling to Build Machine Learning Models for Catalyst Durability.

***Dongjae Shin**[1,2], Jake A. Heinlein[1], Emily K. Schroeder[3], Seunghwa Hong[4], Selin Bac[3], Anastassiya Khan[5], Adam Hoffman[2,5], Phillip Christopher[4], Matteo Cargnello[6], Simon Bare[2,5], Christopher J. Tassone[5], and Kirsten Winther[2]*
(1)Department of Chemical Engineering, Stanford University, Stanford, CA, (2)SUNCAT Center for Interface Science and Catalysis, SLAC National Accelerator Laboratory, Menlo Park, CA, (3)Department of Chemical Engineering, University of California, Santa Barbara, Santa Barbara, CA, (4)Chemical Engineering, University of California, Santa Barbara, Santa Barbara, CA, (5)Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, Menlo Park, CA, (6)Chemical Engineering, Stanford University, Stanford, CA

Evaluating the long-term stability of catalysts is crucial to determine their potential for commercialization. However, current methods for long-term stability testing rely on expensive on-stream studies. Thus, we efficiently generated testing data with the navigation by uncertainty sampling (US) algorithm, resultant data being used for machine-learned (ML) durability models.

CO2 - CO2 CAPTURE AND UPGRADING

CO2 - CO_2 CONVERSION VIA RWGS

Tuesday, June 10, 2025 3:40 PM - 5:40 PM
Centennial Ballroom IV

Chair: Wilson McNeary, National Renewable Energy Laboratory

Co-Chair: Melis Duyar, University of Surrey

Tuning Ru Catalyst for Enhanced CO Production from CH_4 in CO_2 Hydrogenation.

***Kailong Ye**[1], Shaohua Xie[2], and **Fudong Liu**[3]*
(1)University of California, Riverside, Riverside, CA, (2)Department of Civil, Environmental, and Construction Engineering, University of Central Florida, Orlando, FL, (3)Department of Chemical and Environmental Engineering, University of California, Riverside, Riverside, CA

By precisely controlling Ru structures and local environments, the CO_2 hydrogenation pathways on Ru-based catalysts have been clearly elucidated. Moreover, strategies such as creating dual Ru structural sites, engineering Ru-CeO_2 interfaces, and optimizing Ru coordination environments have proven effective in enhancing CO yields.

Intermediate-Temperature Reverse Water-Gas Shift Under Process Relevant Conditions Catalyzed By Dispersed Alkali Carbonates.

Kesha Tamakuwala*, Robert Kennedy, and Matthew Kanan*
Department of Chemistry, Stanford University, Stanford, CA

Alkali carbonate catalysts(K_2CO_3/Na_2CO_3) dispersed on γ-Al_2O_3 enable selective reverse water-gas shift reaction at intermediate temperatures (400-700°C) and elevated pressure, achieving equilibrium CO_2 conversion with 100% CO selectivity. These low-cost, transition metal-free catalysts demonstrate long-term stability, hydrocarbon tolerance, and maintain performance in commercially-relevant form-factors, advancing sustainable fuel and chemical production.

Ceria-Supported Metal-Oxide (MO_x/CeO_2) Catalysts Developed By a One-Pot Chemical Vapor Deposition (OP-CVD) Technique: Structure and Reverse Water Gas Shift Reaction Study.

Amol Pophali[1]*, Ryuichi Shimogawa*[2,3]*, Lihua Zhang*[4]*, Gihan Kwon*[5]*, Kwangsuk Yoon*[6]*, Jangeon Roh*[7]*, Do Heui Kim*[7]*, Hocheol Song*[6]*, Anatoly I. Frenkel*[2,8]*, and Tae Jin Kim*[1]
(1)Materials Science and Chemical Engineering, Stony Brook University, Stony Brook, NY, (2)Stony Brook University, Stony Brook, NY, (3)Mitsubishi Chemical Corporation, Science and Innovation Center, Yokohoma, Japan, (4)Center for Functional Nanomaterials, Brookhaven National Laboratory, Upton, NY, (5)National Synchrotron Light Source II, Brookhaven National Laboratory, Upton, NY, (6)Department of Resource and Environmental Engineering, Hanyang University, Seoul, Korea, Republic of (South), (7)Seoul National University, Seoul, Korea, Republic of (South), (8)Brookhaven National Laboratory, Upton, NY

A novel one-pot chemical vapor deposition (OP-CVD) technique was developed for the synthesis of wide range of MO_x/CeO_2 catalysts. Structural characterizations validated this development and reverse water gas shift (RWGS) reaction tests showed the effectiveness of the prepared catalysts. In-situ DRIFTS and XRD showed reaction mechanisms and structural changes, respectively.

Accelerating Decarbonization By Representing Catalysts with Natural Language.

Mayk C. Ramos, Shane Michtavy, Andrew White, and ***Marc Porosoff***
Department of Chemical Engineering, University of Rochester, Rochester, NY

Representing reverse water-gas shift catalysts with the text of synthesis procedures and reaction conditions enables Bayesian optimization, leading to accelerated catalyst discovery.

Demonstration of Innovative CO_2 to CO Transformation Technology for Carbon Neutrality.

***Risa Sakurai**, Shota Manabe, Haruka Nishiyama, Keisuke Iijima, Noritoshi Yagihashi, and Yuki Nakama*
SEKISUI CHEMICAL CO.,LTD, Tsukuba, Japan

SEKISUI has been developing technologies to efficiently convert CO_2 to CO with Reverse Water Gas Shift by Chemical Looping. Over 90% CO generation yields and 80% H_2 conversion was achieved in the demonstration with actual gas from blast furnace. The details of demonstrations and dissemination plans will be explained.

Mechanistic and Kinetic Relevance of Hydrogen and Water in CO_2 Hydrogenation on Cu-Based Catalysts.

***Ting Lin**[1], Michelle Nolen[2,3], Carrie Farberow[3], Stephanie Kwon[2], and Aditya Bhan[1]*
(1)Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN, (2)Chemical and Biological Engineering, Colorado School of Mines, Golden, CO, (3)Catalytic Carbon Transformation & Scale-Up Center, NREL, Golden, CO

Kinetic effects of H_2, H_2O, and CO_2 during CO_2 hydrogenation are rationalized on catalyst formulations with and without ZnO based on experimental and computational results. We show herein that reaction occurs on Cu surfaces saturated by H* and HCOOH** with methanol synthesis and RWGS involving distinct intermediates and rate-determining steps.

ELECTRO PHOTO - ELECTROCATALYSIS AND PHOTOCATALYSIS

ELECTRO PHOTO - WATER ELECTROLYSIS

Tuesday, June 10, 2025 3:40 PM - 5:40 PM
Centennial Ballroom I

Chair: Joaquin Resasco, The University of Texas at Austin

Co-Chair: Kasun Gunasooriya, University of Oklahoma

Intermittency Accelerates Catalyst Transformations and Degradation during Water Electrolysis.

***Raul Marquez**[1], Jay Bender[2], Ashton Aleman[3,4], Emma Kalokowski[1], Thuy Vy Le[1], Morten Linding Frederiksen[5], Kenta Kawashima[1], Chikaodili Chukwuneke[1], Andrei Dolocan[6], Michaela Burke Stevens[4], Delia Milliron[1,7,8,9], Joaquin Resasco[2,9], Thomas Jaramillo[3,4], and C. Buddie Mullins[1,2,6,8,9]*
(1)Department of Chemistry, The University of Texas at Austin, Austin, TX, (2)McKetta Department of Chemical Engineering, The University of Texas at Austin, Austin, TX, (3)Department of Chemical Engineering, Stanford University, Stanford, CA, (4)SUNCAT Center for Interface Science and Catalysis, SLAC National Accelerator Laboratory, Menlo Park, CA, (5)Department of Biological & Chemical Engineering, Aarhus University, Aarhus, Denmark, (6)Texas Materials Institute, The University of Texas at Austin, Austin, TX, (7)Chemical

Engineering, The University of Texas at Austin, Austin, TX, (8)Center for Electrochemistry, The University of Texas at Austin, Austin, TX, (9)H2@UT, The University of Texas at Austin, Austin, TX

This work reveals the impact of intermittency and reverse currents on catalyst durability in liquid alkaline water electrolyzers. Through systematic *in situ/operando* characterization, we demonstrate that intermittent operation affects electrode discharge, alters the surface composition, degrades catalytic films, accelerates corrosion, and induces local pH swings.

Understanding the Factors That Govern Stability of Ru-Based Pyrochlores for Acidic Oxygen Evolution Reaction.

***Kunal Velinkar**, Michael Allan, and Eranda Nikolla*
Department of Chemical Engineering, University of Michigan, Ann Arbor, MI

This work investigates the stability of Ru-based pyrochlores for acidic OER, showing that smaller A-site cations enhance stability by reducing Ru dissolution. Stability trends correlate with A-site cation radius, oxide reducibility, and Ru–O bond strength, offering insights into structure-stability relationships and design strategies for durable electrocatalysts.

Porous Tantalum Oxide-Supported Ir Catalyst for Reducing Ir Loading in the Anode of Membrane Electrode Assembly for Proton Exchange Membrane Water Electrolyzer.

*Je Yeon Choi[1], Song Gyun Kim[2], Hoseong Yang[2], Yong Won Kim[2], and **Chanho Pak**[1]*
(1)Graduate School of Energy Convergence, Institute of Integrated Technology, Gwangju Institute of Science and Technology, Gwangju, Korea, Republic of (South), (2)Graduate School of Energy Convergence, Gwangju Institute of Science and Technology, Gwangju, Korea, Republic of (South)

This study highlights the benefits of using iridium catalysts supported on hierarchical porous Ta_2O_5 with both mesopores and macropores. The MEA with 0.2 mg_{Ir}/cm^2 presented superior performance and durability at 1 A/cm^2 under PEMWE conditions.

Seawater Electrolysis Using Oxide Encapsulated Ruthenium Oxide Catalysts in Unbuffered pH-Neutral Seawater.

***Daniela Bushiri**[1], Amanda Baxter[1], Onaolapo Odunjo[1], Daniela Fraga Alvarez[2], Yong Yuan[3], Daniel Esposito[1], and Jingguang G. Chen[4]*
(1)Department of Chemical Engineering, Columbia Electrochemical Energy Center, Lenfest Center for Sustainable Energy, Columbia University, New York, NY, (2)Chemical Engineering, Columbia University, New York, NY, (3)Department of Chemical and Biomolecular Engineering, University of Delaware, Newark, DE, (4)Chemistry Division, Brookhaven National Laboratory, Upton, NY

Direct seawater electrolysis offers a pathway to green hydrogen but faces challenges from chlorine evolution competing with oxygen evolution in unbuffered pH-neutral solutions. This

study demonstrates SiO_x and TiO_x overlayers on Ru and RuO_x thin films suppress chloride transport, enhancing OER selectivity and efficiency while balancing the activity and stability.

Identifying Role of Hydronium Cation in Acidic Oxygen Evolution Reaction over IrO_2.

Tianyou Mou[1], *Daniela Bushiri*[2], *Daniel Esposito*[3], *Jingguang G. Chen*[1,2], *and Ping Liu*[1]
(1)Chemistry Division, Brookhaven National Laboratory, Upton, NY, (2)Chemical Engineering, Columbia University, New York, NY, (3)Department of Chemical Engineering, Columbia Electrochemical Energy Center, Lenfest Center for Sustainable Energy, Columbia University, New York, NY

This study highlights the importance of an explicit description of the acidic environment of OER in theoretical modeling, being able to enhance modeling accuracy, gaining better mechanistic insights, and opening new opportunities for optimization of IrO_2-based catalysts.

Theoretical Prediction and Experimental Verification of IrO_x Supported on Titanium Nitride for Acidic Oxygen Evolution Reaction.

Xue Han[1], *Tianyou Mou*[2], *Ping Liu*[2], *and Jingguang G. Chen*[2]
(1)Chemistry Division, Brookhaven National Lab, Upton, NY, (2)Chemistry Division, Brookhaven National Laboratory, Upton, NY

This study highlights the importance of combining theoretical prediction and experimental studies of model catalysts and commercially viable powder catalysts in the discovery of OER catalysts with enhanced activity and stability.

FUNDAMENTALS - FUNDAMENTALS OF CATALYSIS AND SURFACE SCIENCE

FUNDAMENTALS - CATALYST DESIGN AND SURFACE SCIENCE

Tuesday, June 10, 2025 3:40 PM - 5:40 PM
Centennial Ballroom II

Chair: Elizabeth Bickel Rogers, University of Minnesota

Co-Chair: Konstantin Khivantsev, Pacific Northwest National Laboratory

Surface Roughening in Nanoparticle Catalysts.

Cameron Owen[1], *Nicholas Marcella*[2], ***Christopher O'Connor***[1], *Taek-Seung Kim*[3,4], *Ryuichi Shimogawa*[5,6], *Clare Yijia Xie*[7], *Ralph G. Nuzzo*[2], *Anatoly I. Frenkel*[5,8], *Christian Reece*[1], *and Boris Kozinsky*[1,9]
(1)Harvard University, Cambridge, MA, (2)University of Illinois Urbana-Champaign, Urbana, IL, (3)Korea Institute of Energy Research, Daejeon, Korea, Republic of (South), (4)Rowland Institute at Harvard, Harvard University, Cambridge, MA, (5)Stony Brook University, Stony Brook, NY, (6)Mitsubishi Chemical Corporation, Science and Innovation Center, Yokohoma, Japan, (7)Harvard John A. Paulson School of Engineering and Applied Sciences, Harvard

University, Cambridge, MA, (8)Brookhaven National Laboratory, Upton, NY, (9)Robert Bosch LLC Research and Technology Center, Watertown, MA

We demonstrate that reactive MD simulations, powered by machine learned force fields, coupled with in situ infrared and X-ray absorption spectroscopy measurements makes it feasible to gain full atomistic understanding into dynamic structural responses of catalytically relevant metal nanoparticle systems.

The Counterintuitive Influences of Surface Entropy and Surface Hydroxyl Density on Hydrogen Spillover.

Kelle Hart[1] *and Bert Chandler*[2]
(1)Chemistry, Pennsylvania State University, State College, PA, (2)Chemical Engineering, Pennsylvania State Univerisity, State College, PA

Our data show hydrogen spillover coverage increases as surface hydroxyl density decreases. This counterintuitive result provides the first method for invoking spillover in a catalytic reaction. We also find the stabilization of spillover on a metal oxide support likely stems from a surface entropy effect rather than conventional enthalpic stabilization.

Predicting Adhesion Energies of Metal Nanoparticles to Many Oxide Support Surfaces, Metal Chemical Potential Versus Particle Size and Support, and Catalyst Performance.

Charles Campbell[1] *and Nida Janulaitis*[2]
(1)Chemistry and Chemical Engineering Departments, University of Washington, Seattle, WA, (2)Department of Chemical Engineering, University of Washington, Seattle, WA

A simple way to estimate adhesion energies between metal nanoparticles and oxide supports is discovered, which in turn predicts metal atom chemical potential as a function of the particle size and support. This chemical potential allows quantitative prediction of sintering rates and qualitatively corelates with the metal nanoparticle's reactivity.

Bottom-up Design of Microporous SiO_2 Layers on TiO_2 for Alcohol Dehydration Catalysis.

Stephanie Kwon
Chemical and Biological Engineering, Colorado School of Mines, Golden, CO

This work develops bottom-up synthesis procedures to create SiO_2 micropores around Lewis acid-base sites in bulk oxides to enhance their reactivity for alcohol dehydration catalysis.

Engineering Active Sites of Metal/Metal Oxide Catalysts By Oxide Ligand Overlayers.

Jiahua Zhou[1]*, Piaoping Yang*[1]*, Stavros Caratzoulas*[2]*, Weiqing Zheng*[3]*, and Dionisios Vlachos*[2]
(1)University of Delaware, Newark, DE, (2)Delaware Energy Institute, University of Delaware, Newark, DE, (3)Delaware Energy Institute, University of Delaware, Newark, DE, University of Delaware, Newark, DE

This work presents strategy to engineer active sites of Pt catalysts using WOx as oxide ligands, which selectively block Pt terraces. Adjusting WOx coverage tunes site composition, alters reactant adsorption, and shifts selectivity from terrace- to step-dominated pathways. The insights open avenues for improving metal/metal oxide catalysts beyond specific system.

Non-Innocent Supports Enable Single-Site First-Row Metals for Carbon-Oxygen Bond Activation.

Long Qi[1]*, Wenyu Huang*[2]*, Bin Wang*[3]*, and Susannah Scott*[4]
(1)Division of Chemical & Biological Sciences, Ames Laboratory, Ames, IA, (2)Chemistry, Iowa State University, Ames, IA, (3)School of Sustainable Chemical, Biological and Materials Engineering, University of Oklahoma, Norman, OK, (4)Department of Chemical Engineering, University of California, Santa Barbara, Santa Barbara, CA

We demonstrated redox and chemical processes mediated with non-innocent supports for a chemical transformation using single-site first-row transition metals involving reactant binding and multiple bond activations in a single catalytic turnover. Such processes are common in upgrading renewable feedstocks such as biomass and CO_2.

HYDRO ECON - CATALYSIS FOR THE HYDROGEN ECONOMY

HYDRO ECON - LIQUID ORGANIC HYDROGEN CARRIERS

Tuesday, June 10, 2025 3:40 PM - 5:40 PM
Centennial Ballroom III

Chair: Siwen Wang, Toyota Research Institute of North America

Co-Chair: Yizhen Chen, University of Virginia

Design of Pd Catalysts for Liquid Organic Hydrogen Carriers.

Kwangjin An
Ulsan National Institute of Science & Technology, Ulsan, Korea, Republic of (South)

Liquid organic hydrogen carriers (LOHCs) are considered as an attractive approach for transporting and storing hydrogen. In this study, we present a catalyst design strategy to enhance the efficiency of LOHC reactivity by using N-heterocyclic compounds as substrates.

The Role of Support on the Performance of Platinum Catalysts for Methylcyclohexane Dehydrogenation.

Patrick Holcombe*, Kaveh Shariati, Thossaporn Onsree, and Jochen Lauterbach*
Department of Chemical Engineering, University of South Carolina, Columbia, SC

This work analyzes metal oxides and platinum supported on metal oxides to characterize the acidity of supports and gain an understanding of the effect support has on catalyst performance in methylcyclohexane dehydrogenation. Relative amounts and strengths of Lewis and Brønsted acid sites are determined.

Dehydrogenation of Liquid Organic Hydrogen Carriers Catalyzed By Defect-Rich Boron Nitride Catalyst.

Qingju Wang[1], *Zhenzhen Yang*[2], *and Sheng Dai*[2]
(1)Chemistry, University of Tennessee, Knoxville, Knoxville, TN, (2)Chemical Sciences Division, Oak Ridge National Laboratory (ORNL), Oak Ridge, TN

Our study demonstrates a novel flux reconstruction strategy to create highly crystalline metal-free BN catalysts with high surface area and abundant exposed B/N defects, enhancing their dehydrogenation activity towards nitrogen-substituted heterocycles LOHCs for hydrogen economy.

A Computational Study on the Dehydrogenation of Methylcyclohexane to Toluene on Platinum Catalyst.

Andreas Heyden[1], ***Bhawana Rayamajhi***[2], *Wenqiang Yang*[2], *Mubarak Bello*[2], *and Olajide Bamidele*[2]
(1)Department of Chemical Engineering, University of South Carolina, Columbia, SC, (2)Chemical Engineering, University of South Carolina, Columbia, SC

The systematic investigation of stepwise dehydrogenation of MCH to Toluene from the first principle using Density Functional Theory was done to identify the role of the various active sites on three Platinum surface facets and the reaction mechanism and determine the rate and selectivity controlling steps over the active sites.

Mechanistic Insights and Trends of Selectivity for Methylcyclohexane Dehydrogenation on Oxide-Supported Pt, Pd, and Ni Nanoparticles.

Karoline Kvande[1], *Fang Wan*[1], *Zhongyao Zhang*[1], *Sai Chen*[1], *Trenton Otto*[2], *and Enrique Iglesia*[1,3]
(1)Chemical and Biomolecular Engineering, University of California, Berkeley, Berkeley, CA, (2)Chevron Technical Center, Richmond, CA, (3)Chemical Engineering, Purdue University, West Lafayette, IN

This study report similarities among kinetic trends, identity and kinetic relevance of methylcyclohexane dehydrogenation elementary steps on Pt, Pd, and Cu/Ni nanoparticles dispersed on oxides, as well as consequences of metal and support identity on rates and dehydrogenation selectivity. These findings are relevant for the design of catalytic dehydrogenation-hydrogenation cycles.

Surface Structure Effects on Methylcyclohexane Dehydrogenation over Ni Catalysts: A DFT Investigation.

Wenqiang Yang[1], *Mubarak Bello*[1], *Bhawana Rayamajhi*[1], *and Andreas Heyden*[2]
(1)Chemical Engineering, University of South Carolina, Columbia, SC, (2)Department of Chemical Engineering, University of South Carolina, Columbia, SC

Ni(211) is the most active site for MCH dehydrogenation to toluene and also the site prone to excessive dehydrogenation and coking. The findings will contribute to the rational design of improved Ni-based catalysts with high activity, reduced coke formation, and overall enhanced stability.

MICRO MESO - MICROPOROUS AND MESOPOROUS MATERIALS

MICRO MESO - MICROPOROUS AND MESOPOROUS MATERIALS FOR OXIDATION CATALYSIS

Tuesday, June 10, 2025 3:40 PM - 5:40 PM
Hanover Hall CDE

Chair: Pearl Kim, Micromeritics

Co-Chair: Charles Kanyi, Johnson Matthey

Binuclear Ti-Fe Sites in MFI Framework for Synergistically Catalysing Alkene Epoxidation.

Dong Lin[1] *and Richard J. Lewis*[2]
(1)Cardiff University, Cardiff, United Kingdom, (2)School of Chemistry, Cardiff University, Cardiff, United Kingdom

Binuclear Ti-Fe metal sites in MFI framework exhibit a marked improvement in alkene epoxidation compared to analogous materials containing only mononuclear Ti sites. This enhanced performance is attributed to a lower-energy reaction pathway, facilitated by the key oxygen transfer process involving more electrophilic bridging intermediates on binuclear Ti-Fe metal sites.

Investigating the Interplay of Fe Coordination Environment and Reaction Dynamics during MOF-Catalyzed Oxidations.

Joshua Miller[1]*, Rachel A. Yang*[2]*, and Michele Sarazen*[1]
(1)Department of Chemical and Biological Engineering, Princeton University, Princeton, NJ, (2)Department of Chemical Engineering, University of Michigan, Ann Arbor, MI

This work investigates the dynamics of MIL-100(Fe) to construct structure-property relationships for oxidation reactions. Oxidant identity (*tert*-butyl hydroperoxide vs. hydrogen peroxide) and local coordination effects had significant influence on reactivity, selectivity, and deactivation trends. Insights here can be extended to other MOF-catalyzed systems with similar active site requirements.

Oxidation Chemistries over Catalysts Containing M-N_4 Active Sites.

Ethan Iaia[1]*, Ademola Soyemi*[1]*, Ganesh Rana*[2]*, Tibor Szilvasi*[1]*, Martin G. Bakker*[3]*, and James W. Harris*[1]
(1)Department of Chemical and Biological Engineering, The University of Alabama, Tuscaloosa, AL, (2)Department of Chemistry & Biochemistry, The University of Alabama,

Tuscaloosa, AL, (3)Department of Chemistry & Biochemistry, University of Alabama, Tuscaloosa, AL

We compare rates of three different oxidation reactions over metal phthalocyanine and metal nitrogen doped carbon catalysts, which have similar M-N_4 binding sites. M-N_4 sites can accommodate two reactive adsorbates and perform oxidation chemistries through an LH pathway. Insights gained over well-defined phthalocyanine will be applied to less-uniform doped carbons.

Oxidation of Linear Alkanes Using TS-1 and H_2O_2 Toward Chemical Upcycling of Polyolefins.

***Seyeon Park**, Daeyeon Lee, Raymond Gorte, and John Vohs*
Department of Chemical and Biomolecular Engineering, University of Pennsylvania, Philadelphia, PA

Mild oxidation of alkanes from n-C_8H_{18} to n-$C_{36}H_{74}$ using TS-1 catalysts and H_2O_2 demonstrates that alkane concentrations in the aqueous phase significantly impact the oxidation rates. ^{1}H-NMR spectra indicate the 2 position of alkane chains as a preferential reaction site, with notable reactivity at central carbons.

Screening of Indirect Second Sphere Coordination Effects in the MIL-100 Metal-Organic Framework for Methane Partial Oxidation.

Stephen Vicchio
Savannah River National Lab, Aiken, SC

Residual H_2O ligands anchored to the inactive Fe sites within MIL-100(Fe) indirectly alter the chemical reactivity of the Fe active site. Herein, these indirect second sphere coordination effects are further investigated using DFT to identify potential descriptors linking reactivity and the coordinating ligands at the inactive metal centers in MIL-100.

Pairing Hetero-Substituted Zeolites with Tailored Acidity As Tandem Catalysts for Enhanced Light Olefins Production.

***Amir Abutalib**[1,2], Deependra Parmar[2], Jaeyul Kim[2], MD Shahriar Hossain[3], Sangho Chung[4], Lars Grabow[2], Javier Ruiz-Martinez[4], and Jeffrey Rimer[1,2]*
(1)Department of Chemistry, University of Houston, Houston, TX, (2)William A. Brookshire Department of Chemical and Biomolecular Engineering, University of Houston, Houston, TX, (3)William A. Brookshire Department of Chemical and Biomolecular Engineering & Texas Center for Superconductivity (TcSUH), University of Houston, Houston, TX, (4)KAUST Catalysis Center, KAUST, Thuwal, Thuwal, Saudi Arabia

Tandem catalysts with tunable acidity for the enhanced production of olefins were assessed through two reactions: methanol to hydrocarbons (MTH) and oxidative dehydrogenation (ODH). A dual fixed bed reactor configuration was utilized combining gallosilicates and

aluminosilicates, which were both synthesized with distinct zeolite pore topologies (MWW, CHA, and MFI).

POLYMER - CATALYSIS FOR POLYMER SYNTHESIS, UPCYCLING, AND RECYCLING

POLYMER - POLYOLEFIN SYNTHESIS AND HYDROGENOLYSIS

Tuesday, June 10, 2025 3:40 PM - 5:40 PM
Regency Ballroom VI

Chair: Kunlun Ding, Louisiana State University

Co-Chair: Felipe Polo-Garzon, Oak Ridge National Laboratory (ORNL)

KEYNOTE: Reactive Separations and Processivity in Polyolefin Hydrogenolysis.

Aaron Sadow
Division of Chemical & Biological Sciences, Ames Laboratory, Ames, IA

Our team has been investigating heterogeneous catalytic materials and reaction conditions to bypass statistically-controlled scission processes and establish selective conversions of polyolefins into smaller alkanes via hydrogenolysis. Chemical properties of the alkane products and the polyolefin reactants are similar, we have developed methods to create selectivity by leveraging physical differences.

Mechanocatalytic Depolymerization of Polyethylene By Hydrogenolysis Using Metal Hydride Catalysts.

Jouke van Westrenen[1] *and Carsten Sievers*[2]
(1)Chemical and Biomolecular Engineering, Georgia Tech, Atlanta, GA, (2)School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA

Mechanocatalytic hydrogenolysis provides an option for converting polyolefins to smaller hydrocarbons under controlled conditions in a solvent-free process. Thus, it avoids many of the drawbacks of other strategies in literature and could be an economically viable path to the reintegration of plastic waste.

Predicting a Generalized Branched Hydrogenolysis Mechanism on Ru, Ir, and Pt Surfaces for Polymer Upcycling Applications.

Andy Simonson*, Lydia Thies, and David Hibbitts*
Department of Chemical Engineering, University of Florida, Gainesville, FL

Hydrogenolysis chemistry can upcycle polymers to generate value from plastic waste. We present a fundamental study investigating C–C hydrogenolysis mechanisms at branch points of alkanes on Ir, Pt, and Ru surfaces using density functional theory investigations of model compounds to predict macromolecular reactions during polymer upcycling.

Catalysts for Nylon-6 Depolymerization to ε-Caprolactam: Understanding the Structure-Performance Relationship..

Prabin Dhakal[1], *Derek Creaser*[2], *and Louise Olsson*[2]
(1)Chemistry and chemical engineering, Chalmers University Of Technology, gothenburg, Sweden, (2)Chemical Engineering, Chalmers University of Technology, Gothenburg, Sweden

We have demonstrated a heterogeneous catalytic pathway for nylon depolymerization using only hydrogen. By investigating the influence of various metal oxide support properties, we provide valuable insights for designing efficient catalysts. These findings contribute to advancing polymer recycling and upcycling, promoting more sustainable processes in a circular economy.

Polyolefin Melt-Phase Effects on Alkane Hydrogenolysis over Pt Catalysts.

Andreas Heyden[1] *and* ***Mehdi Zare***[2]
(1)Department of Chemical Engineering, University of South Carolina, Columbia, SC, (2)Chemical Engineering, University of South Carolina, Columbia, SC

Using a hybrid quantum mechanical/molecular mechanical (QM/MM) approach, we systematically study polyolefin melt phase effects on small alkanes hydrogenolysis over Pt(111) catalyst surface in a polymer melt.

OTHER EVENTS

TUESDAY POSTER SESSION

Tuesday, June 10, 2025 6:00 PM - 8:00 PM
Grand Hall

A New Method for the Simulation of Catalyst Deactivation in Fluidized Bed Reactors.

Andrea Pappagallo[1], *Hugo Pétremand*[1], *Tilman Schildhauer*[2], *and* ***Emanuele Moioli***[3]
(1)Paul Scherrer Institute, Villigen, None, Switzerland, (2)Paul Scherrer Institut, Villigen PSI, Switzerland, (3)Politecnico di Milano, Milano, None, Italy

This work describes a new methodology for the description of catalyst deactivation in fluidized bed reactors. The methodology includes the description of particle motion in the reactor and the estimation of the time-on-stream evolution in a CO/CO2 methanation reactor.

Selective Conversion of 2,3-Butanediol to Aviation Fuel and Chemical Precursors Via Dioxolane Intermediates.

Michael Cordon[1], *Peter Neate*[2], *Xiaokun Yang*[2], *Chenjiao Bu*[3], *Liangliang Huang*[3], *Meijun Li*[1], *and Andrew D. Sutton*[1]
(1)Manufacturing Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN, (2)Chemistry Division, Los Alamos National Laboratory, Los Alamos, NM, (3)School of Sustainable Chemical, Biological and Materials Engineering, University of Oklahoma, Norman, OK

This work addresses a bottleneck in 2,3-butanediol conversion processes for sustainable fuels and chemicals production. Using coupled catalyst and process design principles, catalysts were tailored to form the isobutanal intermediate critical for dioxolane formation which enables the sustainable and commercial viability of biomass-derived 2,3-butanediol separation and valorization processes.

Understanding Glycine Oxidation Mechanism: Pathway Towards Nutrient Recovery from Waste Sludge.

Samuel Olusegun[1], *Haldrian Iriawan*[2], *Nianhan Tian*[3], *Andrew Medford*[3], *Yang Shao-Horn*[2], *and Joseph Gauthier*[1]
(1)Chemical Engineering, Texas Tech University, Lubbock, TX, (2)Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, MA, (3)School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA

Understanding the glycine oxidation mechanism provides fundamental insights into electrochemical waste sludge oxidation into value-added products and could inform methods to improve the reaction rate and selectivity towards desired value-added products. This work combines theoretical and experimental approaches to develop a deeper mechanistic understanding of the glycine oxidation reaction

Evaluation of the Potential of Producing SAF and Renewable Diesel Fractions from Upgrading Bio-Oils Using Dispersed Catalyst.

Yi Zhang *and Jacques Monnier*
Natural Resources Canada, CanmetENERGY-Ottawa, Ottawa, ON, Canada

This study evaluated the potential of producing biojet and renewable diesel fractions by upgrading biomass fast pyrolysis oil and catalytic pyrolysis oil using dispersed unsupported MoS_2 catalyst, and assessed how close the final products are to meet jet and diesel fuels standards (ASTM D7566 and D975, respectively).

Harnessing Ultrasound Irradiation for Selective Radical-Driven Aldehyde Oxidation to Carboxylic Acids.

Ari Fischer[1], *Teseer Bahry*[2], *Zhangyue Xie*[1], *Kaicheng Qian*[3], *Renhong Li*[4], *James Kwan*[5], *Francois Jerome*[2], *Sabine Valange*[2], *Wen Liu*[1], *Prince N. Amaniampong*[2], *and Tej Choksi*[1]
(1)School of Chemistry, Chemical Engineering and Biotechnology, Nanyang Technological University, Singapore, Singapore, (2)Institut de Chimie des Milieux et Matériaux de Poitiers, CNRS, Poitiers, France, (3)Zhejiang Sci-Tech University, Hangzhou, Zhejiang, China, (4)National Engineering Lab for Textile Fiber Materials and Processing Technology, Zhejiang Sci-Tech University, Hangzhou, China, (5)Engineering Science, University of Oxford, Oxford, United Kingdom

Ultrasound irradiation generates free radicals enabling aqueous radical oxidation chemistry. The kinetics of one such process, glyoxal oxidation, are described robustly by combining density

functional theory calculations with experiments. These descriptions inform experimental conditions that afford selective aldehyde oxidation in favor of deleterious C-C cleavage.

Biocrude Upgradation Via Hydrodeoxygenation Using Ni-Mo Doped Hydrochar Catalysts Derived from Sawdust.

Priyanka Tirumareddy, *Ajay Dalai, and Philip Boahene*
Chemical and Biological Engineering, University of Saskatchewan, Saskatoon, SK, Canada

Biocrude was produced via hydrothermal liquefaction of canola and mustard meal, achieving 42 wt.% yield at optimized conditions. Catalytic upgrading with Ni-Mo doped hydrochar derived from sawdust reduced oxygen content from 9-10 wt.% to 2-4 wt.%, significantly enhancing biocrude quality for sustainable renewable fuel production.

Synergistic Effect of Metal and Acid Sites in Chemical Recycling of Plastic Wastes.

Junho Suh *and Do Heui Kim*
Seoul National University, Seoul, Korea, Republic of (South)

It was found that through the bifunctional mechanism over Ru/BEA, high conversion of PE, low production of methane, and improved product distribution toward naphtha range could be achieved.

One Pot Synthesis of Fully Formulated Sustainable Aviation Fuel from Brown Grease Via Multifunctional Catalysts.

Clara Mongelli[1], Great Umenweke[2,3], ***Robert Pace III***[3]*, and Eduardo Santillan-Jimenez[2,3]*
(1)Université de Bourgogne Franche-Comté, Dijon, France, (2)Department of Chemistry, University of Kentucky, Lexington, KY, (3)Center for Applied Energy Research, University of Kentucky, Lexington, KY

Multifunctional nickel copper catalysts supported on zeolites and zeotypes were employed in the upgrading of brown grease to fully formulated sustainable aviation fuel. 10% Ni-2.5% Cu supported on ZSM-5 was found to have quantitative conversion and good selectivity to all four hydrocarbon types found in aviation fuel.

Carbon Dioxide to Ethylene Conversions on Iron-Based Catalysts.

Bin Liu
Chemical Engineering, Kansas State University, Manhattan, KS

This study helps provide molecular insights into the active sites, reaction mechanisms and CO_2 conversion product selectivities for the important Fe-based catalysts.

CuO-ZnO Oxides Derived from Lamellar Structures As Catalysts for the Hydrogenation of CO_2 to Methanol.

Renatto A. Angeli, Janaina Fernandes Gomes, Luana Paula, Jose Assaf, and ***Janaina F. Gomes***
Chemical Engineering Department, Federal University of São Carlos, São Carlos, Brazil

The conversion of CO_2 into methanol is typically carried out using copper-based mixed oxides. Although these oxides have high reactivity, they also exhibit low catalytic stability. In this context, this work proposes modifications to classical methods for obtaining Cu-Zn-based metal precursors, investigating the impact of urea and cetyltrimethylammonium bromide.

通过优化活性位点接近度和 CO 中间体促进反铁基催化剂上co 2加氢制烯烃.

Wei Wang[1]*, Bowen Li*[2]*, Caiqi Wang*[1]*, Norbert Kruse*[1]*, and Hongfei Lin*[1]
(1)The Gene and Linda Voiland School of Chemical Engineering and Bioengineering, Washington State University, Pullman, WA, (2)Department of Chemical Engineering, Northeastern University, Boston, MA

This work develops inverse Fe-based catalysts for CO_2 hydrogenation to olefins, optimizing active site proximity and CO intermediate transport. The inverse catalysts achieve 53.9% olefin selectivity at 48.7% CO_2 conversion, outperforming traditional catalysts. In situ DRIFTS shows a combined RWGS and CO hydrogenation pathway, enhancing CO_2 conversion and olefin selectivity.

Understanding Sulfur-Induced Deactivation in Ru/Al_2O_3 Catalysts for CO_2 Hydrogenation Via Combined *in-Situ* and *Ex-Situ* Methods.

Clara Larghi[1]*, Alessandro Porta*[1]*, Carlo Giorgio Visconti*[1]*, Janos Szanyi*[2]*, and Luca Lietti*[1]
(1)Dipartimento di Energia, Politecnico di Milano, Milan, Italy, (2)Pacific Northwest National Laboratory, Richland, WA

Sulfur contaminants in CO_2 flows strongly hinder the methanation process. This study used *ex-situ* and *in-situ* poisoning to analyze sulfur's impact on the morphology and activity of a 4% Ru/Al_2O_3 catalyst. Additionally, a kinetic model developed was able to effectively describe the catalyst's deactivation.

Sustainable CO_2 Electrolysis to Concentrated Formate in the CEM-Based Electrolyzer..

Haocheng Xiong[1]*, Bingjun Xu*[2]*, and Qi Lu*[3]
(1)Department of Chemical Engineering, Tsinghua University, Beijing, China, (2)Catalysis Center for Energy Innovation, Department of Chemical and Biomolecular Engineering, University of Delaware, Newark, DE, (3)Chemical Engineering, Tsinghua University, Beijing, China

I will present various CO_2 electrolysis strategies to produce concentrated formate products up to 5.3 M using a cation exchange membrane-based flow-type electrolyzer. This approach demonstrated substantial profitability for valuable chemical production from CO_2 in the TEA analysis, even without considering potential subsidies and carbon taxes.

Catalytic Roles of Reactive Hydrogen in CO_2 activation Via Reverse Water Gas Shift on Rh and Pt Surfaces.

Riccardo Colombo[1], *Gabriele Spanò*[1], *Luca Nardi*[1], *Ya-Huei (Cathy) Chin*[2], *and Matteo Maestri*[1]
(1)Laboratory of Catalysis and Catalytic Processes - Dipartimento di Energia, Politecnico di Milano, Milano, Italy, (2)Department of Chemical Engineering and Applied Chemistry, University of Toronto, Toronto, ON, Canada

Despite extensive investigations, Reverse Water Gas Shift mechanism over supported metal nanoparticles remains unclear. To address these uncertainties, we performed a rigorous kinetic investigation on Pt and Rh nanoparticles supported on alumina, deriving apparent reaction orders, activation energies and two rate equations based on different CO_2 activation pathways.

Material and Process Optimization of Reactive Carbon Capture to Methanol Using Cu-ZnO-Al_2O_3 Dual Function Materials.

Chae Jeong-Potter, *Martha A. Arellano-Treviño, Wilson McNeary, Alexander J. Hill, Daniel A. Ruddy, and Anh To*
Catalytic Carbon Transformation and Scale-Up Center, National Renewable Energy Laboratory, Golden, CO

We report the development and evaluation of Cu-Zn-Al based dual function materials for combined capture and conversion of CO_2 to methanol. Through a rigorous design of experiments, the DFM composition (alkali identity and loading) and process conditions (hydrogenation parameters) were optimized, resulting in increased MeOH selectivity from 53% to 97%.

Computational Investigation into Supported and Inverted Cu-ZrO_2 Catalysts for Selective CO_2 Hydrogenation to Methanol.

Anshuman Goswami[1,2], *Junjie Chen*[1,2], *Alessandro Gallo*[1,2], *Thomas Jaramillo*[1,2], *and Frank Abild-Pedersen*[1,2]
(1)Department of Chemical Engineering, Stanford University, Stanford, CA, (2)SUNCAT Center for Interface Science and Catalysis, SLAC National Accelerator Laboratory, Menlo Park, CA

We utilize Density Functional Theory (DFT) calculations for atomistic models of supported and inverted Cu-ZrO_2 systems. We evaluate reaction pathways and energetics for energetically favorable configurations in both systems. Through this, we finally elucidate the role of supported and inverted catalyst systems in assisting selective CO_2 hydrogenation to methanol.

Integrated CO_2 Capture and Utilization over Cu-K_2CO_3/MgO Dual Functional Catalyst.

Saiyed Tasnim Md Fahim[1], *Bruno Henrique Arpini*[2], *and Kandis Leslie Gilliard-Abdulaziz*[3]
(1)Sonny Astani Department of Civil and Environmental Engineering, University of Southern California, Los Angeles, CA, (2)Chemical Engineering, University of Southern California, Los

Angeles, CA, (3)Sonny Astani Civil and Environmental Engineering Department, University of Southern California, Los Angeles, CA

This work showed the preparation and application of a dual functional Cu-K_2CO_3/MgO catalyst for CO_2 capture and selective conversion to CO, an important step towards methanol synthesis.

设计CO2加氢制备C2 +烃和含氧化合物的反应路径和产物效率.

Hongfei Lin[1]*, Caiqi Wang*[1]*, Wei Wang*[1]*, Bowen Li*[2]*, and Norbert Kruse*[1]
(1)The Gene and Linda Voiland School of Chemical Engineering and Bioengineering, Washington State University, Pullman, WA, (2)Department of Chemical Engineering, Northeastern University, Boston, MA

This study investigates CO2 hydrogenation to C2+ hydrocarbons and oxygenates using CoM-based catalysts (M = Cu, Mn, Fe) with a potassium promoter. It highlights the synergistic effect of CO_2 activation and C-C coupling in product selectivity. In situ DRIFTS shows that formate intermediates enhance C-C coupling for selective product formation.

Catalytic Functionalities of Ni-Based Catalysts for CO_2 hydrogenation By Hydrogen Transfer from Isopropanol.

Julieth García Sánchez[1]*, Josefine Schnee*[2]*, Alejandro Karelovic*[3]*, Luz Marina Ballesteros Rueda*[4]*, Daviel Gómez*[5]*, Patricia Concepción*[5]*, and* ***Victor Gabriel Baldovino Medrano***[6]
(1)Chemical Engineering, Centro de Investigaciones en Catálisis, Universidad Industrial de Santander, Bucaramanga, Santander, Colombia, (2)Sorbonne Université, Paris, France, (3)Chemical Engineering, Universidad de Concepción, (4)Universidad Industrial de Santander, Bucaramanga, Colombia, (5)Instituto de Tecnología Química, Valencia, Spain, (6)Chemical Engineering, Centro de Investigaciones en Catálisis (CICAT), Universidad Industrial de Santander, Bucaramanga, Santander, Colombia

From a thermodynamic point of view, the hydrogenation of CO_2 by hydrogen transfer from isopropanol would be possible and the ability to carry out these reactions depends on catalytic functionalities such as acid-base properties and Ni loading; but it is limited by the competition between reactants on the catalyst surface.

Pathway of CO_2 Conversion over a Ru-K_2CO_3/CNF Dual Functional Material for Direct Air Capture.

Freek Karaçoban*, Tomas Haasterecht, van, and Johannes Hendrik Bitter*
Wageningen University, Wageningen, Netherlands

In Ru/K_2CO_3 on carbon, a dual functional material for CO_2 capture (from air) and conversion special sites are present which can retain captured CO_2 until a temperature relevant for the methanation is reached.

Novel Thermal Catalytic CO_2 Conversion without External Hydrogen: A Tandem Process for Methane, Bio-Lubricant, and Hydrogen Production Via Methyl Palmitate Ketonization.

Piyasan Praserthdam[1] *and Supareak Praserthdam*[2]
(1)Chemical Engineering, Chulalongkorn University, Bangkok, -, Thailand, (2)Chemical Engineering, Chulalongkorn University, Bangkok, Thailand

This study introduced a tandem thermal approach to converting CO_2 into methane without external hydrogen and methyl palmitate ketonization. TiO_x catalysts with varying oxygen vacancy levels were investigated. Co-feeding CO_2 improves not only methane production but also hydrogen production.

One-Step CO_2 Hydrogenation to Hydrocarbons on K Promoted Fe Catalyst on an Alginate-Based Carbon Support..

Pio Gramazio[1]*, Jia Yang*[1,2]*, Mei Ju Goemans*[1]*, Joakim Tafjord*[1]*, Rune Myrstad*[3]*, Erling Rytter*[1]*, Magne Hillestad*[1]*, and Edd Blekkan*[1]
(1)Department of Chemical Engineering, Norwegian University of Science and Technology, Trondheim, Norway, (2)College of Smart Energy, Shanghai Jiao Tong University, Shangai, China, (3)SINTEF Industry, Kinetics and Catalysis Research Group, Trondheim, Norway

This work provides an interesting way of valorizing CO_2 streams into high added-value liquid fuels. An innovative synthesis, based on alginate, was employed to produce K, Fe carbon-supported catalysts. The catalyst was able to hydrogenate CO_2, with a conversion up to 40%, and a selectivity towards Fischer-Tropsch products of 80%.

Dynamic Reconstruction Behavior of Complex Oxides in Dry Reforming of Methane: In Situ Generation of Stable Nicu Alloy Active Sites.

Junyan Zhang[1]*, Meijia Li*[1]*, Yuanyuan Li*[1]*, Kevin Siniard*[2]*, Alexander Ivanov*[1]*, Harry M. Meyer III*[1]*, Shize Yang*[3]*, Zili Wu*[1]*, Zhenzhen Yang*[1]*,* ***Felipe Polo-Garzon***[1]*, and Sheng Dai*[1]
(1)Chemical Sciences Division, Oak Ridge National Laboratory (ORNL), Oak Ridge, TN, (2)Chemistry, University of Tennessee, Knoxville, TN, (3)Yale University, New Haven, CT

Dry reforming of methane operates at high reaction temperatures, leading to catalyst deactivation. Tightly anchored Ni-Cu bimetallic nanoparticles were in situ exsoluted from a solid oxide solution ($NiMgCuZnO_x$) to catalyze DRM and repel coke.

High Performance M (Ga, Ce, Mn, Mg, La)-Promoted Cu-ZnO-ZrO_2 Catalysts for CO/CO_2 Hydrogenation to CH_3OH.

Shihang Meng[1]*,* ***Yujing Weng***[1]*, Qi Sun*[1]*, and* ***Yulong Zhang***[2]
(1)Chemical Engineering, Henan Polytechnical University, Jiaozuo, China, (2)Chemical Engineering, Henan Polytechnical University, Jiaozuo, Henan, China

The Ga promoted $CuZnOZrO_2$ catalyst were prepared by coprecipitation with Na_2CO_3. CO/CO2 co-hydrogenation to methanol were carried out to study the catalyst performance CO and CO2 conversion collectively. The Ga promoted CZZ catalyst showed notable enhancement of CO_2 adsorption and exhibited excellent performance for CO/CO_2 co-conversion with high methanol yield.

Deciphering Transition-Metal B-Site Reactivity, Selectivity, and Stability for Oxidative C_1 Hydrocarbon Upgrading on Perovskite Oxides.

Rachel A. Yang *and Eranda Nikolla*
Department of Chemical Engineering, University of Michigan, Ann Arbor, MI

Perovskite oxides with systematically varied transition metal cation identities demonstrate distinct reactivities, C_2 selectivities, and stabilities for the oxidative coupling of methane. Reaction pathways are a function of intrinsic metal properties and cation compositions that can be tuned and leveraged for more atom-efficient C_1 conversion to chemicals and fuels.

Unraveling the Silver-Catalyzed Methanol to Formaldehyde Reaction: Understanding the Sub-Reactions, Kinetics and Restructuring.

Tina Bergh[1]*, Youri van Valen*[1]*, Ole Håvik Bjørkedal*[2]*, Ann Kristin Lagmannsveen*[3]*, and Hilde Johnsen Venvik*[1]
(1)Department of Chemical Engineering, Norwegian University of Science and Technology (NTNU), Trondheim, Norway, (2)Dynea AS, Lillestrøm, Norway, (3)K.A. Rasmussen, Hamar, Norway

We study the silver-catalyzed methanol to formaldehyde (MTF) reaction and its sub-reactions. The reaction data obtained from our annular reactor setup using a cylindrical silver catalyst provides mechanistic insights relevant to industrial conditions, while thorough nanoscale characterization (SEM, FIB, 4D-STEM) highlights the effects of various reactants on catalyst restructuring.

Light Alkane Conversion through Ammonia Assisted Reforming and Dehydrogenation.

Yizhi Xiang
Department of Chemical and Biomedical Engineering, University of Missouri Columbia, Columbia, MO

We proposed to convert light alkane through ammonia assisted reforming and dehydrogenation, for energy and chemical production. From a fundamental point of view, we will discuss the catalytic active sites and mechanism of these new catalytic reactions based on extensive catalyst characterization and kinetic analyses.

Mechanochemical Synthesis of Multicomponent Bismuth-Based Molybdate Catalysts for Propylene Ammoxidation to Produce Acrylonitrile.

ChangJin Han *and Do Heui Kim*
Seoul National University, Seoul, Korea, Republic of (South)

The bismuth molybdenum-based multi-metal oxide catalysts were mechanochemically synthesized using the ball milling method without the use of nitric acid and exhibited excellent performance in propylene ammoxidation. The physicochemical properties and catalytic activities of the iron or cobalt phase added to the bismuth molybdenum phase were investigated.

Catalytic Activity of MoO_x@SiO_2 Yolk-Shell Structures in Propane Dehydrogenation and Subsequent Propylene Metathesis.

Anna Rokicinska[1], Mariya Myradova[2], Mateusz Mandrela[1], Dominika Waśniowska[1], Marek Debosz[1], Piotr Michorczyk[2], and ***Piotr Kustrowski***[1]
(1)Faculty of Chemistry, Jagiellonian University, Krakow, Poland, (2)Department of Organic Chemistry and Technology, Cracow University of Technology, Krakow, Poland

MoO_x@SiO_2 nanoreactors with a yolk-shell structure were developed for efficient propane dehydrogenation combined with subsequent metathesis of produced propylene. The key role in achieving high activity in both industrially important processes was played by controlled dispersion of the active phase within the composite.

High-Yield Ethanol to Acetone Reaction Using Induction Heating.

Ryan Thompson[1], *Ben Ko[1], Han Wang[1], Carlos L. Pueyo[2], Jianping Chen[3], Roel Sanchez-Carrera[4], and Erdem Sasmaz[1]*
(1)Chemical and Biomolecular Engineering, University of California, Irvine, Irvine, CA, (2)BASF, Ludwigshafen am Rhein, Germany, (3)BASF, Beachwood, OH, (4)BASF, Iselin, NY

Induction heating has been shown to be an effective method for electrifying heating. The production of acetone from ethanol using Fe_2O_3-ZnO was studied in a packed-bed reactor with steel receptors. Improvements in temperature gradients in the catalyst bed were shown. Magnetic effects were also hypothesized and analyzed in adsorbed intermediates.

Unifying Dehydrogenation and Coupling of Isoalkane Feedstocks to SAF-Range Precursors in a Single Reactor..

Alexander J. Hill[1], *Anh To[2], Claire Nimlos[2], Susan E. Habas[2], and Daniel Ruddy[2]*
(1)National Renewable Energy Laboratory, Golden, CO, (2)Catalytic Carbon Transformation and Scale-Up Center, National Renewable Energy Laboratory, Golden, CO

This work explores mixed beds of dehydrogenation and olefin coupling catalysts to conduct dehydrogenative coupling of isoalkanes to SAF-range olefins in a single reactor. Tuning acid properties of the olefin coupling catalysts catalysts improves compatibility with dehydrogenation conditions. Combining these two reactions enables equilibrium conversion of isoalkanes to be surpassed.

Conversion of Ethanol to 1,3-Butadiene over Supported Cobalt Catalyst with Induction Heating.

John Pham[1], *Han Wang*[1], *Ben Ko*[1], *Carlos L. Pueyo*[2], *Jianping Chen*[3], *Roel Sanchez-Carrera*[4], *and Erdem Sasmaz*[1]
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Induction heating, showing great potential in decarbonization efforts, is utilized to investigate the promising enhancement of the selectivity of the (bio)ethanol-to-1,3-butadiene reaction over a bifunctional $Co/ZrO_2/SiO_2$ catalyst. The results suggest that the magnetic field and SiO_2 (SBA-16)-ZrO_2 interactions contribute to the catalyst activity improvement.

DFT and Microkinetic Study of the Mechanism of Propene Metathesis on MoO_x/SiO_2 and $MoO_x/(AlO_y\text{-}SiO_2)$ Catalysts.

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Density functional theory study of the mechanisms of propene metathesis on activated MoO_4/SiO_2 and $MoO_4/AlO_4/SiO_2$ showed that transition and intermediate states are significantly stabilized for $MoO_4/AlO_4/SiO_2$ compared to MoO_4/SiO_2 indicating higher activity. This work will address key atomic-scale details of how catalyst structure influences catalytic activity on supported MoO_x/SiO_2 catalysts.

Iso-Butanol Production from Methanol/Ethanol Mixtures Via the Guerbet Reaction Using Hydrotalcite Ni/Cu-Al Catalysts.

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In this study, a sustainable method of producing iso-butanol was introduced via Guerbet using Ni/Cu-Al catalyst. The mixture of methanol/ethanol was mainly converted into iso-butanol. 5 wt% of 10Ni/2Cu-Al showed the best performance with 124 mmol/L of iso-butanol and 7.7 % of ethanol conversion at 185 °C, and 4h.

Single Nickel Site Catalyst on Mesoporous Silica for Light Olefin Oligomerization.

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Nickel-substituted polyoxometalates on mesoporous silica exhibit excellent stability and promising performance in light olefin oligomerization. Our work offers valuable mechanistic insights into the impact of pore size on catalyst deactivation, which can be applied to other porous materials. Rates and selectivity for pure and mixed feeds are also showcased.

Active and Selective Nature of Cezn and Cucezn for the Oxidative Dehydrogenation of Propane with Carbon Dioxide.

*Cedric Karel Fonzeu Monguen[1,2], Samuel Daniel[2,3], Hannington Nevin Otieno[2,3], **Patrick Lott**[1], Olaf Deutschmann[1], and Zhen-Yu Tian[2,3]*
(1)Institute for Chemical Technology and Polymer Chemistry, Karlsruhe Institute of Technology, Karlsruhe, Germany, (2)Institute of Engineering Thermophysics, Chinese Academy of Sciences, Beijing, China, (3)University of Chinese Academy of Sciences, Beijing, China

The CeZn binary oxide catalyst exhibited attractive performance for CO_2-ODHP. Loading Cu into the (Ce/Zn) structure was found to promote propane conversion and propene yield with CO_2. Thus, the novel catalyst exhibits high potential for application in the petrochemical industry.

Ethane Dehydrogenation with CO_2 Using LDH-Derived Mixed Oxides of V, Mn, and Ga.

***Gabriel Liscia Catuzo**, Rosembergue G. L. Gonçalves, and Elisabete Assaf*
Instituto de Química de São Carlos/Universidade de São Paulo, São Carlos, Brazil

Layered double hydroxide-derived catalysts doped with V, Mn, and Ga were evaluated for ethane dehydrogenation with CO_2. The MgZnGa catalyst showed the highest ethylene yield of 479 μmol $min^{-1}.g^{-1}$ even after 5 h of reaction, owing to its resistance to deactivation and the retention of active sites.

Copper-Based Catalysts for DME Steam Reforming: Investigating Reaction Mechanisms for Hydrogen Production.

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(1)Chemistry Division, Los Alamos National Laboratory, Los Alamos, NM, (2)Los Alamos National Laboratory, Los Alamos, NM, (3)Illinois State University, Normal, IL

We synthesized copper-based catalysts with a CeO_2 core and zeolite shell for DME steam reforming. The catalysts exhibit different reaction mechanisms depending on copper loading, with formate and methyl formate intermediates observed. DFT calculations confirm the feasibility of these pathways, offering insights for enhancing hydrogen production in the hydrogen economy.

Catalytic Pyrolysis of Plastic Waste for the Synthesis of Hydrogen and Nanocarbons.

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The alarming rise in plastic waste necessitates innovative solutions. Thermo-catalytic conversion transforms plastics into hydrogen and CNTs, addressing pollution and energy needs. Conventional Fe/Al2O3 and Ni/Al2O3 and novel flyash acts as catalyst. This sustainable approach supports clean energy production and a circular economy, reducing environmental impact.

Ammonia Production from the Catalytic Decomposition of Hydroxylammonium Nitrate As Green Energetic Source for Clean Space.

Rachid Amrousse
University of Chouaib Doukkali, Faculty of Sciences, El Jadida, Morocco

This study explores ammonia (NH3) production via the thermal decomposition of hydroxylammonium nitrate (HAN), a green propellant, using an iridium-based catalyst. The research combines experimental and theoretical methods to confirm NH3 generation, suggesting HAN as a sustainable energy source for space propulsion systems.

Defect-Induced Nanocrystalline Colored Titania - Inspiring Next Generation Photocatalyst: Application in Cellulose Reforming for Hydrogen Production.

Parasuraman Selvam
Department of Chemistry & NCCR, IIT-Madras, CHENNAI, India

Defect-induced colored titania photocatalysts were evaluated for photoreforming of cellulose which gave remarkable activity as compared to the white TiO_2. Importantly, the CO_2 evolution was much lower for the colored samples than that of the corresponding white titania which suggests the importance of intrinsic defects for the photocatalytic reaction.

Multifunctional Graphene-Nickel Single-Atom Catalyst for AEM Water Electrolysis and UV/Chlorine Treatment.

Lee Jihoon*, Yang Eunju, and Yoon Yeojoon*
Department of environmental and energy engineering, Yonsei university, Wonji-si, Gangwon-do, Korea, Republic of (South)

We developed a low-cost graphene-nickel single-atom catalyst for AEM water electrolysis using an impregnation method. The catalyst's effectiveness was demonstrated in both AEM water electrolysis and a UV/chlorine reactor for water treatment. This integrated approach demonstrates the catalyst's multifunctional potential in hydrogen production and water treatment applications.

Mechanistic Understanding of Iron-Aluminum Composites in Methane Cracking for Turquoise Hydrogen and Fibrous Carbon Production.

Shih-Yuan Chen
Department of Energy and Environment, National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Ibaraki, Japan, Japan

From an industrial perspective, CH_4 conversion over FeAl mixed oxides was studied and modeled to predict Fe-based catalyst performance for turquoise hydrogen and valuable carbon production. A strategy to improve catalyst longevity was proposed, enhancing the commercial feasibility of CH_4 cracking and increasing the industrial value of nanostructured carbon materials.

Development of Nickel Catalysts with Core-Shell Structure for Ethanol Steam Reforming.

Andrelaine de Souza Bernardes[1]*, Leticia Forrer Sosa*[2]*, and Pedro Romano*[3]
(1)Chemistry School, Federal University of Rio de Janeiro (UFRJ), Rio de Janeiro, Brazil, (2)Universidade Federal do Rio de Janeiro, Rio de Janeiro, Brazil, (3)Campus D. de Caxias, Federal University of Rio de Janeiro, Rio de Janeiro, Brazil

This study focuses on synthesizing and evaluating nickel-based core-shell catalysts (Ni-SiO_2@CeO_2) for steam ethanol reforming to produce hydrogen. Cerium oxide (CeO_2) is employed as a shell to enhance stability, prevent coke deposition, and reduce nickel deactivation, promoting an economically viable and sustainable hydrogen production process from renewable ethanol sources.

A First-Principles Based Microkinetic Investigation of the Dehydrogenation of C_7H_{14} to C_7H_8 on Pt(111).

Alvaro Posada-Borbon[1]*, Tobias Möslinger*[2]*, and Henrik Grönbeck*[1]
(1)Department of Physics and Competence Centre for Catalysis, Chalmers University of Technology, Göteborg, Sweden, (2)Department of Physics, Chalmers University of Technology, Göteborg, Sweden

We interrogate the dehydrogenation of methylcyclohexane (MCH) to toluene and a competing demethylation to benzene on Pt(111) through DFT calculations and microkinetic modelling. Kinetic analysis shows the dehydrogenation reaction is controlled by the adsorption/desorption of MCH and toluene. The work provides handles for the rational design of LOHC dehydrogenation catalysts.

Niobia Supported Cu-Zn Catalysts for Sour Water Gas Shift Reaction.

Ludmila P. C. Silva[1]*, Ana Carla Coutinho*[1]*, Luis E Terra*[1]*, and* ***Fabio B. Passos***[2]
(1)Department of Chemical and Petroleum Engineering, Fluminense Federal University, Niteroi, Brazil, (2)Department of Chemical and Petroleum Engineering, Universidade Federal Fluminense, Niteroi, Brazil

Sulfur compounds poison typical water-gas shift reaction (WGSR) catalysts required to increase H_2 production. Here we present an investigation on the use of niobia as support for CuZn catalysts, addressing how active sites interact with sulfur poison and WGSR reactants.

Hydrogen Production from Water on Molybdenum Carbide: A Mechanistic Study.

Milad Ahmadi Khoshooei
Northwestern University, Evanston, IL

This work focused on elaborating mechanisms of activating water in the presence of a carbonaceous source for hydrogen production over a molybdenum carbide catalyst. Isotopic labeling, spectroscopic analysis, and kinetic experiments revealed that the catalyst is prone to oxidation in the presence of water.

Improving Quality and Increasing Throughput in Catalyst Manufacturing Unit Operations.

Benjamin Glasser *and William Borghard*
Chemical and Biochemical Engineering, Rutgers University, Piscataway, NJ

By combining our expertise in particle technology and optimization we are developing and promoting science-based methods for designing, scaling up and optimizing catalyst manufacturing processes. A combination of experiments and computer models has been used to improve the understanding and performance of unit operations used to make catalysts.

Highly Dispersed Bimetallic Catalysts for Semi Hydrogenation of Acetylene with Galvanic Displacement.

An Zhang *and Weijian Diao*
Chemical Engineering, Villanova University, Villanova, PA

This study offers a general synthesis strategy for Pd-Cu bimetallic system with controlled surface composition and structure. It has the potential to be applied to other bimetallic catalysts with suitable metal precursors and reaction conditions. GD is a promising method for immobilizing secondary active components onto the supported metallic catalysts.

Synthesis of MFI Zeolites with Small Crystallite Sizes to Generate Stable Product Selectivity from Alkene Oligomerization.

Sanghyun Ahn*, Elizabeth Bickel Rogers, Songhyun Lee, Evan E. Sowinski, and Rajamani Gounder*
Charles D. Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN

Synthesis recipes were developed to prepare small crystallite-size (<50 nm) MFI zeolites that meet commercial manufacturing targets to enable future catalyst scale-up efforts, and evaluated

against conventionally prepared larger-crystallite zeolites, to demonstrate improved olefin oligomerization rate and product stability with time-on-stream.

Aqueous-Based Granulation Method Towards Clean Energy Applications.

Divakar Reddy Aireddy[1], *Christopher Marin*[2], *Biswanath Dutta*[3], *Eric Popczun*[2], *Christina Wildfire*[4], *and Douglas Kauffman*[2]
(1)Reaction Engineering Team, National Energy Technology Laboratory (/Leidos), Morgantown, WV, (2)National Energy Technology Laboratory, Pittsburgh, PA, (3)NETL Support Contractor, Morgantown, WV, (4)National Energy Technology Laboratory, Morgantown, WV

An aqueous-based granulation method is developed to combat the structural changes associated with binder-based granulation techniques. Microwave-assisted methane reforming studies showed an improved catalyst efficiency for these aqueous-based granules compared to the powder catalysts. This granulation method has been extended to other practical applications (chemical looping gasification and air separations).

Evaluation of Fumed and Precipitated Silica Extrudates: Balancing Surface Area, Crush Strength, and Pore Volume.

Chris Bauer
Smart Effects, Evonik Corporation, Piscataway, NJ

This study evaluates fumed and precipitated silica extrudates, highlighting their impact on catalyst support properties. By optimizing formulations and processing conditions, the research aims to achieve high mechanical strength, surface area, and porosity, offering potential improvements in industrial catalyst applications.

The Growth of Titanium-doped Ceria Thin Films by Pulsed Laser Deposition for CO_2 Splitting with H_2O.

Rosa Virginia Melinda[1], *David King*[2], *Nishan Paudyal*[1], *Jinke Tang*[2], *and Jing Zhou*[1]
(1)Chemistry, University of Wyoming, Laramie, WY, (2)Physics and Astronomy, University of Wyoming, Laramie, WY

This study utilized pulsed laser deposition method coupled with glancing angle deposition technique to synthesize titanium-doped ceria thin films with controlled nanostructures, morphologies, and compositions. This allows for a fundamental investigation of the interaction with CO_2 and H_2O for thermochemical cycles of CO_2 conversion to chemicals and fuels.

Catalytic Consequences of Catalyst Pellet Architecture on the Direct Production of Dimethoxymethane from Methanol..

Sebastian Cook[1], ***William Broomhead***[2], *Adam Johnston*[3], *Ya-Huei (Cathy) Chin*[1], *and Jose Herrera*[3]

(1)Department of Chemical Engineering and Applied Chemistry, University of Toronto, Toronto, ON, Canada, (2)Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA, (3)Department of Chemical and Biochemical Engineering, Western University, London, ON, Canada

The considerations required to scale up a lab-scale catalyst formulation to industrial-scale pellets requires are presented. Active phase dispersion and distribution need to be carefully controlled to minimize temperature gradients and optimize catalyst performance.

Design and Assessment of Pt-Fe/SiO2 Catalysts for Stoichiometric Methane Combustion: Does Fe Really Contribute?.

Carol Bibiana Espinosa Lobo[1], Julieth García Sánchez[1], Edwing Velasco Rozo[2], and ***Victor Gabriel Baldovino Medrano***[3,4]
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We probed Pt-Fe phases in the stoichiometric combustion of methane doing as follows: (1) synthesizing Pt-Fe/SiO_2 catalysts of uniform particle sizes; (2) testing without transport artifacts. Thus, iron and platinum establish a synergistic and constant effect only around 390°C. Otherwise, iron has a null role in these catalysts.

Improved Catalytic NO Oxidation over Pt Supported on Sulfuric Acid Treated TiO_2.

Wo Bin Bae[1]*, Jiseok Park[2], Sung Bong Kang[3], and Jun Hee Jang[1]*
(1)Department of Chemical Engineering, Rowan University, Glassboro, NJ, (2)School of Environment and Energy Engineering, Gwangju Institute of Science and Technology, Gwangju, Korea, Republic of (South), (3)Department of Environment and Energy Engineering, Gwangju Institute of Science and Technology, Gwangju, Korea, Republic of (South)

In this study, we demonstrate that the increase of acidic sites on the TiO_2 surface during the catalyst synthesis promotes the dispersion and formation of the metallic phase of Pt with the beneficial effects of sulfur species introduced on the surface of catalyst supports.

Opportunities and Challenges of Thin-Film Technology for Thermocatalytic Applications.

Daniel Amkreutz
PVcomB, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany

The application of thin-film technology in thermocatalysis is mostly applied for model systems today. However, it was demonstrated that for specific reactions, thin film catalysts can

outperform power catalysts. We present an overview on the concept of thin-film catalysis with a focus on deposition, characterisation and potential.

Effect of Binder Selection in Cu-Zn-Y/Beta Extruded Catalysts for Ethanol Upgrading to Olefins.

Hunter Jacobs[1]*, Stephen Purdy*[1]*, Meijun Li*[1]*, Shivangi Nandkumar Borate*[2]*, James W. Harris*[2]*, and Andrew D. Sutton*[1]
(1)Manufacturing Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN, (2)Department of Chemical and Biological Engineering, The University of Alabama, Tuscaloosa, AL

Metal-loaded dealuminated beta zeolites have previously been identified as promising catalysts in direct ethanol upgrading to olefins. In order for these materials to be viable for scale-up efforts, extruded forms must be also developed. This work shows that extrudate binder selection can have drastic effects on catalyst structure and performance.

Dual-Templated Syntheses, Characterization, and Application of MFI/Ton-Type Zeolite Intergrowth.

Soonhyoung Kwon *and Rajamani Gounder*
Charles D. Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN

An MFI/TON intergrown zeolite was synthesized via a dual co-templating approach, combining MFI's three-dimensional channels with TON's one-dimensional channels. Characterization confirmed the intergrowth, and catalytic testing showed high p-xylene selectivity similar to TON, indicating the zeolite retains TON-like selectivity within a single crystalline material.

Harnessing Drying Dynamics to Control Nanoparticle Size in Silica Supported Pt Catalysts.

Ismail Paykar[1]*, Simon Friedrich*[2]*, Chigozie Ezeorah*[3]*, Frank Gupton*[4]*, John Regalbuto*[5]*, and Christopher Williams*[5]
(1)Chemical Engineering Department, University of South Carolina, Columbia, SC, (2)Virginia Commonwealth University, Richmond, VA, (3)Chemistry and Biochemistry, University of South Carolina, Columbia, SC, (4)Chemical and Life Science Engineering, Virginia Commonwealth University, Richmond, VA, (5)Chemical Engineering, University of South Carolina, Columbia, SC

Drying dynamics control nanoparticle size and active sites in silica-supported Pt catalysts. Balancing convective flow and molecular back-diffusion during drying reduces particle size from 11.2 nm to 2.8 nm, significantly enhancing the active surface area. These findings integrate crystallization and transport principles to optimize catalyst synthesis and performance.

Synthesis of Supported Metal Nanoparticles Using a Surface Support As a Reducing Agent: Characterization and Catalytic Performance in HMF Electrooxidation to Fdca.

Nataliya Shcherban[1,2]*, Moritz Krebs*[2]*, Ivan Kopa*[1]*, Eko Budiyanto*[2]*, Dmitry Murzin*[3]*, and Ferdi Schüth*[2]
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Application of the support (g-C_3N_4) surface as a reducing agent resulted in the formation of smaller and more uniform metal nanoparticles in comparison with a traditional reduction of metal precursors with hydrazine. Supported metal nanoparticles demonstrated higher catalytic performance in the electrochemical oxidation of HMF.

Controlling Metal Nanoparticle Size on Carbon Supports with Surface Tension.

Nathan Thornburg and ***John Regalbuto***
Chemical Engineering, University of South Carolina, Columbia, SC

By oxidizing carbon supports, the surface hydrophilicity increases with a decrease in the point of zero charge. With powder X-ray diffraction and scanning transmission electron microscopy (STEM), there is a scientifically significant effect on nanoparticle size and the percentage of atomic isolation from increased support hydrophilicity.

Synthesis Strategies for Porous High-Entropy Oxides and Their Activity in Thermocatalytic CO2 Hydrogenation.

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(1)Empa, Duebendorf, Switzerland, (2)AGH University of Science and Technology, Krakow, Poland

As the field of high-entropy oxides (HEOs) is expanding into applications like catalysis, synthesis strategies control physical properties are needed Here we utilize different synthesis strategies (hydrothermal, precipitation, and solvothermal) to produce porous high-entropy precursors. Selected calcined HEOs were then tested for activity in the thermocatalytic CO2 hydrogenation reaction.

The Importance of Full Reduction and the Choice of Precursor on the Site Distribution of Rh on TiO_2 and Activity for CO Oxidation.

Vishwas Reddy Akavaram[1]*, Zhanyuan Liu*[2]*, Dionisios Vlachos*[3]*, John Vohs*[4]*, and Ayman M. Karim*[5]
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Engineering, University of Pennsylvania, Philadelphia, PA, (5)Department of Chemical Engineering, Virginia Polytechnic Institute and State University, Blacksburg, VA

This study identifies optimal pretreatment conditions for complete Rh reduction and precursors favoring single atoms, enabling investigation of CO oxidation kinetics on single atoms, nanoparticles, and their mixtures. It also examines how precursor environments influence the size and uniformity of Rh species on Rh/TiO_2.

Nenu-5 a New Route to Prepare Mo_2c with High Specific Surface Area for Use in Catalysis.

Adrian Ortega[1], Mario Caccia[2], and ***Javier Narciso***[1]
(1)University of Alicante, Alicante, Spain, (2)Alfred University, Alfred, Spain

In this work, a new synthetic route of Mo_2C from MOF is presented, where Mo_2C has been obtained with catalytic activity superior to Pt, even an order of magnitude higher than conventional carbide. The hydrogenation reaction of nitroarenes is presented as an example.

Enhancing Hydrothermal Stability of Alumina-Based Carrier and Its Characterization.

Xueqin Wang[1]*, Jing Su[2], Seth Riehemann[1], and Yeping Cai*[1]
(1)R&D Center-Louisville, Clariant Co., Louisville, KY, (2)R&D Center-Shanghai, Clariant Co., Shanghai, China

Catalysts made over alumina-based carriers are widely used for water-forming reactions or reactions containing water feed. Alumina phase transition to Boehmite at steam environment is hydrodynamically favored. Promoters prevent water attack. SEM is a good tool to identify Boehmite precursor formed on the alumina surface.

Hybrid Kinetic Modeling for Dynamic Catalytic Systems.

Kenneth Kusima[1] *and Lars Grabow*[2,3]
(1)William A. Brookshire Department of Chemical and Biomolecular Engineering, University of Houston, Houston, TX, (2)Center for Programmable Energy Catalysis (CPEC), Minneapolis, MN, (3)William A. Brookshire Department of Chemical and Biomolecular Engineering & Texas Center for Superconductivity (TcSUH), University of Houston, Houston, TX

Traditional kinetic models such as microkinetic and lumped/global models face limitations in dynamic conditions. Kinetic Monte Carlo simulations may overcome some limitations but are computationally intensive. Hybrid kinetic models, integrating machine learning and mechanistic methods, enhance adaptability, accuracy, and robustness for applications in dynamic or programmable catalysis.

Enhanced CO_2 Hydrogenation to Methane: The Role of Feed Modulation and Electric Field.

Debasish Sarkar, Rajagopalan V. Ranganathan, Jeremy Hartvigsen, ***Debtanu Maiti****, and*

Rebecca Fushimi
Catalysis and Transient Kinetics Group, Idaho National Laboratory, Idaho Falls, ID

The synergistic role of feed modulation and electric field effects has been explored towards enhanced CO_2 hydrogenation to methane on Ru/CeO_2 catalysts. The improvement of reaction performance is attributed to a combination of accelerated surface protonics, and dynamic distribution of surface coverages, leading to changes in reaction pathways.

Coverage Effects for Dynamic Modulation of Formic Acid Oxidation.

Atharva Burte *and Omar Abdelrahman*
William A. Brookshire Department of Chemical and Biomolecular Engineering, University of Houston, Houston, TX

Comprehending the pseudo-steady state coverages or rather the time-averaged coverages under oscillatory conditions deeply enhances the scope of understanding the fundamentals of dynamic catalysis. Researchers would better tune and modulate catalytic turnovers beyond formic acid oxidation with this deeper understanding.

Investigating Dynamic Redox Properties of Bismuth Molybdates in Selective Propylene Oxidation.

Tanmayi Bathena[1]*, Kenneth Kusima*[2]*, Bhuvaneswari M Shivakumaran*[3]*, Venkateshkumar Prabhakaran*[3]*, Shutthanandan Vaithiyalingam*[3]*, Konstantinos Goulas*[4]*, Ajay S. Karakoti*[3]*, and Lars Grabow*[2]
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This study examines catalytic effects of crystal restructuring in bismuth molybdates during propylene oxidation to acrolein. The dynamic redox properties of supported vs unsupported samples show irreversible repositioning of active sites and active phases that effect the overall activity

Exploring Adsorbate-Induced Dynamic Structuring and Transport Properties of Supported Liquid Metal Catalysts Using DFT & Reaxff.

Gunnar Sly[1]*, Kathryn MacIntosh*[1]*, Adri van Duin*[2]*, Robert Rioux*[3]*, and Michael Janik*[4]
(1)Chemical and Biomedical Engineering, The Pennsylvania State University, University Park, PA, (2)Mechanical Engineering, The Pennsylvania State University, University Park, PA, (3)Department of Chemical Engineering, The Pennsylvania State University, University Park, PA, (4)Chemical Engineering, The Pennsylvania State University, University Park, PA

The structures of PdGa low-melting temperature alloys used in catalytic propane dehydrogenation are explored with a combination of DFT and ReaxFF. Surface interactions with

H and C_x intermediates are examined through adsorption isotherms, induced Pd surface segregation, and reactive simulations in experimentally relevant gaseous environments.

A Bulk Phase Transformation Drives Ammonia Synthesis on Barium Hydride.

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(1)Atomistic Simulations, Italian Institute of Technology, Genova, Italy, (2)Department of Materials Science, University of Milano-Bicocca, Milan, Italy, (3)Italian Institute of Technology, Genova, Italy

A successful heterogeneous catalyst relies on dynamic behavior under operating conditions. Machine learning simulations confirm this for BaH_2 in ammonia synthesis via chemical looping. BaH_2 transforms into a superionic compound under N_2, enabling high ionic mobility and efficient ammonia formation after H_2 exposure, showcasing its dynamic catalytic nature.

Unveiling the Dynamics of Cu/ZIF-8 Catalysts during CO_2 Hydrogenation Using Forced Dynamic (Operando) Conditions.

Pia Dally[1] *and Pedro Castano*[2]
(1)Imaging and Characterization Core Lab, KAUST, Thuwal, -, Saudi Arabia, (2)King Abdullah University of Science and Technology (KAUST), Thuwal, Saudi Arabia

Our ongoing research develops an advanced workflow using forced dynamic operando reactors and high-pressure pulsing, combined with in-situ and operando techniques. This approach aims to thoroughly analyze the dynamic behavior of Cu/ZIF-8 during CO_2 hydrogenation, offering insights beyond those possible with kinetic modeling alone

Investigating the Effect of a Back-Gate on the Filling of Trap Density of States in Ultrathin TiO_2 Films.

Shreya Singh *and C. Daniel Frisbie*
Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN

We discuss a back-gated electrode structure with TiO_2 simultaneously acting as the semiconductor in the metal-insulator-semiconductor stack and as the working electrode in the electrochemical cell. We perform chronoamperometry measurements to show that back-gate potential affects filling of trap states in the TiO_2 film, independent of the working electrode potential.

Generalizing Reactive Surfaces of Ir Complex Metal Oxide Catalysts for the Oxygen Evolution Reaction in Acidic Electrolytes.

Harrison Lippie *and Joaquin Resasco*
McKetta Department of Chemical Engineering, The University of Texas at Austin, Austin, TX

Ir-based double perovskites for the OER in acidic media converge to similar surface activities and structures at steady-state. Non-Ir elements leach, forming a disordered IrO_x surface with higher specific area and activity than rutile IrO_2. Differences in short-term activity relate to stability, but long-term performance equalizes across perovskites.

Thermodynamic Insights of CO_2 Reduction in Solid Oxide Electrolysis Cells with Sulfur Containing Feed Flows.

Johari Dramiga
Lehigh University, Bethlehem, PA

Understanding the kinetic consequences of S poisoning on SOEC cathode electrocatalysts to improve efficiency and mitigate contaminate induced degradation. Competitive adsorption between CO_2 and SO_2 coupled with thermodynamics of respective dissociation reactions, can result in surface converge effects which reduce catalytic performance.

Visible Light As a Leverage to Accelerate the Reverse Water Gas Shift Reaction over Cu-$Ce_x(Ti_{1-x})O_2$ Catalysts.

Miha Okorn[1,2]*, Petar Djinović*[1,2]*, Nataša Novak Tušar*[1,2]*, and Kristijan Lorber*[1]
(1)Department of Inorganic Chemistry and Technology, National Institute of Chemistry, Ljubljana, Slovenia, (2)University of Nova Gorica, Nova Gorica, Slovenia

The Cu/Ce(Ti)O_2 nanorod catalysts demonstrate significant potential for the light-assisted RWGS reaction, yielding significantly higher R_{CO} compared to thermal catalysis at moderate temperatures. This work is focused in the areas of structural and in-situ spectroscopic characterization for better understanding of the mechanistic origins of visible light on the catalytic process

Enhancing Electrocatalytic Conversion of CO_2 Via Bicarbonate Reduction to Formate Via Indium-Bismuth Alloys.

Yukun Hu[1]*, Yuke Li*[2]*, Jia Zhang*[2]*, and Andrew Wong*[3]
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For the first time, we have designed, synthesized, and characterized novel indium-bismuth alloy phases, achieving exceptional electrochemical bicarbonate reduction reaction (BRR) performance with formate Faradaic efficiencies ranging from 83.67% at 100 $mA \cdot cm^{-2}$ to 60.24% at 400 $mA \cdot cm^{-2}$ with mechanistic insights into improving BRR selectivity by theory and experiments.

The Microenvironment Frontier for Electrochemical CO_2 Conversion.

Andrew Wong[1] and ***Yukun Hu***[2]
(1)Materials Science and Engineering, National University of Singapore, Singapore, Singapore, (2)Chemical & Biomolecular Engineering, National University of Singapore, Singapore, --- None ---, Singapore

For electrochemical CO2 reduction, focusing on the microenvironment offers many new possibilities to towards developing selective CO2 conversion. This overview talk shares perspectives for tuning electrochemical CO2 reduction in terms of activity of critical species (CO2, CO, and H2O). Strategies inspired by these perspectives will be discussed.

A New Member to Electrocatalyst Family.

Xianqin Wang
Chemical and Materials Engineering, New Jersey Institute of Technology, Newark, NJ

A new member, polynitrogen, was synthesized by accelerating the rate-limiting step with the UV irradiation. N8 is found to be more stable and more active than the Pt/C commercial catalyst in DMFCs. A four-electron process at N8 is confirmed with the SHINERS experiments and DFT calculations.

Atomic-Level Insights on Electrocatalytic Decarboxylation of Acetic Acid over Anatase-Supported Pt Clusters.

Alexander von Rueden*, Juan A. Lopez-Ruiz, and Mal Soon Lee*
Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA

Our work reveals the atomic structures that metallic/oxidized Pt clusters and adsorbates adopt on anatase supports. By correlating these structures with our density functional theory-calculated electrocatalytic decarboxylation/oxygen evolution energetics and experimental activities, we provide a fundamental understanding that will help guide the electrocatalytic valorization of biomass-derived molecules.

Effects of Mixed Solvents on CO_2 Electrocatalytic Reduction.

Huy Nguyen *and Matthew Neurock*
Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN

We examine the effects of mixed solvents between water and polar aprotic solvents for CO2 electrochemical reduction over gold electrodes and show reactivity can be tuned using different solvents. This work highlights the importance of solvent effects in controlling the electrochemical reactions, facilitating the design of electrolytes for electrocatalysis.

Electrochemical Stability of Iridium Metal - Effect of Surface Structure.

Maira Amjad[1] *and Ian McCrum*[2]

(1)Material Science and Engineering, Clarkson University, Potsdam, NY, (2)Chemical & Biomolecular Engineering, Clarkson University, Potsdam, NY

The stability of iridium and iridium oxide in the electrochemical environment is influenced by the adsorption of electrolyte species including hydrogen, hydroxide, and oxygen on the surface. Our work builds on prior work quantifying the thermodynamic stability of defect-free iridium for OER electrocatalysis.

Detection of Hydroxylamine Intermediate Opens a New Perspective on Ammonia Selectivity in Metal-Catalyzed Nitrate Reduction.

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In the catalytic reduction of nitrates and nitrites in drinking water, undesired ammonia formation is the main drawback yet hindering industrial application. Despite that most studies claim nitrites, ammonia, and nitrogen as exclusive products, we additionally found hydroxylamine under typical reaction conditions, which questions the ammonia selectivities reported in literature.

Enhancing Activity and Stability of Pd-on-TiO_2 Single-Atom Catalyst for Low-Temperature CO Oxidation through *in Situ* Local Environment Tailoring.

Yubing Lu[1]*, Fan Lin*[1]*, Coogan Thompson*[2]*, Libor Kovarik*[1]*, John L. Fulton*[1]*, Zdenek Dohnalek*[1]*, Ayman M. Karim*[2]*,* ***Huamin Wang***[1]*, and Yong Wang*[1]
(1)Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA, (2)Department of Chemical Engineering, Virginia Polytechnic Institute and State University, Blacksburg, VA

The development of efficient Pd single-atom catalysts for CO oxidation is hindered by limited reactivity and thermal stability. Here, we report a TiO_2-supported Pd catalyst with enhanced CO oxidation activity and thermal stability, achieved by adjusting the local coordination of Pd atoms through H_2 treatment.

Site-Specific Monomeric Fe Sites Catalyze the N_2O Decomposition Reaction.

Daniel Camilo Cano Blanco[1,2]*, Jörg W.A. Fischer*[3]*, Gunnar Jeschke*[3]*, Oliver Kröcher*[1,2]*, and Davide Ferri*[1]
(1)Paul Scherrer Institute, Villigen, Switzerland, (2)EPFL, Lausanne, Switzerland, (3)ETH Zurich, Zurich, Switzerland

Herein, we present an *operando* multi-spectroscopy investigation, complemented by spectroscopic-based kinetic analyses, that unveils mechanistic details of N_2O decomposition over Fe-SSZ-13. We demonstrate the site selectivity of the process, involving the redox of specific Fe

ions with the reduction as rate-determining step. These findings advance Fe-zeolite development for after-treatment processes

Aftertreatment System Design for H_2-ICE Using Kinetic Modeling: Promises and Challenges.

Joseph Buttacci*, Keka Mandal, Rajbala Rajbala, Erin Thomson, Manohar Prasad, and Ujjal Das*
Johnson Matthey, Wayne, PA

H_2-ICE is gaining popularity as an alternative to diesel because of carbon free emissions. An aftertreatment system is still required to capture harmful nitrogen oxides. We will highlight the differences between diesel and H_2 emissions and demonstrate the use of kinetic modeling to reduce resources for H_2-ICE system design.

Alloying and Segregation Effects in Palladium-Alloy Catalysts.

Willow Dew[1]*, Sander O. Velle*[1]*, Ingeborg-Helene Svenum*[2]*, and Hilde Venvik*[1]
(1)Chemical Engineering, Norwegian University of Science and Technology, Trondheim, Norway, (2)SINTEF Materials and Nanotechnology, Trondheim, Norway

Supported Pd/Al_2O_3 and $Pd\text{-}Ag/Al_2O_3$ catalysts of varying particle sizes were synthesized and their activity tested in CH_4 oxidation and CO oxidation in comparison with $Pd_{75}Ag_{25}$ (100) and (111) single crystals in order to better understand alloying and segregation effects, using physisorption, chemisorption, X-ray diffraction, X-ray photoelectron spectroscopy, and electron microscopy.

Systematic Studies of Catalyst Structure-Property Relationships in CO_2 Hydrogenation to Methanol.

Shuxuan Feng[1] *and Weixin Huang*[2]
(1)Chemistry, Univerisity of North Dakota, Grand Forks, ND, (2)University of North Dakota, Grand Forks, ND

In this work, we demonstrate the influence of various metal coordination environments on catalytic activity and selectivity in CO_2 hydrogenation to methanol, providing insights to guide the design of tailored catalysts with enhanced performance for utilizing CO_2 as a sustainable carbon feedstock in methanol production.

Determining the Atomistic Structures of Oxy-Carbides and Understanding Their Stability for Oxidative Reactions..

Tej Choksi[1]*, **Nurul Farhana Binti Abd Ghaffar***[2]*, Wen Liu*[2]*, Asmee Prabhu*[2]*, Lavie Rekhi*[2]*, Luan Q. Le*[2]*, and Pieremanuele Canepa*[3]
(1)School of Chemistry, Chemical Engineering and Biotechnology, Nanyang Technological University, Singapore, No State, Singapore, (2)School of Chemistry, Chemical Engineering and

Biotechnology, Nanyang Technological University, Singapore, Singapore, (3)Materials Science and Engineering, National University of Singapore, Singapore, Singapore

We develop a physics-based model to determine the most thermodynamically stable oxy-carbide surfaces of VC and TiC across different chemical potential of oxidants (eg: CO_2/CO, H_2O/H_2, and O_2). The model is developed through density functional theory (DFT) calculated co-adsorbate interactions between oxygen atoms on the surface, partitioned into pair-wise interactions.

Automatic Formulation and Exact Solutions to the Master Equation for Multisite Microkinetic Models in Catalysis.

***Jiankai Ge**, Kevin Adams, and Baron Peters*
Chemical and Biomolecular Engineering, University of Illinois at Urbana-Champaign, Urbana, IL

We present master equation microkinetic models (ME-MKMs) that combine the analytic simplicity of mean-field models with the accuracy of kinetic Monte Carlo. ME-MKMs capture adsorbate interactions, surface diffusion, and reaction kinetics, providing accurate rate predictions and parameter estimation capabilities, making them a powerful tool for heterogeneous catalysis studies.

Identification of the Roles of Carbonaceous Species in Pd-Catalyzed Selective Hydrogenation.

*Peng Zhai[1], Divakar Reddy Aireddy[2], Ye Xu[1], and **Kunlun Ding**[1]*
(1)Cain Department of Chemical Engineering, Louisiana State University, Baton Rouge, LA, (2)National Energy Technology Laboratory, Morgantown, WV

In this work, we investigated the roles of carbidic carbon and surface carbonaceous carbon in Pd-catalyzed acetylene hydrogenation. We reveal that the structure of surface carbonaceous species plays a decisive role in hydrogenation selectivity.

Exploring the Role of Oxygen Vacancies in Promoting Electro-Oxidations on NiOOH for Chemical Manufacturing and Water Treatment.

***Quy P. Nguyen**[1], Vi Thi Thuy Phan[2], Le Thy Thy Ho[1], Ian Burgess[2], and Bin Wang[1]*
(1)School of Sustainable Chemical, Biological and Materials Engineering, University of Oklahoma, Norman, OK, (2)Department of Chemistry, University of Saskatchewan, Saskatoon, SK, Canada

The fundamental findings reported here is anticipated to comprehend understanding of the mechanistic insights and the structure-activity relationship in electro-catalysis on O/OH-vacant NiOOH, shaping rational guidelines for surface-defect engineering to boost the activity and selectivity for the wide ranges of applications.

CO-Induced Reconstruction of Alumina-Supported Transition Metal Clusters.

Sakshi Satyanand[1]*, George Yan*[2]*, Dionisios Vlachos*[2]*, Stavros Caratzoulas*[2]*, Ayman M. Karim*[3]*, Raymond Gorte*[4]*, and John Vohs*[4]
(1)Chemical and Biomolecular Engineering, University of Delaware, Newark, DE, (2)Delaware Energy Institute, University of Delaware, Newark, DE, (3)Department of Chemical Engineering, Virginia Polytechnic Institute and State University, Blacksburg, VA, (4)Department of Chemical and Biomolecular Engineering, University of Pennsylvania, Philadelphia, PA

We investigate the fundamental question of CO induced restructuring of supported sub-nanometer transition metal clusters on dry and hydroxylated γ-Al_2O_3. We employ *ab initio* simulations to study cluster morphology at cryogenic, room, and high temperatures in different CO coverage.

Towards Understanding Entropic Effects in Multimetallic Catalysts.

Sai Varanasi[1]*, Jinwon Oh*[2]*, and Matteo Cargnello*[1]
(1)Chemical Engineering, Stanford University, Stanford, CA, (2)Materials Science, Stanford University, Stanford, CA

Fundamentally understanding what specific changes in the geometric and electronic structure make a high entropy alloy active and stable will allow for the ability to efficiently tune catalyst properties. We show a step-by-step approach, investigating the activity of a single metal, bimetallic, trimetallic, tetrametallic, and high entropy alloy pentametallic catalyst.

Leveraging Epitaxial Metal-Support Interface for Structure-Function Relationship Studies in Thermal Catalysis.

Aswathi Rajeevan[1]*, Matthew Moegling*[1]*, Julia de Barros Dias Moreira*[2]*, Libor Kovarik*[2]*, Janos Szanyi*[2]*, and* ***Linxiao Chen***[1]
(1)Department of Chemical, Biomolecular, and Corrosion Engineering, The University of Akron, Akron, OH, (2)Pacific Northwest National Laboratory, Richland, WA

This work presents a novel epitaxial-growth-based method that allows the rigorous study of particle density effect by isolating it from size and shape effects. Deploying the platform, we demonstrate the effects of multi-particle physisorption of polyolefin chains in hydrogenolysis kinetics.

New Methods for Determining Ad-/Desorption Energies.

Lin Bigom-Eriksen *and* ***Jakob Munkholt Christensen***
Department of Chemical Engineering, Technical University of Denmark, DK-2800 Lyngby, Denmark

We demonstrate new methods for analysis of TPD spectra on the basis of a new adsorption isotherm. We also present new equations for determining both adsorption energies and adsorbate-adsorbate interaction energies on the basis of TPD experiments.

Elucidating Rate Determining Steps in the Presence of Isothermal Multiplicity during Catalytic Oxidation Reactions.

Austin Morales[1]*, Jonathan Ratcliff*[1]*, Daniel Hodonj*[2]*, Patrick Lott*[2]*, Olaf Deutschmann*[2]*, Michael Harold*[1]*, and Praveen Bollini*[1]
(1)William A. Brookshire Department of Chemical and Biomolecular Engineering, University of Houston, Houston, TX, (2)Institute for Chemical Technology and Polymer Chemistry, Karlsruhe Institute of Technology, Karlsruhe, Germany

Recently developed mathematical formalisms for elucidating rate determining steps such as the degree of rate control provide unique insights into the rate governing phenomena behind different branches (solutions) of multivalued rates observed during isothermal methane (CH_4) and carbon monoxide (CO) oxidation over catalyst surfaces.

Understanding Structure Sensitivity and Surface Coverage in the Electrocatalytic Hydrogenation of *Cis,Cis*-Muconic Acid on Palladium.

Deep M. Patel, Prathamesh Prabhu, Jean-Philippe Tessonnier, and ***Luke T. Roling***
Department of Chemical and Biological Engineering, Iowa State University, Ames, IA

The electrocatalytic hydrogenation of *cis,cis*-muconic acid can yield adipic acid from biomass feedstocks. This presentation highlights the importance of Pd terrace sites in enabling adipic acid formation, focusing on fundamentals of surface structure and surface coverage to uncover a tandem mechanism occurring sequentially as outer-sphere and inner-sphere electrochemical processes.

Isotopic Studies of Reaction Pathways within Propylene Epoxidation over Promoted Silver Catalysts.

Joseph Esposito[1] *and Aditya Bhan*[2]
(1)Chemical Engineering and Material Science, University of Minnesota, Minneapolis, MN, (2)Chemical Engineering and Materials Science, University of Minnesota Twin Cities, Minneapolis, MN

Kinetic and isotopic tracer experiments isolate rate-determining generation of a common oxidant intermediate which readily scrambles with carbon dioxide and initiates either propylene epoxidation or combustion over heavily promoted Ag catalysts. The mechanistic influence of chlorine promotion within propylene epoxidation involves primarily the selectivity-determining step.

Identifying Methanol Adsorbate Geometries on (101)-Faceted Anatase Titania Nanocrystals.

Benjamin Moskowitz[1], *Carrington Moore*[2], *Anthony Savoy*[2], *Mark Engelhard*[1], *Gregory Collinge*[1], *Mal Soon Lee*[1], *Janos Szanyi*[1], *Feng Gao*[1], *Simone Raugei*[1,2], *Jean-Sabin McEwen*[2], *Huamin Wang*[1,2], *and Yong Wang*[1,2]
(1)Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA, (2)The Gene and Linda Voiland School of Chemical Engineering and Bioengineering, Washington State University, Pullman, WA

Understanding the binding of oxygenates to metal oxides at the atomistic level is crucial for efficiently upgrading biomass to fuels and chemicals. We integrate *in situ* diffuse reflectance infrared spectroscopy, density functional theory, and molecular dynamics to reveal the geometries of methanol adsorbates on anatase titania nanocrystals.

Kinetics and Thermodynamics of CO Adsorption Onto Mononuclear Pd Ions Supported on Ceria.

Nicholas Nelson
Catalysis Science, Pacific Northwest National Laboratory, Richland, WA

The variations of CO adsorption kinetics and thermodynamics onto 0.034 wt.% Pd/CeO_2 under different pretreatment conditions reveal structural changes in the coordination sphere of site-isolated metal centers. This provides insight into atom mobility under reaction conditions and can be used to inform rational catalyst design strategies.

Stable CeO_x Nanoglue-Confined Copper Species for CO Oxidation and Water-Gas Shift Reaction.

Ying Zheng *and Jingyue Liu*
Department of Physics, Arizona State University, Tempe, AZ

This work studies the synthesis of atomically dispersed and stable Cu species and how they interact with Ce^{3+}-rich CeO_x nanoislands, peppered onto high-area silica support, to form strongly bound Cu–[O_x]–Ce complexes that act as stable active centers for CO oxidation and water-gas shift reaction.

Molecular-Level Insights into Adsorption and Reaction Sites in Heterogeneous Catalysts from Solid-State NMR.

Zachariah Berkson
Chemical Engineering, Arizona State University, Tempe, AZ

Advanced solid-state NMR techniques provide direct, molecular-level insights into the types, structures, and interactions of surface sites, reaction products, and/or adsorbates in heterogeneous Mo- and W-based olefin metathesis catalysts. In particular, NMR parameters of the transition metal centers (e.g., ^{95}Mo) provide site-specific descriptors for electronic structure and reactivity.

Modeling Solvent Effects on Alcohol Elimination within Zeolite Pores.

Benjamin Jackson[1], *Mal Soon Lee*[1], *Manish Shetty*[1], *Sungmin Kim*[1], *Donald M. Camaioni*[1], *Oliver Gutiérrez-Tinoco*[1], *and Johannes Lercher*[1,2]
(1)Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA, (2)Technical University of Munich, Garching b. München, Germany

The role solvents play in alcohol dehydration and solid-liquid interfaces is poorly understood. Here, cyclohexanol dehydration catalyzed by Brønsted acid sites (BAS) within pores of BEA zeolites is used as a model system to systematically explore the influence of various solvents on the mechanism and rate of dehydration.

SBA-15 Nano Catalysts Evaluated in the Hdo of Phenol As an Oxygen Compound Derived from Bio-Oils.

Luis Jorge Rodriguez Castillo[1], *Franklin J. Méndez*[2], *Jorge García-Macedo*[2], *Lina A. Calzada*[3], *Elim Albiter*[3], *Gabriela Zavala*[4], *Juan A. Alcantara*[4], *Felix Cancino*[4], *Carlos Eduardo Santolalla-Vargas*[4], *and Victor Florencio Santes Hernandez*[4]
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This work proposes the synthesis, evaluation and characterization of HDO catalysts. For this, the synthesis of NiMo materials over a SBA15-Gallium supports using the hydrothermal method is described to analyze its catalytic activity and selectivity in the HDO reaction of phenol in order to improve the quality of synthetic biofuels.

Activation of Carbon Monoxide CO in H-Mor Zeolite Via Protonation.

Ja Hun Kwak[1], *Hristiyan A. Aleksandrov*[2], *Nicholas Jaegers*[3], *Georgi Vayssilov*[2], *Janos Szanyi*[4], *and* ***Konstantin Khivantsev***[5]
(1)Ulsan National Institute of Science and Technology, Ulsan, Korea, Republic of (South), (2)Faculty of Chemistry, University of Sofia, 1126 Sofia, Bulgaria, (3)University of California at Berkeley, Berkeley, CA, (4)Pacific Northwest National Laboratory, Richland, WA, (5)Physical and Computational Sciences Directorate and Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA

Our study provides insights into reactivity of zeolitic protons. CO forms protonated HCO^+ species, which opens up a new chapter in understanding zeolites and their reactivity.

Adsorption of Azo Dyes Using ZnO/SiO_2 hybrid Aerogels and Xerogels.

Al-Zahraa Fatima El Cheikh[1], *Houssam El-Rassy*[2], *Mohammad Ahmad*[3], *and Witold Kwapinski*[4]
(1)1Department of Chemical and Environmental Science, university of limerick, Limerick, Ireland, (2)Department of Chemistry, American University of Beirut, Beirut, Lebanon, (3)B & W Basstne Department of Chemical Engineering and Advanced Energy, American University of Beirut, Beirut, Lebanon, (4)University of Limerick, Limerick, Ireland

Nano-ZnO/SiO_2 aerogels and xerogels were synthesized via sol-gel co-gelation of zinc and silica precursors. Characterization confirmed nanoporous ZnO crystals dispersed in a 3D silica matrix. The composites adsorbed Congo Red dye (Q_m is up to 100 mg/g), with adsorption following Freundlich and Langmuir isotherms. They exhibited reusability over five cycles.

Tailoring Morphology and Surface Properties of Microporous Carbon Catalysts Derived from Metal-Organic Frameworks.

Akihiro Okada[1], *Shintaro Takeda*[1], *Shin R. Mukai*[2], *and* ***Isao Ogino***[2]
(1)Graduate School of Chemical Sciences and Engineering, Hokkaido University, Sapporo, Japan, (2)Faculty of Engineering, Hokkaido University, Sapporo, Japan

Metal-organic framework materials (MOFs) are promising precursors for synthesizing supported metal electrocatalysts. Using two different types of ZIFs, a sub-class of MOFs, with similar building units but different morphologies, we demonstrate how particle size and shape influence the catalytic properties of the corresponding carbon-based catalysts in the oxygen reduction reaction.

How Local Order Leads to Shape-Selectivity in Disordered Materials: FAU-FER Interzeolite Transformation Intermediates and Its Exceptional Catalytic Properties.

Julia de Souza[1], *Alexandre Young*[2], *Pedro Romano*[3], *Javier García-Martínez*[4], *and João Monnerat*[5]
(1)LIPCAT, Rio de Janeiro, Brazil, (2)LIPCAT (UFRJ), Rio de Janeiro, Rio de Janeiro, Brazil, (3)Campus D. de Caxias, Federal University of Rio de Janeiro, Rio de Janeiro, Brazil, (4)Molecular Nanotechnology Lab, Department of Inorganic Chemistry, University of Alicante, Alicante, Spain, (5)Chemistry Institute, Federal University of Rio de Janeiro, Rio de Janeiro, Rio de Janeiro, Brazil

This study explores the innovative development of Interzeolite Transformation Intermediates (ITIs) during FAU-to-FER transitions. These hybrid materials combine high mesoporosity with remarkable shape selectivity, enhancing accessibility for bulky reactants. A standout ITI demonstrated tenfold catalytic activity improvements and exceptional stability, revolutionizing applications in energy transition and complex molecule synthesis.

Tuning Zeolite Catalysts Using Organic Additives: Molecular Modelling Studies.

Matthew Robinson *and Andrew Logsdail*
School of Chemistry, Cardiff University, Cardiff, United Kingdom

Pyridine-based additives can tune the selectivity of the mordenite-catalysed ethanol dehydration reaction, a potential green route from bio-ethanol to ethylene (a highly-demanded chemical feedstock). The additive can also be decorated with other functional groups to further enhance/diminish its adsorptive behaviour and open up wider applications.

Structure-Property Evolution of Metal-Organic Frameworks (MOFs)-Derived Catalysts.

Bibesh Gauli[1]*, Swarit Dwivedi*[2]*, Akshat Tanksale*[1]*, and Alan Chaffee*[3]
(1)Chemical Engineering, Monash University, Clayton, VIC, Australia, (2)Chemical and Biological Engineering, Monash University, Clayton, VIC, Australia, (3)Chemistry, Monash University, Clayton, VIC, Australia

This work aims to study the thermal decomposition mechanisms and understand the structure-activity evolution of ZIF-8-derived catalysts for CO_2 hydrogenation to methanol. The metal-support interactions in these catalysts will be finetuned by adjusting the pyrolysis temperature and environment to enhance catalytic activity.

An Accelerated Approach Towards Predicting Coverage-Dependent Surface Free Energies on Transition Metal Surfaces.

Asmee Prabhu and ***Tej Choksi***
School of Chemistry, Chemical Engineering and Biotechnology, Nanyang Technological University, Singapore, Singapore

Ab initio phase diagrams have a pivotal role in identifying thermodynamically stable surfaces. Yet, exploring the configurational space of adsorbates on surfaces to construct phase diagrams is computationally intractable using density functional theory. We present a physics-based pre-trained model that builds ab initio phase diagrams on-the-fly, for promoter-decorated (hkl) surfaces.

Exploring the Use of Global Optimization and Universal Potentials – CO Oxidation over Pd-Based Alloys.

Tor S. Haugland[1] *and* ***Ingeborg-Helene Svenum***[1,2]
(1)Sintef Industry, Trondheim, Norway, (2)Department of Chemical Engineering, NTNU, Trondheim, Norway

The segregation behavior of Pd-based alloy surfaces under conditions relevant for CO oxidation have been studied using machine-learning potentials together with global optimization methods, which enables a fast and systematic sampling of the surface composition depending on coverage.

The Ratings Concept As a Combined First-Principles and Microkinetic Modeling Tool for an on-Line Optimization of Integrated Carbon Capture and Conversion.

Supareak Praserthdam *and Piyasan Praserthdam*
Chemical Engineering, Chulalongkorn University, Bangkok, -, Thailand

The Ratings concept, based on Density Functional Theory, enhances the efficiency of the Integrated Carbon Capture and Conversion process. It follows a two-step approach: identifying catalysts using reactivity (RT-R) and stability (RT-S) ratings and optimizing performance through on-line adjustments. Sensitivity analysis shows temperature has a greater impact than feed ratio.

Variable Reaction Coordinate Transition State Theory for Computing Rate Constants for Barrierless Desorption.

Youbin Kim[1] *and C Franklin Goldsmith*[2]
(1)Brown University, Providence, RI, (2)School of Engineering, Brown University, Providence, RI

Variational Transition State Theory (VTST), an extension of Transition State Theory, addresses its limitations in predicting reaction rates, particularly for gas-phase molecular dissociation. This study focuses on Variable Reaction Coordinate TST (VRC-TST), highlighting its strengths in evaluating multi-dimensional partition functions for gas-phase and gas-surface reactions.

Novel Algorithms for Efficient Exploration of Potential Energy Surfaces.

Sandra Liz Simon*, Nitin Kaistha, and Vishal Agarwal*
Department of Chemical Engineering, Indian Institute of Technology Kanpur, Kanpur, India

Efficient exploration of potential energy surfaces and discovery of minimum energy paths and transition states are key to understanding chemical reaction mechanisms. However, the high computational cost of quantum mechanical calculations poses a challenge. This work introduces two novel algorithms to reduce this cost and accelerate transition state discovery.

Na-Y Zeolite Water Interaction: A Multimodal Analysis Using Gcmc, Machine Learning Potentials and *Operando* X-Ray Diffraction.

Agnieszka Seremak[1]*, Ruben Goeminne*[2]*, Izar Capel Berdiell*[1]*, Lars Lundegaard*[3]*, Pablo Beato*[3]*, Veronique Van Speybroeck*[2]*, and Stian Svelle*[1]
(1)Department of Chemistry, University of Oslo, Oslo, Oslo, Norway, (2)Ghent University, Ghent, Belgium, (3)Haldor Topsøe A/S, Kgs. Lyngby, Denmark

The study used GCMC and MLP-MD methods to analyze cation distribution and framework dynamics in zeolite Na-Y during dehydration. Results showed framework contraction upon water removal and expansion due to cation migration. Findings matched XRD data, highlighting the approach's accuracy and the need for advanced methods in complex system studies.

Graph Based Grand Canonical Basin Hopping: A Case Study for Global Optimization for Amorphous Oxides and Metal Clusters.

Kaustubh Sawant *and Philippe Sautet*
Chemical and Biomolecular Engineering, University of California, Los Angeles, Los Angeles, CA

Global optimization of periodic atomistic models using DFT/ML methods is challenging, particularly for complex amorphous materials. We developed an open-source Python package that employs graph-based grand canonical basin hopping, featuring a standardized library of structural moves for basin hopping and integration with common modeling codes.

Multi-Scale Modelling of MOF-Derived Catalysts.

Swarit Dwivedi[1], Rajan Lakshman[1], Adri C.T van Duin[2], Alan Chaffee[3], and ***Akshat Tanksale***[1]
(1)Chemical and Biological Engineering, Monash University, Clayton, VIC, Australia,
(2)Chemical Engineering, The Pennsylvania State University, University Park, PA,
(3)Chemistry, Monash University, Clayton, VIC, Australia

We report a multi-scale atomistic simulation methodology to simulate the chemical transformation in MOFs under high temperatures. We report the formation of MOF-derived porous carbon catalysts, including metal-embedded carbonaceous matrix and single/dual-atom catalysts. We report the key descriptors of parent MOF morphologies that govern the structure of MOF-derived materials.

Modeling Interfacial Hydrogen Atom Transfer Kinetics Using a Nonadiabatic Proton-Coupled Electron Transfer Framework.

Noah South[1] *and Robert Warburton*[2]
(1)Chemical and Biomolecular Engineering, Case Western Reserve University, Cleveland, OH,
(2)Department of Chemical and Biomolecular Engineering, Case Western Reserve University, Cleveland, OH

This work uses methane decomposition to develop and apply general computational techniques that model kinetics of interfacial hydrogen atom tunneling. Preliminary results indicate that nonadiabatic proton-coupled electron transfer theory best describes the kinetics and supports the assertion that hydrogen atom tunneling is prevalent in thermal catalysis.

Geometrical Restraints for Enhanced Sampling Simulations in Heterogeneous Catalysis.

Gustavo Perez Lemus*, Yinan Xu, Yezhi Jin, Pablo Zubieta, and Juan J. de Pablo*
Pritzker School of Molecular Engineering, University of Chicago, Chicago, IL

By integrating geometric restraints into enhanced ABF methods in PySAGES and leveraging ML-based potentials, we improve convergence and accuracy of free energy calculations for methane activation on Ni surfaces. Overly tight constraints reduce entropic contributions, while selective minimal constraints maintain accuracy and match known free

energy results.

Constant Potential Molecular Dynamics for Electrocatalytic Interface.

Yuanyue Liu
The University of Texas at Austin, Austin, TX

Electrochemical interface is a complex system with a number of factors that are challenging to model at atomic level, such as solvation, surface charge, and their couplings and dynamics. I will present our efforts to solve these problems by developing "constant potential + hybrid solvation + dynamic model" (CP+HS+DM).

Effect of Electric Potential on Electrochemical CO_2 Reduction at Ag(111)-H_2o Interface.

Xiongwei Tian[1,2]*, Axel Tosello Gardini*[1]*, Umberto Raucci*[1]*, Hai Xiao*[2]*, Yuqun Zhuo*[2]*, and Michele Parrinello*[1]
(1)Italian Institute of Technology, Genova, Italy, (2)Tsinghua University, Beijing, China

Using neural network molecular dynamics and enhanced sampling techniques, we reveal how the applied constant potential conditions uniquely influence interfacial water dynamics and CO_2 electro-reduction process, offering deeper insights into the effect of electric potential on electrocatalytic mechanisms which is crucial for future reaction optimization.

Synthesis–Structure–Function Relationships of Oxide-Supported Ruthenium Catalysts for Ammonia Reforming.

Gabrielle A. Kliegle[1]*, Jacob Miller*[1]*, Kathleen D. Brown*[1]*, Alexander J. Hill*[1]*, Matthew M. Yung*[1]*, and Nicholas Thornburg*[2]
(1)Catalytic Carbon Transformation and Scaleup Center, National Renewable Energy Laboratory, Golden, CO, (2)Center for Energy Conversion & Storage Systems, National Renewable Energy Laboratory, Golden, CO

In this work, we synthesize ruthenium catalysts to investigate the effects of metal oxide support identity and alkali promotion, uncovering descriptors of ammonia reforming fixed-bed kinetics. These findings enable an alternative hydrogen production pathway by elucidating synthesis–structure–function relationships that inform on rational catalyst design for ammonia decomposition.

Non-Thermal Plasma Ammonia Synthesis over Porous Silica.

Vashanti Storr[1] *and Maria L. Carreon*[2]
(1)Chemical Engineering, University of Arkansas, Fayettevile, AR, (2)Chemical Engineering, University of Arkansas, Fayetteville, AR

This work investigates earth-abundant silica materials with tailored porosity and morphology, including mesoporous and macroporous structures like spheres and gyroids, to elucidate ammonia synthesis pathways under non-thermal plasma. By optimizing textural properties, this study enhances the development of efficient catalysts for sustainable, decentralized ammonia production, particularly suited for remote regions.

Two-Step Transient Catalytic System for NO_x-to-Ammonia.

***Masaru Ogura**, You Hatanaka, and Takeshi Ohnishi*
Institute of Industrial Science, The University of Tokyo, Tokyo, Japan

We develop a new technology "reNOx" to recover NOx as a resource of ammonia. NOx enrichment is attained by use of selective NOx adsorbent from combustion exhaust as the first stage of the process, followed by the reNOx process by hydrogen to obtain almost pure ammonia.

Ammonia Cracking for Hydrogen Production – Effect of Promoters on Non-Noble Metal Catalysts.

***Ljubiša Gavrilovic**, Jean-Patrick Pinheiro, Saima Sultana Kazi, and Julien Meyer*
Institute for Energy Technology, Kjeller, Oslo, Norway

Series of Ni and Co based catalysts were synthesized using wet impregnation. The catalysts were characterized using H_2 chemisorption, XRD, TPR and BET/BJH. The effect Ce (1-5wt%) promotion on Ni activity, and Mo (1-5wt%) on Co activity were studied. Ammonia cracking was investigated at different temperatures (400-800 °C) and GHSVs.

Promoting Ru Electron Density By Basic Hydroxyapatite Supports for H_2 Storage As NH_3 Under Mild Conditions.

*Sabrina Akrour[1], Alexandre Vimont[2], Sandra Casale[1], Guylène Costentin[1], and **Cyril Thomas**[1]*
(1)Sorbonne Université, Laboratoire de Réactivité de Surface, Paris, France, (2)Normandie Université, Laboratoire Catalyse et Spectrochimie, Caen, France

These results not only highlight the potential of modified HAps as supports for Ru in NH_3 synthesis, but also provide a clear proof of concept of the critical role of the basic properties of the support on the electronic density of the Ru particles and on the activation of N_2.

Ternary Hydride Catalysts for Low Temperature Ammonia Synthesis.

***Selin Ernam**, Anastasiia Karabanova, Xiufu Sun, and Peter Vang Hendriksen*
Energy Conversion and Storage, Technical University of Denmark, Lyngby, Denmark

This study focuses on hydride-based catalysts for low temperature nitrogen activation for ammonia synthesis. We report the catalytic activity and stability of Li_4RuH_6, and a novel quaternary hydride.

Co/Fe Ratio Effect on the Stability of $LaSrCoFeO_3$ Perovskites for Ammonia-Fueled Solid Oxide Fuel Cells.

Alicia San Martin Rueda[1], *Faranak Foroughi*[2], *Ingeborg-Helene Svenum*[1,3], *David Waller*[2], *and Magnus Rønning*[1]
(1)Department of Chemical Engineering, NTNU, Trondheim, Norway, (2)Yara Technology Center, Porsgrunn, Norway, (3)SINTEF Materials and Nanotechnology, Trondheim, Norway

Ammonia-fueled SOFCs have been claimed as an efficient alternative for single-step chemical energy conversion to electricity. Materials with long-term stability are required for this application. LSCF perovskites are viable catalysts for both anode and cathode. Studying these materials can lead to the optimization of suitable catalysts for such purposes.

Economically Competitive Production of Oleo-Furan Sulfonate Detergents from Furfural and Fatty Alcohols.

Truc Phung[1], *Nicholas L. Gadinas*[2], *Kyle B. Reem*[2], *Emily Pond*[2], *and Konstantinos Goulas*[3]
(1)School of Chemical, Biological and Environmental Engineering, Oregon State University, Corvallis, OR, (2)Oregon State University, CORVALLIS, OR, (3)Oregon State University, Corvallis, OR

Oleo-furan sulfonates are advanced detergents derived from fatty acids and furanic derivatives, offering superior properties over petrochemical-based alternatives. Traditional production via furan acylation with fatty acid anhydrides is thermodynamically limited. We propose an alternative pathway using dehydrogenative aldol condensation of fatty alcohols with furfural, coupled with transfer hydrodeoxygenation using isopropanol.

Modified ZIF-67 for CO_2 Capture and Valorization through Cycloaddition: FT-IR 'Operando' Studies.

David Villalgordo Hernández[1], *Andrea Jouve*[2], *Silvia Bordiga*[2], *Enrique V. Ramos Fernandez*[1], *and Javier Narciso*[1]
(1)University of Alicante, Alicante, Spain, (2)Department of Chemistry, University of Turin, Turin, Turin, Italy

ZIF-67 affinity towards CO_2 was greatly enhanced through exchanging up to 60% of its ligand with 1,2,4-Triazole without altering its structure. An FT-IR in-depth study has been carried out to better understand this process' coordinating impact. CO_2 cycloaddition reaction was followed in 'operando' conditions to test the reaction's mechanism.

Synthesis of ZIF-8 on Brass Monoliths Prepared By 3D Selective Laser Melting for CO_2 Conversion.

Leidy Patricia Figueroa Quintero, *Javier Narciso, and Enrique V. Ramos Fernandez*
University Institute of Materials (IUMA), Inorganic Chemistry Department, University of Alicante, Alicante, Spain

This work reports the integration of ZIF-8 into brass monoliths fabricated by 3D-SLM, managing to combine advanced catalytic properties with high mechanical strength. The synthesized materials achieved 90% conversion in CO_2 cycloaddition, underlining their impact as a sustainable and efficient solution for CO_2 capture and valorization.

Na-Promoted Bimetallic Hydroxide Nanoparticles for Aerobic C-H Activation: Catalyst Design Principles and Insights into Reaction Mechanism.

Beyzanur Erdivan, Eylul Calikyilmaz, Yunus Emre Turkmen, and ***Emrah Ozensoy***
Chemistry, Bilkent University, Ankara, Turkey

Na-promoted bimetallic $Fe_xMn_{1-x}(OH)_y$ hydroxides capable of catalyzing aerobic C–H (alkylarene) oxidation reactions at low temperatures were developed, without the need for an initiator. Through a systematic synthetic effort, we scanned a wide nanoparticle synthesis parameter space to lay out a detailed set of catalyst design principles.

Continuous Injection Isothermal Titration Calorimetry for the Determination of Adsorption Kinetics at Solid-Liquid Interfaces.

Jeong Hwan Lee[1]*, Sophia Minadaki*[2]*, Ran Wang*[1]*, Antonios Armaou*[1]*, and Robert Rioux*[3,4]
(1)Chemical Engineering, The Pennsylvania State University, University Park, PA, (2)Chemical Engineering, University of Patras, Patras, Greece, (3)Department of Chemistry, The Pennsylvania State University, University Park, PA, (4)Department of Chemical Engineering, The Pennsylvania State University, University Park, PA

Continuous injection isothermal titration calorimetry (CI-ITC) was developed to determine the kinetic parameters for adsorption processes at the solid-liquid interface. We demonstrated complete characterization of the kinetics and thermodynamics of thiol adsorption to Au nanoparticles. CI-ITC is a novel approach to characterize solid-liquid interfacial kinetics, relevant to heterogeneous catalysis.

Exploring the Growth Kinetics of Carbon Nanotubes Using Transient Pressure Pulsing.

Audrey Dannar[1]*, Jack Peden*[2]*, Adam Boies*[2,3]*, and Christian Reece*[1]
(1)Rowland Institute at Harvard, Harvard University, Cambridge, MA, (2)Cambridge University, Cambridge, United Kingdom, (3)Stanford University, Stanford, CA

Upconversion of hydrocarbons to carbon nanotubes (CNTs) is a promising method of generating CO-free H_2 on the industrial scale. High-quality CNTs could offset the cost of H_2, but fundamental insight is needed to control growth. We utilize *in-situ* kinetic measurements of C_2 gas decomposition to reveal competing CNT growth mechanisms.

Aqueous Phase Reforming (APR) of Glycerol over Platinum Supported on Al_2O_3 Catalyst.

Lioudmila Nossova and ***Gianni Caravaggio***
CanmetENERGY-Ottawa, Natural Resources Canada (NRCan), Ottawa, ON, Canada

The glycerol's APR reaction over 5 wt% Pt/Al_2O_3 catalyst for H_2 production in a batch reactor is investigated in the present work. The effect of the operating parameters (reaction time, temperature, glycerol and catalyst concentration) on the H_2 productivity and selectivity was investigated.

Modification of Metal–Organic Framework: ZIF-8 By Ligand Exchange for the Adsorption and Removal of Mercury.

Maria Karla Lopez González[1], *Enrique V. Ramos Fernandez*[1], *and Javier Narciso*[1,2]
(1)University of Alicante, Alicante, Spain, (2)Alicante Institute for Health and Biomedical Research, Alicante, Spain

The urgent need to remove mercury from wastewater drives the search for new materials. Sulfur-modified ZIF-8 shows great potential as an adsorbent. This study develops six innovative materials, with Int.Z1.1-1 emerging as the most effective, exhibiting optimal structural and chemical properties for environmental water remediation applications.

Selective Hydrogenation of Furfural on Ptsn Alloy Surfaces.

Mengxiong Qiao[1], *Wenrui Chai*[2], *Sharfa Farzandh*[3], *Sumit Beniwal*[3], *Fangliang Li*[3], *Graeme Henkelman*[2], *and Donna Chen*[4]
(1)Chemistry and biochemistry, University of South Carolina, Columbia, SC, (2)Department of Chemistry and Biochemistry, University of Texas at Austin, Austin, TX, (3)Chemistry and Biochemistry, University of South Carolina, Columbia, SC, (4)Chemistry, University of South Carolina, Coulmbia, SC

Selective hydrogenation of furfural to furfuryl alcohol on PtSn catalysts was investigated by combination of experimental studies on single-crystal surfaces and density functional theory calculations. The ordered Pt_3Sn catalyst has high activity and selectivity to furfuryl alcohol compared with Pt(111), as well as other alloy surfaces with different Sn compositions.

Atomically Precise $Cu_{14}H_1$ Nanoclusters for Electrocatalytic CO_2 Reduction.

Manju Maman[1], *Anik Sarkar*[1], *Beenish Bashir*[2], *John Bacsa*[3], *Zhenming Du*[1], *Guoxiang (Emma) Hu*[2], *Gangli Wang*[1], *and Xuefei Li*[1]
(1)Department of Chemistry, georgia state university, Atlanta, GA, (2)school of chemistry and biochemistry, georgia institute of technology, Atlanta, GA, (3)Department of Chemistry, Emory University, Atlanta, GA

We synthesized atomically precise $Cu_{14}H_1$ nanoclusters and evaluated their performance for electrochemical CO_2 reduction. The clusters exhibit high selectivity over the hydrogen evolution reaction, with preliminary gas chromatography indicating hydrocarbon formation. This study provides fundamental insight into active site structure and supports the design of selective catalysts for CO_2 conversion.

Micro-Scale Reactor Systems for Investigating Biomass/Biooil Upgrading.

Tricia Marchese[1]*,* ***Erica Razook***[1]*, Marco Castaldi*[1]*, and Lucas Dorazio*[2]
(1)Chemical Engineering, The City College of New York, New York, NY, (2)BASF, Iselin, NJ

The poster summarizes development of a micro-scale lab reactor for testing high concentrations (50% up to 100 wt%) of biooil in gasoil mixtures. The reactor enables evaluation of catalyst performance in impacting coke formation, and addresses limitations of traditional methods in advancing biomass upgrading for renewable fuel production.

Two-Dimensional (2D) Mxene Supported Ruthenium Catalysts for Plastic Waste Hydrogenolysis: Mass Transport Versus Confinement in Interlayer Spacing.

Ali Kamali *and Dongxia Liu*
Department of Chemical and Biomolecular Engineering, University of Delaware, Newark, DE

Two-dimensional MXene supports confine Ru nanoparticles, enhancing accessibility and mass transport for hydrogenolysis of polyethylene into valuable liquid fuels. It further suppresses methane formation, and elevates liquid selectivity, illustrating MXene's promise for efficient, selective thermochemical upcycling of plastic waste.

Thermal Stability Study of Rh Single Atom Catalyst on Titanate Perovskites and TiO_2 thin Films, Al_2O_3 and $MgAl_2O_4$.

Zhanyuan Liu*, Raymond Gorte, and John Vohs*
Department of Chemical and Biomolecular Engineering, University of Pennsylvania, Philadelphia, PA

CO-DRIFTS was employed to investigate the dynamics of the deposited Rh single atoms at temperatures up to 500°C under reducing conditions. This study demonstrated a large variation in the thermal stability of the Rh single atoms on the various supports, which were ranked as: Al_2O_3>$MgAl_2O_4$>TiO_2/Al_2O_3>$SrTiO_3/MgAl_2O_4$>$CaTiO_3/Al_2O_3$.

Robust, Thermally Stable and Versatile Single Atom Catalysts Based on Earth Abundant Materials.

Brandon Burnside[1]*, Juliana Bertoldi*[1]*, Ryan Alcala*[1]*, Jesse Larence*[2]*, Shan Jiang*[3]*, Wei Ling Huang*[3]*, Geunho Han*[4]*, Andrew T. DeLaRiva*[5]*, Hien N. Pham*[5]*, Abhaya K. Datye*[1]*, Justin M. Notestein*[4]*, Jeffrey T. Miller*[3]*, and Hua Guo*[6]
(1)Department of Chemical & Biological Engineering and Center for Micro-Engineered Materials, University of New Mexico, Albuquerque, NM, (2)University of New Mexico, Albuquerque, NM, (3)Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN, (4)Department of Chemical & Biological Engineering, Northwestern University, Evanston, IL, (5)Department of Chemical and Biological Engineering and Center for Micro-Engineered Materials, University of New Mexico, Albuquerque, NM, (6)Department of Chemistry, University of New Mexico, Albuquerque, NM

We developed a robust thermally stable single atom catalyst based on earth abundant materials. We show a nickel single atom catalyst that is capable of performing both oxidation and hydrogenation mechanism without needing pretreatment to alter the active site. While also showing excellent selectivity in all tested reactions.

Understanding pH Effects and Intrinsic Reaction Kinetics in Electrocatalysis: The Reference Potential Scale Matters.

Nitish Govindarajan
School of Chemistry, Chemical Engineering, and Biotechnology, Nanyang Technological University, Singapore, Singapore

Understanding the intrinsic kinetics of electrocatalytic processes is essential to develop electrified interfaces with high efficiency and selectivity for energy conversion. Here, we highlight the importance of the potential reference – absolute vs. pH dependent scale in interpreting intrinsic reaction kinetics and mechanisms of multistep electrocatalytic processes.

First Principles Insights into Effect of Charge Condensation on Water Gas Shift Reaction Mechanism.

Venkata Rohit Punyapu[1] *and Rachel Getman*[2]
(1)Chemical and Biomolecular Engineering, The Ohio State University, Columbus, OH, (2)Department of Chemical and Biomolecular Engineering, The Ohio State University, Columbus, OH

We show that surface charge condensation can significantly alter Water Gas Shift reaction energetics on Pt catalysts. Positive charge strengthens intermediate binding and shifts reaction barriers, offering a new strategy for tuning catalytic activity through charge manipulation combined with microkinetic modeling.

Rational Design of Interface-Controlled Materials: Bridging Structure-Property Relationships in Heterogeneous Catalysis.

Jiaqi Yu
Department of Chemistry, Northwestern University, Evanston, IL

In heterogeneous catalysis, catalysts are fundamentally connected with reaction kinetics and thermodynamics. While researchers traditionally leverage this relationship to develop catalysts based on reaction principles, our approach reverses this paradigm by designing materials to unveil deeper mechanistic insights. This poster will present our efforts in this direction.

Comparing Constructions of Supported Nanoparticlesvia Machine Learning Interatomic Potentials.

Tristan Maxson *and Tibor Szilvasi*

Department of Chemical and Biological Engineering, The University of Alabama, Tuscaloosa, AL

Idealized constructions common to nanoparticle analysis are evaluated and we find that all fail relative to direct optimization. This work using MLIPs indicates that researchers must exercise a high level of caution when applying idealized construction to catalytic descriptors for supported nanoparticles when an atomistic model has not been optimized.

Lithium Silicates for Isothermal Sorption-Enhanced Steam Methane Reforming (SE-SMR).

Michael Smith[1]*, Snehesh Shivananda Ail*[2]*, Terena Tsao*[3]*, Charles Coe*[1]*, and Marco J. Castaldi*[3]
(1)Chemical Engineering, Villanova University, Villanova, PA, (2)Catalyst Technologies, Johnson Matthey, (3)Chemical Engineering, City College of New York, New York, NY

A novel surfactant-mediated synthesis of lithium orthosilicate which isothermally and reversibly absorbs CO2 at 600 - 650° C has been evaluated in packed-bed reactor studies for sorption-enhanced steam-methane reforming (SE-SMR) show 25 - 30% increase above equilibrium in H_2 production

Seeing Catalysis Dynamics Live at the Atomic Scale: New *in Situ* Transmission Electron Microscopy Workflows Under Reactive Gas Environments.

Lee Casalena
Thermo Fisher Scientific, Portland, OR

Recent advances in environmental TEM enable real-time atomic-scale imaging and spectroscopy under reactive gas environments. New workflows integrate high-stability optics, in situ EELS, pulsed beams, and damage mitigation strategies, allowing researchers to observe dynamic structural and chemical changes in catalysts under near-operando conditions.

Influence of Organocations on the Kinetics and Mechanism of Electrocatalytic Hydrogen Evolution in Alkaline Media.

Isaac Boateng *and Jason Bates*
Chemical Engineering, University of Virginia, Charlottesville, VA

Organocations strongly influence alkaline HER rates, yet the mechanistic basis for this effect remains unclear. This study combines mechanism-derived rate expressions with the coverage-dependence of Tafel slopes to discriminate among candidate HER mechanisms, revealing that organocations decrease the rate of the kinetically relevant step without changing the overall HER mechanism.

Scalable Transformation of Pyrolysis Oil into Biographite Anode for Lithium-Ion Batteries.

Shaikat Chandra Dey[1], *Brian Worfolk*[2], *William Joe Sagues*[3], *Ravindra Kumar Bhardwaj*[4], *Bertrand Tremolet de Villers*[4], *Steven Rowland*[4], *Mark Nimlos*[5], *and Sunkyu Park*[6]
(1)Forest Biomaterials, North Carolina State University, Realigh, NC, (2)Worfolk Consulting, Realigh, NC, (3)North Carolina State University, Raleigh, NC, (4)National Renewable Energy Laboratory, Golden, CO, (5)National Renewable Energy Lab, Golden, CO, (6)Forest Biomaterials, North Carolina State University, Raleigh, NC

This study explored five different pathways to address iron-induced foaming in pyrolysis oil. Following the optimal pathway, the pyrolysis oil was catalytically converted into biographite anode for lithium-ion battery application.

Elucidating Molybdenum Trioxide (MoO_3) Deactivation during the Ambient Pressure Hydrogenation of Lignin-Derived MODEL Compounds.

Mahmudul Khan *and Brent H. Shanks*
Department of Chemical and Biological Engineering, Iowa State University, Ames, IA

Understanding the deactivation of molybdenum trioxide under reaction conditions is crucial for the rational catalyst design for biomass processing. We show that the deactivation kinetics of lignin-derived molecules are oxygenate-dependent, and the catalyst does not remain universally stable, even after the formation of a stable oxycarbohydride phase, limiting pretreatment potential.

Synthesis and Characterization of Pt Single-Atom and Clusters on Transition Metal Carbide Catalyst Supports.

Bipin Lamichhane[1], ***Dahee Lee***[2], *Bishal Gautam*[2], *Arturo Ponce*[3], *Fang Xu*[2], *and Shyam Kattel*[1]
(1)Physics, University of Central Florida, Orlando, FL, (2)Chemistry, The University of Texas at San Antonio, San Antonio, TX, (3)Physics and Astronomy, The University of Texas at San Antonio, San Antonio, TX

Transition metal carbides (TMCs) exhibit strong metal-support interaction that is crucial for the long-term stability of Pt single-atom catalysts (SACs). DFT calculations comparing Pt SACs supported on various TMCs were verified experimentally using a case study of Pt/HfC. The results provide guidance on selecting stable Pt SACs supported by TMCs.

Breaking the C-X Bond: A Kinetic Analysis of the Room Temperature Dehalogenation of Halobenzenes Catalyzed By Rh/Al_2O_3.

Olivia De Luca[1], *Lauren Babb*[2], *Maria Blankemeyer*[2], *Charlotte Suh*[2], *Chloe Deitz*[2], *Christian Geci*[3], *Brian Frederick*[3], *Thomas Schwartz*[4], *and Rachel Austin*[2]
(1)Chemistry, Barnard College of Columbia University, New York, NY, (2)Chemistry, Barnard College, New York, NY, (3)Chemistry/FIRST, University of Maine, Orono, ME, (4)Chemical and Biomedical Engineering, University of Maine, Orono, ME

This study examines Rh/Al_2O_3-catalyzed hydrogenolysis of halobenzenes, showing that reaction rates depend on C–X bond strength when Rh is in its metallic form. These findings clarify the catalytic mechanism of C-X bond breakage and inform the design of efficient, earth-abundant metal catalysts for remediating persistent halogenated environmental pollutants.

Effect of Plasma Power on Intermediate Species and Reaction Temperature in the Presence and Absence of Catalysts for Dry Reforming of Methane Application.

Md Monir Hossain *and Ruigang Wang*
Chemical Engineering and Materials Science, Michigan State University, East Lansing, MI

This study investigates the impact of plasma power on reactor temperature and catalytic reaction pathway in dry methane reforming (DRM). Plasma-induced temperature rise enhances catalytic activity when the catalyst exceeds its thermal activation threshold. The research demonstrates how plasma power influences product distribution, activating new reaction pathways at higher temperatures.

Exploring Catalyst Compositions for Microwave-Assisted Methane Dehydroaromatization.

Biswanath Dutta[1], Swarom Kanitkar[1], Duy Hien Mai[1], Evgeniy Myshakin[1], and ***Daniel Haynes***[2]
(1)NETL Support Contractor, Morgantown, WV, (2)National Energy Technology Laboratory, Morgantown, WV

Flaring natural gas wastes resources and increases CO_2 emissions. Microwave-assisted methane dehydro-aromatization (MDA) offers a sustainable alternative, converting methane into valuable chemicals. This study enhances CH_4 conversion and selectivity toward aromatics, minimizing coke formation by modifying synthesis methods and incorporating catalytic promoters.

PLENARY LECTURES

2025 MICHEL BOUDART AWARD PLENARY LECTURE BY BERT WECKHUYSEN

Wednesday, June 11, 2025 8:00 AM - 9:00 AM
Centennial Ballroom

Chair: Carsten Sievers, Georgia Institute of Technology

Operando **Spectroscopy of Heterogeneous Catalysts: Foundation, Developments & Applications.**

Bert M. Weckhuysen
Utrecht University, Utrecht, Netherlands

Operando spectroscopy has turned into an important field of research. This methodology approaches industrial-like reaction environments and catalyst materials complexity. Further closing this "*operando* gap" results in more insights in reaction and deactivation mechanisms, providing practical leads to develop new catalyst formulations and monitor the "catalyst health" during real-life operation.

BIOMASS - BIOMASS AND WASTE VALORIZATION CATALYSIS

BIOMASS - LIGNIN
Wednesday, June 11, 2025 9:30 AM - 11:30 AM
Regency Ballroom VI

Chair: Ana Alba-Rubio, Clemson University **Co-Chair:** Huamin Wang, Pacific Northwest National Laboratory

KEYNOTE: Advancing the RCF Lignocellulose Biorefinery: From Molecular Insights to Practical Safer Applications.

Bert Sels
Center for Surface Science and Catalysis, KU Leuven, Leuven, Belgium

This presentation will offer a comprehensive exploration of the complexities of catalysis in biomass recycling, providing innovative solutions to current challenges and promoting the transition to a more sustainable, circular economy.

Selective Oxidation of Humins to Maleic Acid Using Transition-Metal-Substituted Keggin-Type Polyoxometalate Catalysts.

Tobias Esser, André Wassenberg, Jan-Christian Raabe, ***Dorothea Voß****, and Jakob Albert*
Hamburg University, Hamburg, Germany

In this study we could for the first time show the selective oxidation of humins to maleic acid using tailor-made POM catalysts to gain a deeper understanding of the structure-activity-selectivity relationships in the selective catalytic oxidation of furanic compounds.

Acid Pretreatment Effects on the Structure and Catalytic Depolymerization of Corn Cob Lignin.

Nakisha Mark[1]*, Sandip Kumar Singh*[1]*, Anoop Uchagawkar*[1]*, Erik Hagberg*[2]*, Thomas Binder*[3]*, and Bala Subramaniam*[3,4]
(1)Center for Environmentally Beneficial Catalysis, University of Kansas, Lawrence, KS, (2)Archer Daniels Midland Company, Decatur, IL, (3)Center for Environmentally Beneficial Catalysis, The University of Kansas, Lawrence, KS, (4)Chemical & Petroleum Engineering, The University of Kansas, Lawrence, KS

Sulfuric acid as a catalyst in the acetosolv process eliminates β-O-4 linkages and introduces sulfur into the extracted lignin causing sulfur poisoning of Pd/C catalyst used in lignin catalytic fractionation. In contrast hydrochloric acid avoids these challenges and improve monomer yields. The findings provide guidance for effective lignin valorization strategies.

Tuning Performance of Ni–Mo Catalysts for the Hydrodeoxygenation of Lignin Oils to Fuels.

Tove Kristensen[1,2]*, Sara Blomberg*[1]*, Marcus Jawerth*[3]*, Christian Dahlstrand*[3]*, and Christian P.*

Hulteberg[2,4]
(1)Department of Process and Life Science Engineering, Lund University, Lund, 221 00, Sweden, (2)Hulteberg Chemistry Engineering AB, Malmö, 212 25, Sweden, (3)Ren Fuel K2B AB, Uppsala, 754 50, Sweden, (4)Division of Chemical Engineering, Department of Process and Life Science Engineering, Lund University, Lund, Scania, Sweden

In this work, a beneficial tailoring approach of a La- and Ce-promoted $NiMo/Al_2O_3$ catalyst with enhanced potential for long-term activity in the industrial HDO of lignin oils to fuels is demonstrated. A high deoxygenation degree of a lignin oil feedstock is achieved and diffusion limitation and carbon polymerization are suppressed.

Synergistic Cu-ReO_x Catalysis for Hydrogen-Free Transfer Hydrogenation of Furfural: Pathway to Value-Added Chemicals and Fuels.

Debarun Banerjee[1,2,3], *Jack Clegg*[2], *and Sreedevi Upadhyayula*[3]
(1)UQ-IITD Research Academy (UQIDRA), Indian Institute of Technology Delhi, New Delhi, Delhi, India, (2)School of Chemistry and Molecular Biosciences, University of Queensland, Brisbane, QLD, Australia, (3)Chemical Engineering, Indian Institute of Technology Delhi, New Delhi, India

This study explores a hydrogen-free catalytic process for the selective transfer hydrogenation of furfural to value-added chemicals and fuels. The approach offers a tunable pathway for high-conversion, sustainable production of furfuryl alcohol and 2-methylfuran, providing insights into catalyst design and reaction mechanism for similar transformations.

C1 - CATALYSIS OF C1 CHEMISTRY

C1 - METHANOL CONVERSION

Wednesday, June 11, 2025 9:30 AM - 11:30 AM
Centennial Ballroom IV

Chair: Benjamin Moskowitz, Pacific Northwest National Laboratory

Co-Chair: Marc Porosoff, University of Rochester

True Activation Energies Relevant to Methanol-to-Olefins Chemistry.

Dipti Bhave[1], *Oleksiy V. Shvets*[2], *Mykhailo M. Kurmach*[2], *Nataliya Shcherban*[3], *and Friederike Jentoft*[1]
(1)Department of Chemical Engineering, University of Massachusetts Amherst, Amherst, MA, (2)L.V. Pisarzhevsky Institute of Physical Chemistry, National Academy of Sciences of Ukraine, Kyiv, Ukraine, (3)Department of porous substances and materials, L.V. Pisarzhevsky Institute of Physical Chemistry, National Academy of Sciences of Ukraine, Kyiv, Ukraine

The kinetics of surface reactions relevant to methanol-to-olefins conversion were monitored spectroscopically, and the activation energies for ring contraction of cycloalkenyl cations and for cyclization of alkadienyl cations were determined. The influence of zeolite framework topology, acid site density and isomorphous substitution by boron, gallium, and iron will be discussed.

On the Redox Mechanism of Methanol Carbonylation on the Dispersed ReO_x/SiO_2 Catalyst.

Neil Tran *and Alexander V. Mironenko*
Chemical and Biomolecular Engineering, University of Illinois Urbana-Champaign, Urbana, IL

This study investigates methanol carbonylation on ReO_x/SiO_2 catalyst using DFT, NBO analysis, and the energetic span model. We find that Re reduction is crucial for catalyst activation. C–C coupling is favorable in Re(III), but challenges arise with C–O scission, suggesting multinuclear sites enable the high catalytic activity.

Impact of Mesoporosity and Alkaline-Earth Metal Species in the Deactivation of Zeolite Y in the Methanol-to-Hydrocarbons Reaction.

Claudia Fabris[1]*, Tomás Cordero-Lanzac*[2]*, Izar Capel Berdiell*[1]*, Sebastian Prodinger*[3]*, Silvia Bordiga*[4]*, and Stian Svelle*[1]
(1)Department of Chemistry, University of Oslo, Oslo, Oslo, Norway, (2)Department of Chemical Engineering, University of the Basque Country (UPV/EHU), Bilbao, Spain, (3)Topsøe A/S, Kgs. Lyngby, Kgs. Lyngby, Denmark, (4)Department of Chemistry and NIS Centre, University of Turin, Torino, Italy

This systematic study highlighted how the modification of the catalyst materials influences the MTH reaction, with a rationalization for different Si/Al: mesoporosity affected the kinetics of deactivation while alkaline-earth metal species suppressed the aromatic selectivity, thus extending the catalyst lifetime.

Brønsted Acid-Site Density Controls the Mechanistic Cycle and Product Selectivity in the Methanol-to-Hydrocarbons Reaction in BEA Zeolite.

Juan Carlos Navarro de Miguel Sr.
King Abdullah University of Science and Technology, Thuwal, Saudi Arabia

The methanol-to-hydrocarbons reaction on beta zeolite is controlled by Brønsted acid-site density. Low density favors the olefinic cycle, boosting propylene selectivity, while high density promotes the aromatic cycle, increasing ethylene and aromatics production. Operando UV-vis spectroscopy links monoenylic carbocations to the olefinic cycle and polyalkylated aromatics to the aromatic cycle.

Ceria Facet Effect on Microwave-Assisted Dry Reforming of Methane.

Sinmyung Yoon[1]*, Alfred Worrad*[2]*, and Dionisios Vlachos*[1]
(1)Delaware Energy Institute, University of Delaware, Newark, DE, (2)University of Delaware, Newark, DE

This work presents a novel investigation of facet-engineered CeO_2 catalysts for MW-assisted DRM, establishing structure-performance relationships that provide new design principles for electrified catalysis.

Dynamic Active Sites on the Mo/HZSM-5 Catalyst for Methane Dehydro-Aromatization (MDA).

Han Chau[1]*, Md Sifat Hossain*[2]*, Shengguang Wang*[1]*, Debasish Sarkar*[1]*, Debtanu Maiti*[1]*, Sheima Khatib*[2]*, and Rebecca Fushimi*[1]
(1)Catalysis and Transient Kinetics Group, Idaho National Laboratory, Idaho Falls, ID,
(2)Chemical Engineering, Virginia Tech, Blacksburg, VA

The dynamic nature of active sites in Mo/HZSM-5 catalysts was elucidated by transient kinetic investigations in the Temporal Analysis of Products (TAP) reactor. This work sheds light on the genesis of molybdenum (oxy-) carbide active sites and catalyst deactivation upon exposure to methane under non-oxidative and oxidative methane dehydro-aromatization pathways.

C2+ - CATALYSIS OF C2+ CHEMISTRY

C2+ | C3+ OLEFINS C-C COUPLING, ISOMERIZATION, AND OXIDATION REACTIONS

Wednesday, June 11, 2025 9:30 AM - 11:30 AM
Hanover Hall FG

Chair: Alan Allgeier, University of Kansas

Co-Chair: Weixin Huang, University of North Dakota

Bilayered Supported $MoO_x/AlO_x/SiO_2$ Catalyst for Olefin Metathesis.

Eli Ream[1]*, Joseph Thompson*[1]*, Adhika Setiawan*[1]*, Srinivas Rangarajan*[2]*, and* ***Israel Wachs***[1]
(1)Department of Chemical and Biomolecular Engineering, Lehigh University, Bethlehem, PA,
(2)Chemical and Biomolecular Engineering, Lehigh University, Bethlehem, PA

Surface modification of SiO_2 with AlO_x was used to tune the molecular structure and activity of surface MoO_x for olefin metathesis. The isolated surface $(O=)_2Mo^{6+}(\text{-O-Al})(\text{-O-Si})$ sites on bilayered supported $MoO_x/AlO_x/SiO_2$ allow a more energetically favorable mechanism, resulting in enhanced performance over MoO_x/SiO_2. This work provides new insights regarding support effects.

Deciphering the Active Sites of Tandem $M_1@M_2O_x$ Catalysts for Selective Alkane Chemistry.

Snehitha Srirangam *and Siddharth Deshpande*
Department of Chemical Engineering, University of Rochester, Rochester, NY

We investigate Oxidative Propane Dehydrogenation (ODHP) on $M_1@M_2O_x$ catalyst, In_2O_3-Pt/Al_2O_3, a highly stable catalyst[1], at an atomic level using a novel data-driven framework. We

find Indium oxide to stabilize selective ODHP by blocking Pt(322) defect sites and preventing deep dehydrogenation.

[1] Yan., H. et al., *Science* 371, 1257–1260 (2021)

Carbonaceous Deposits As the Active Sites for Butene Isomerization.

*Karoline L. Hebisch[1], Pawel Chmielniak[1], and **Carsten Sievers**[2]*
(1)School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA, (2)School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA

This work elucidates the synergistic effects of carbonaceous deposits and solid acidity in confined spaces on the example of ferrierite-catalyzed skeletal butene isomerization. A combination of kinetic studies and spectroscopic analyses provides insights into the reaction location and active species, laying the foundation for prolonging catalyst lifetime.

The Role of Carbonates in the Selective Epoxidation of Propylene on Promoted Ag Catalysts.

***Joseph Esposito**[1] and Aditya Bhan[2]*
(1)Chemical Engineering and Material Science, University of Minnesota, Minneapolis, MN, (2)Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN

Kinetic experiments in tandem with post-reaction surface characterization reveal three required promoters—solid K^+ and gaseous, co-fed CO_2 and trace NO—feature co-dependent promotional interactions. Alkali promotion is shown to stabilize surface carbonates, generated by co-fed CO_2, which deactivate the catalyst in the absence of NO and improve selectivity.

Spectroscopic Insights into the Effects of Pretreatment and K Promotion on Direct Propylene Epoxidation over Cu/SiO_2.

***Hashim Alzahrani**[1,2,3] and **Juan Bravo-Suarez**[2]*
(1)Center for Environmentally Beneficial Catalysis, The University of Kansas, Lawrence, KS, (2)Chemical & Petroleum Engineering, The University of Kansas, Lawrence, KS, (3)Chemical and Materials Engineering Department, King Abdulaziz University, Jeddah, Saudi Arabia

A systematic study investigated K promotion and gas pretreatment effects on propylene epoxidation over Cu/SiO_2. The results revealed a synergy between Cu oxidation states and K, suggesting K-modified Cu^{1+} as the selective site for propylene oxide formation, likely formed through K-Cu interactions when the catalyst starts in a reduced state.

Selective Propene Oxidation: A Transient Kinetic Investigation.

*Debasish Sarkar[1], **Debtanu Maiti**[1], M. Ross Kunz[1], Kenneth Kusima[2], Lars Grabow[3], and*

Rebecca Fushimi[1]
(1)Catalysis and Transient Kinetics Group, Idaho National Laboratory, Idaho Falls, ID, (2)William A. Brookshire Department of Chemical and Biomolecular Engineering, University of Houston, Houston, TX, (3)William A. Brookshire Department of Chemical and Biomolecular Engineering & Texas Center for Superconductivity (TcSUH), University of Houston, Houston, TX

This work delves into the intrinsic kinetics of selective oxidation of propene to acrolein on industrial bismuth molybdate catalysts. Effect of dynamic availability of oxygen sites on different redox states of the catalyst and at various reaction temperatures has been explored towards tuning the product selectivity.

ELECTRO PHOTO - ELECTROCATALYSIS AND PHOTOCATALYSIS

ELECTRO PHOTO - ELECTROCATALYSIS FOR CO2 CONVERSION 1

Wednesday, June 11, 2025 9:30 AM - 11:30 AM
Centennial Ballroom I

Chair: Astrid M Müller, University of Rochester

Co-Chair: Nitish Govindarajan, Nanyang Technological University

Hydronium Ions Inhibit CO_2 Reduction on Coinage Metals.

Max Huelsey[1]*, Bryan Tang*[2]*, and Yogesh Surendranath*[3]
(1)Department of Chemistry, Technical University of Munich, Garching, Germany, (2)Chemistry and Chemical Biology, Harvard University, Cambridge, MA, (3)Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA

We uncover by transient electrochemical methods paired with electrochemical mass spectrometry the mechanistic basis of the lack of CO_2 reduction in acidic medium. Supporting electrolyte cations are required to increase the interfacial pH under electrolysis conditions allowing CO_2 reduction to occur.

Controlling Temperature to Engineer the Local pH of CO_2 Electrolyzers for Selective Multi-Carbon Products Synthesis.

Victor Brandão *and Carsten Sievers*
School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA

Surface enhanced Raman spectroscopy was coupled with product analysis to investigate how potential and temperature control local pH and the local concentrations of bicarbonate and carbonate for selective multi-carbon products formation under CO_2 reduction conditions.

Activation and Regeneration of an Indium-Bismuth Electrocatalyst for CO_2 Reduction Via Quasi Simultaneous *in Situ* XAS and XRD in a Gas Diffusion Electrode System.

Mariangela Biggiero[1]*, Hugo P. Iglesias van Montfort*[2]*, Vaishnavi Ganesh*[1]*, Jan den Hollander*[1]*, Joris Janssens*[1]*, Roos Grote*[1]*, Kirill A. Lomachenko*[3]*, Tom Burdyny*[2]*, Brian Rawls*[4]*, Florian Meirer*[1]*, Ward van der Stam*[1]*, Annelie Jongerius*[4]*, Bettina Baumgartner*[5]*, and Bert M. Weckhuysen*[1]
(1)Inorganic Chemistry and Catalysis, Institute for Sustainable and Circular Chemistry, Utrecht University, Utrecht, Netherlands, (2)Chemical Engineering, TU Delft, Delft, Netherlands, (3)European Synchrotron Radiation Facility, Grenoble, France, (4)Avantium, Amsterdam, Netherlands, (5)Van 't Hoff Institute for Molecular Sciences, University of Amsterdam, Amsterdam, Netherlands

Industrial implementation of an indium-bismuth catalyst for CO_2 electroreduction towards formate requires understanding of catalyst composition, activation and regeneration. To this end, we investigate catalyst oxidation state and crystalline structure in a Gas Diffusion Electrode cell during industrial-like conditions, combining quasi in simultaneous *in situ* X-ray Absorption Spectroscopy and Diffraction.

Analysis of the Role and Reactivity of Bicarbonate on Silver Gas Diffusion Electrodes for Electrochemical CO_2rr.

Claire Yin[1]*, Nirala Singh*[2]*, and Suljo Linic*[1]
(1)Chemical Engineering, University of Michigan, Ann Arbor, MI, (2)Department of Chemical Engineering, University of Michigan, Ann Arbor, MI

We present a combined experimental and modeling approach to explore the role of bicarbonate in CO2RR by quantifying its and water's contributions to the hydrogen evolution reaction (HER) on a silver electrocatalyst in a gas diffusion electrode flow cell.

How Interfacial Fields Influence Electrocatalytic Rates.

Joaquin Resasco
McKetta Department of Chemical Engineering, The University of Texas at Austin, Austin, TX

Electrocatalytic rates are strongly affected by the electrolyte in which the reaction is run. Here, we propose that the electric field present at the catalyst surface is sensitive to the identity of the cation in the electrolyte. This interfacial field alters the energetics of the reaction and consequently catalytic performance.

Carbon-Neutral Syngas Production Via Electrolysis: In-Situ/Operando Investigation of Cathode Behavior Under Reaction Conditions.

Seval Gunduz*, Dhruba Jyoti Deka, Jaesung Kim, Serra Yesilata, and Umit Ozkan*
William G. Lowrie Department of Chemical & Biomolecular Engineering, The Ohio State University, Columbus, OH

Our research targets acquiring a fundamental understanding of the structure-performance relationship within perovskite-type electrode materials for high-temperature co-electrolysis of

CO_2 and H_2O. In-situ and operando characterization techniques showed migration of B-site atoms to the surface, leading to significant changes in the electrode activity, stability, and product composition.

FUNDAMENTALS - FUNDAMENTALS OF CATALYSIS AND SURFACE SCIENCE

FUNDAMENTALS - ZEOLITES AND ACID-BASE CATALYSIS 1

Wednesday, June 11, 2025 9:30 AM - 11:30 AM
Centennial Ballroom II

Chair: James W. Harris, The University of Alabama

Co-Chair: Siddarth Krishna, University of Wisconsin-Madison

Correlating Atomic-Scale Compositions, Structures, and Reaction Properties of Bifunctional Pt/H^+usy Zeolite Catalysts.

Anna Pischer[1], *Bradley F. Chmelka*[2], *Stacey Zones*[3], *and Michael Girgis*[4]
(1)Chemical Engineering, University of California, Santa Barbara, Santa Barbara, CA, (2)Department of Chemical Engineering, University of California Santa Barbara, Santa Barbara, CA, (3)Chevron Energy Technology Company, Richmond, CA, (4)Chevron Research, Richmond, CA

This study uses advanced solid-state 2D, ^{195}Pt, and *in situ* NMR methods to provide detailed new atomic-level insights on the impact of dealumination treatments on the locations and distributions of Al^{IV} sites within zeolite frameworks. These insights are correlated with their catalytic activities, offering insights to improve catalyst performance.

Impact of Polar and Non-Polar Interaction on Alcohol Adsorption in MFI Frameworks.

Benjamin Jackson[1], *Mal Soon Lee*[1], *Ruixue Zhao*[2], *Sungmin Kim*[1], *Fuli Deng*[2], *Xiaomai Chen*[2], *Yue Liu*[2,3], *Roger Rousseau*[1], *and Johannes Lercher*[1,2]
(1)Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA, (2)Technical University of Munich, Garching b. München, Germany, (3)Shanghai Key Laboratory of Green Chemistry and Chemical Processes, School of Chemistry and Molecular Engineering, East China Normal University, Shanghai, China

Combined computational and experimental methods elucidate the role of hydrophobic zeolite pore wells and hydrophilic acid-base sites in the adsorption of C1–C4 alcohols on Si-MFI (without BAS) and H-MFI (with BAS) zeolites at the atomic scale which is crucial for design of catalysts with enhanced activity and selectivity.

Investigating Heterogeneity of Partial Confinement in External-Surface Pockets of SSZ-70 Zeolite Catalysts.

Shankar Ramaswamy[1], *Stacey I. Zones*[2], *and Alexander Katz*[2]
(1)Department of Chemical and Biomolecular Engineering, University of California - Berkeley,

Berkeley, CA, (2)Chemical and Biomolecular Engineering, University of California, Berkeley, Berkeley, CA

We investigate the effect of varying degrees of partial confinement within external-surface pockets of zeolite SSZ-70 on epoxidation catalysis. Our data demonstrate a lack of heterogeneity when only one silanol environment is possible, and a high degree of heterogeneity when silanols are localized at different depths within the pockets.

Quantifying the Kinetics of Framework Dealumination during Hydrothermal Aging of Proton-Form CHA Zeolites.

Tania Class-Martinez[1]*, Craig Waitt*[2]*, Steven Yeo*[2]*, Subramanian Prasad*[3]*, Ahmad Moini*[4]*, William Schneider*[2]*, and Rajamani Gounder*[1]
(1)Charles D. Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN, (2)Chemical and Biomolecular Engineering, University of Notre Dame, Notre Dame, IN, (3)BASF Corporation, Iselin, NJ, (4)BASF Environmental Catalyst and Metal Solutions, Iselin, NJ

Dealumination kinetics measured during hydrothermal aging of proton-form chabazite (CHA) zeolites, with varying amounts of framework Al (Al_f) and 6-MR paired Al site arrangements, reveal that Al_f-O hydrolysis and extra-framework Al agglomeration are both kinetically relevant steps to extents that depend on hydrothermal aging conditions (e.g., temperature, H_2O pressure).

Deactivation, Site Requirements, and Product Inhibition over Au/TS-1 Bifunctional Propene Epoxidation Cascades.

Ryoh-Suke Sekiya[1]*, Enrique Iglesia*[1,2]*, and Rajamani Gounder*[1]
(1)Charles D. Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN, (2)University of California, Berkeley, Berkeley, CA

Dioxygen activation rates and O-based propylene oxide (PO) selectivities are reported for bifunctional propene epoxidation cascades on Au/TS-1 to demonstrate the structural stability of encapsulated Au domains during catalysis, catalytic functions provided by TS-1 for parasitic side reactions, and promotional and inhibitory roles of water on Au.

Surface Tuning of Promoted MoO_x Catalysts for Selective Hydrodeoxygenation of Carboxylic Acids As Hydrogen Carriers.

Thomas Salas*, Laura Alejandra Gomez Gomez, Daniel E. Resasco, and Steven P. Crossley*
School of Sustainable Chemical, Biological and Materials Engineering, University of Oklahoma, Norman, OK

Acetic acid/ethanol systems are candidate liquid organic hydrogen carriers but require kinetically controlled catalysis to achieve sufficient selectivity to the hydrogen carrier form. Promoted MoO_3 catalysts show enhanced activity with high selectivity for the selective

hydrodeoxygenation of acetic acid. The catalyst can be optimized with pretreatment and kinetic analysis.

HYDRO ECON - CATALYSIS FOR THE HYDROGEN ECONOMY

HYDRO ECON - ELECTROCATALYSIS 1

Wednesday, June 11, 2025 9:30 AM - 11:30 AM
Centennial Ballroom III

Chair: Sen Zhang, University of Virginia

Co-Chair: Samira Siahrostami, Simon Fraser University - Burnaby Campus

Atomically Thin Layer of Iridium Oxide over Cobalt Oxide Nanocrystals for Water Electrolysis.

Gengnan Li
Center for Nanoscale Materials, Argonne National Laboratory, Lemont, IL

An atomically thin layer of iridium oxide has been uniformly dispersed onto cobalt oxide nanocrystals to improve the efficient use of iridium. The resulting iridium cobalt oxide outperforms the commercial iridium oxide for acidic oxygen evolution reaction.

Intrinsic Metal-Support Interactions Break the Activity-Stability Dilemma in Electrocatalysis.

Lingxi Zhou *and Ruitao Lv*
Tsinghua University, Asian (Including Pacific Islander), Beijing, China

We report a steam-assisted synthesis armed with machine learning screening of an integrated ruthenium-titanium-manganese electrode, featuring intrinsic metal-support interactions. These atomic-scale interactions with self-healing capabilities radically address the activity-stability dilemma across all pH levels. This breakthrough highlights the potential of intrinsic metal-support interactions for enhancing electrocalysis in diverse applications.

Ionic Liquid-Based Electrocatalytic Systems for Sustainable Synthesis at Intermediate Temperatures.

Clare Yijia Xie[1]*, Devan Solanki*[2]*, and Zachary Schiffer*[1]
(1)School Of Engineering And Applied Sciences, Harvard University, Cambridge, MA,
(2)Harvard John A. Paulson School of Engineering and Applied Sciences, Harvard University, Cambridge, MA

This work advances intermediate-temperature electrochemistry by designing ionic liquid-based systems for sustainable synthesis at 100–250°C. Combining voltage with intermediate temperatures enables efficient electrocatalytic reactions that are challenging or impossible under ambient conditions. We use an ionic liquid electrolyte to explore fundamental thermodynamics and kinetics of benzaldehyde reduction, a prototypical hydrogenation.

Theory Guided Design of $MoO_3/NiMoO_4$ Heterostructures Hybridized Active Pt Co-Catalyst for Efficient Water Splitting.

Nikhil Komalla *and Nelson Dzade*
Energy and Mineral Engineering, The Pennsylvania State University, State College, PA

By combining novel synthesis with catalytic activity measurements, and advanced theoretical modelling, we present a cost-effective bifunctional Pt-$MoO_3/NiMoO_4$ electrocatalyst that shows excellent water-splitting efficiency comparable to current industrial-grade (noble metals) catalysts, with low overpotentials and robust durability, resulting from synergistically improved charge transfers.

KEYNOTE: Catalyst and Electrode Design for Durable Alkaline-Membrane Electrolysis.

Shannon Boettcher
and Energy Storage and Distributed Resources Division, Lawrence Berkeley National Laboratory, Berkeley, CA

Alkaline-exchange-membrane electrolyzers promise high performance for H_2 production with earth-abundant catalysts and low-cost materials but are unstable. In this talk I will present new strategies to understand and design electrode catalysts and ionomer-electrolyte interfaces demonstrating <10 μV/h degradation at >2 $A \cdot cm^{-2}$ and <2 V while operating in pure water.

LIQUID - CATALYSIS IN LIQUID, SUPERCRITICAL, AND MULTIPHASE SYSTEMS

LIQUID - SOLVENT EFFECTS AND MOLECULAR DYNAMICS

Wednesday, June 11, 2025 9:30 AM - 11:30 AM
Regency Ballroom VII

Chair: Jimmy A. Faria, University of Twente

Co-Chair: Graham Leverick, Tufts University

Functional Assessments of Solvent on Solid Brønsted Acid Catalyzed Unimolecular C–O Scission Catalysis.

Junfeng Guo *and Ya-Huei (Cathy) Chin*
Department of Chemical Engineering and Applied Chemistry, University of Toronto, Toronto, ON, Canada

Correlative experiments across reactant-solvent and probe-solvent pairs show a probe molecule's excess adsorption free energy and its difference in charge distribution from the transition state captures the excess activation free energy during solid acid-catalyzed C-O scission, predicting solvent effect on rates and advancing understanding of acid catalysis at liquid-solid interfaces.

Impacts of pH and Surface Charge on Oxygen Reduction at Au(100)-Water Interfaces from Ab Initio Molecular Dynamics Simulations.

Alexander von Rueden[1]*, Mal Soon Lee*[1]*, Vassiliki-Alexandra Glezakou*[2]*, Roger Rousseau*[3]*, and Manos Mavrikakis*[4]
(1)Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA, (2)Physical and Computational Sciences Directorate and Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA, (3)ORNL, Oak Ridge, TN, (4)Department of Chemical and Biological Engineering, University of Wisconsin-Madison, Madison, WI

Our work uncovers the atomic-level participation of interfacial water and co-adsorbed OH groups in the oxygen reduction reaction on the Au(100) surface. This fundamental understanding is crucial for guiding the development of improved electrocatalysts.

Molecular Insights into the Effect of Silanol Nest Defects on Solvent Structure and Diffusion Around the Active Site in Sn-BEA..

Woodrow Wilson[1]*, John Lane*[1]*, William Humphreys*[1]*, Vivek Bharadwaj*[2]*, and Neeraj Rai*[1]
(1)Dave C. Swalm School of Chemical Engineering and Center for Advanced Vehicular Systems, Mississippi State University, Mississippi State, MS, (2)National Renewable Energy Laboratory, Golden, CO

Large scale reactive molecular dynamics simulations utilizing equivariant neural network interatomic potentials trained on density functional theory calculations show that multiple solvent molecules can adsorb to the active sites of Sn-BEA zeolite depending on solvent type, active site location, and presence of silanol nest defects.

Sub-Monolayer Sn Coverages on Pd Surface Promotes Catalytic Nitrate Reduction Reaction.

Janek Betting*, Leon Lefferts, and Jimmy A. Faria*
Catalytic Processes and Materials (CPM) - TNW Faculty, University of Twente, Enschede, Netherlands

In this study, the ideal composition of porous and practically non-porous SnPd catalysts prepared via in-situ controlled surface deposition are established experimentally and using DFT calculations in the context of mass transport effects in a multiphase reaction system for nitrate reduction reaction and the complexity of bimetallic catalysts.

Ammonia: A Vital Additive in the Epoxidation of Propylene over TS-1 Extrudates.

Matias Alvear[1]*, Tapio Salmi*[2]*, and Ive Hermans*[1]
(1)Department of Chemical & Biological Engineering, University of Wisconsin-Madison, Madison, WI, (2)Laboratory of Industrial Chemistry and Reaction Engineering (TKR), Åbo Akademi University, Turku, Finland

The present study aims to analyze the effect of this crucial additive on the epoxidation process. By utilizing extrudates, spectroscopy and a DFT study, it is possible to observe the challenges in

achieving high selectivity with this shaped catalyst, while also allowing a clear understanding of the additive's significance.

Solvent-Manipulated C-O Elimination Reactivity of Alkanols in Beta-Type Zeolite Confinements.

Sungmin Kim[1], *Feng Chen*[1], *Benjamin Jackson*[2], *Hui Shi*[3], *Manish Shetty*[1,4], *Mal Soon Lee*[1], *Wenda Hu*[1,5], *Jian Zhi Hu*[1], *Donald M. Camaioni*[1], *Oliver Gutiérrez-Tinoco*[1], *and Johannes Lercher*[1,6]
(1)Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA, (2)Pacific Northwest National Laboratory, Richland, WA, (3)Technische Universität München, Muchen, Germany, (4)Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX, (5)Washington State University, Pullman, WA, (6)Department of Chemistry and Catalysis Research Center, Technische Universität München, Garching, Germany

We address how solvents, combined with the steric constraints of H-BEA micropore, influence the local organization of solvent and substrate molecules. The generalized model with the standard chemical potential at initial and transition states allows for the estimation and prediction of C-O elimination rates with different solvents.

SYNTHESIS - CATALYST SYNTHESIS AND MANUFACTURING

SYNTHESIS - MATERIAL ENGINEERING AND MANUFACTURE

Wednesday, June 11, 2025 9:30 AM - 11:30 AM
Hanover Hall CDE

Chair: Yeping Cai, Clariant Co.

Co-Chair: James Crawford, Montana State University

Precision Structure Engineering of High-Entropy Oxides Under Ambient Conditions.

Kevin Siniard[1], *Zhenzhen Yang*[2], *and Sheng Dai*[2]
(1)Chemistry, University of Tennessee, Knoxville, TN, (2)Chemical Sciences Division, Oak Ridge National Laboratory (ORNL), Oak Ridge, TN

High-entropy oxides (HEOs) are promising in catalysis for their stability and tunability but face challenges in synthesis under mild conditions. This study develops an ambient in situ lattice engineering approach to integrate HEOs into CeO_2, achieving high surface area, abundant defects, and superior catalytic performance compared to ex situ methods.

Lattice Oxygen Activation in High-Entropy Oxide Catalysts Via Li and Al Doping.

Hailing Yu[1] *and Sheng Dai*[2]
(1)University of Tennessee, Knoxville, Knoxville, TN, (2)Chemical Sciences Division, Oak Ridge National Laboratory (ORNL), Oak Ridge, TN

This study adopts a Li and Al oxide doping strategy to modify the surface structure of high-entropy oxide catalysts, significantly enhancing lattice oxygen activation. The optimized catalysts exhibit enhanced performance in oxidation reactions, showcasing a promising strategy for advancing heterogenous catalytic applications.

Multivariate Bayesian Optimization of Cobalt Oxide Nanoparticles for CO_2 Hydrogenation Catalysis.

*Lanja R. Karadaghi[1], Emily M. Williamson[1], Ahn T. To[2], Allison P. Forsberg[1], Kyle D. Crans[1], Craig L. Perkins[3], Steven C. Hayden[3], Nicole J. LiBretto[2], Frederick G. Baddour[2], Daniel A. Ruddy[2], Noah Malmstadt[1], **Susan Habas**[2], and Richard L. Brutchey[1]*
(1)Department of Chemistry, University of Southern California, Los Angeles, CA, (2)Catalytic Carbon Transformation and Scale-Up Center, National Renewable Energy Laboratory, Golden, CO, (3)Materials Science Center, National Renewable Energy Laboratory, Golden, CO

We present a multivariate Bayesian optimization, coupled with a data-driven classifier, to map the synthetic design space for CoO nanoparticles and optimize them for catalytically relevant features. An optimized CoO/SiO_2 catalyst was evaluated for CO_2 hydrogenation and the high performance was attributed to particle stability and consistent H* surface coverage.

Impact of so_2 on Exsolution and Dissolution of Ni-Fe Nanoparticles from $LaFe_{0.9}Ni_{0.1}O_3$ Perovskite Oxide.

***Musa Najimu**[1], Sahanaz Parvin[2], Courtney Brea[3], Neelesh Kumar[2], Yiqing Wu[4], Zili Wu[5], Jonas Baltrusaitis[2], Israel Wachs[6], and Kandis Leslie Gilliard-Abdulaziz[1]*
(1)Sonny Astani Civil and Environmental Engineering Department, University of Southern California, Los Angeles, CA, (2)Chemical and Biomolecular Engineering, Lehigh University, Bethlehem, PA, (3)Georgia Institute of Technology, Atlanta, GA, (4)Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN, (5)Chemical Sciences Division, Oak Ridge National Laboratory (ORNL), Oak Ridge, TN, (6)Department of Chemical and Biomolecular Engineering, Lehigh University, Bethlehem, PA

Our study shows that highly stable sulfate and sulfite species influence the number, density, and composition of exsolved NiFe nanoparticles. While NiFe catalysts enhance thermocatalytic water splitting activity, the formation of stable sulfur-adsorbed species adversely influences the surface exsolution nucleation pathway and catalyst performance.

Single-Step Syngas-to-Dimethyl Ether Synthesis on Nanoparticle-Derived Pdzn/ZnO/Mp-HZSM-5 and $Pd/CeO_2/Al_2O_3$ Catalysts.

*Bing Wang[1], Zairan Yu[2], Shuang Chen[2], Nicola Da Roit[3], Michael Zimmermann[1], Yuemin Wang[2], and **Silke Behrens**[1]*
(1)Institute of Catalysis Research and Technology (IKFT), Karlsruhe Institute of Technology (KIT), Eggenstein-Leopoldshafen, Germany, (2)Karlsruhe Institute of Technology, Institute of Functional Interfaces, Eggenstein-Leopoldshafen, Germany, (3)Karlsruhe Institute of Technology, Karlsruhe, Germany

The influence of the methanol and dehydration catalyst on the catalytic performance in the single-step syngas-to-dimethyl ether process is shown for different types of bifunctional model catalysts which were prepared using nanoparticle precursors. Material structure aspects are discussed.

Particle Flow, Mixing and Heat Transfer in Rotary Calcination and Drying: Effect of Wall Friction and Baffles.

William Borghard[1]*, Carlin Leung*[1]*, Marcella Raymundo Alves*[1]*, Alberto Cuitino*[2]*, Nina C. Shapley*[1]*, and Benjamin Glasser*[1]
(1)Chemical and Biochemical Engineering, Rutgers University, Piscataway, NJ, (2)Mechanical and Aerospace Engineering, Rutgers, the State University of New Jersey, Piscataway, NJ

In catalyst manufacturing, rotary calciner wall friction has a significant effect on heating time and temperature uniformity. Completely smooth walls can double heating time. One baffle can remedy this. This has implications for improving the design and operation of calciners and dryers, which are known to be extremely energy intensive.

C1 - CATALYSIS OF C1 CHEMISTRY

C1 - COX ACTIVATION AND OXYGENATE PRODUCTION

Wednesday, June 11, 2025 1:00 PM - 3:20 PM
Centennial Ballroom IV

Chair: Felix Herold, Norwegian University of Science and Technology

Co-Chair: Thomas Lin, Stanford University

KEYNOTE: Tailored Materials for Engineering Activity, Stability and Selectivity in CO_2 Conversion Catalysts.

Matteo Cargnello[1] *and Chengshuang Zhou*[2]
(1)Chemical Engineering, Stanford University, Stanford, CA, (2)Molecular Foundry, Lawrence Berkeley National Lab, Berkeley, CA

We present multiple catalyst systems to tune selectivity in CO_2 hydrogenation reactions at mild pressure. We use compositionally tunable metal catalysts (Ru/In), porous polymer overlayers, and oxide supports to control metal/support and metal/ligand interactions and reaction selectivity towards the preparation of useful fuels and chemicals.

Plasma-Assisted Dry Reforming of Methane Using CeO_2 Nanorods Supported Single Atom Bimetallic Ni-Ru Catalysts.

Md Monir Hossain *and Ruigang Wang*
Chemical Engineering and Materials Science, Michigan State University, East Lansing, MI

This study investigates the impact of deposition-precipitation and hydrothermal methods on Ni-Ru bimetallic catalysts supported on CeO_2 nanorods for plasma-assisted dry reforming of

methane. Preliminary results reveal differences in chemisorption behaviors. In-situ Raman and DRIFTS analyses will provide insights into structural changes and reaction mechanisms for optimizing methane reforming.

Co-Promoted Co/SiO_2 with ZnO-MnO ALD for Improved Higher Oxygenate Synthesis.

Nadine Humphrey[1]*, Stacey F. Bent*[2]*, and Simon Bare*[3]
(1)Department of Chemical Engineering, Stanford University, Stanford, CA, (2)Chemical Engineering, Stanford University, Stanford, CA, (3)Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, Menlo Park, CA

Co-promoted Co/SiO_2 with ZnO-MnO ALD increases selectivity towards higher oxygenates to 20% and enhances catalyst activity over ZnO promotion alone. This work uses ALD as a dispersed, controlled, and uniform process relating catalyst structure to performance, expanding on the promotion effects on Co in designing catalysts for higher alcohol synthesis.

2D Nanoscale MoS_2 Catalysts for Direct Conversion of Methane to Oxygenates.

Steven Farrell[1]*, Juan Jimenez*[2]*, Ayaskanta Sahu*[3]*, Sanjaya D. Senanayake*[2]*, and Eli Stavitski*[1]
(1)National Synchrotron Light Source II, Brookhaven National Laboratory, Upton, NY, (2)Chemistry Division, Brookhaven National Laboratory, Upton, NY, (3)Chemical and Biomolecular Engineering, New York University, Brooklyn, NY

Methane is difficult to transport as a gas. We present MoS_2, a low-cost material that forms 2D nanosheets, as a selective and efficient catalyst for the conversion of methane to liquid oxygenates, competitive with costly precious metals. We also probe *in situ* behavior with X-ray absorption spectroscopy under realistic conditions.

Enhancing Rh-Fe Interaction to Achieve Higher Ethanol Selectivity in CO_x Hydrogenation.

Gokce Gulfidan[1]*, Hao Xu*[2]*, Wenda Hu*[3]*, Robert A. Dagle*[4]*, Jothi Kothandaraman*[4]*, and Yong Wang*[5]
(1)Chemical Engineering, Washington State University, Pullman, WA, (2)Chemical and Bio Engineering, Washington State University, Pullman, WA, (3)The Gene and Linda Voiland School of Chemical Engineering and Bioengineering, Washington State University, Pullman, WA, (4)Pacific Northwest National Laboratory, Richland, WA, (5)Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA

The conversion of CO_x (CO and CO_2) into ethanol is essential for sustainable carbon utilization. This study demonstrates enhanced ethanol selectivity in CO_x hydrogenation using Rh-based catalysts promoted by Fe. Improved Rh-Fe interactions on silica support and co-loading boost selectivity under mild conditions, highlighting the importance of active site structure.

Evaluating Enhanced Stability of Si-Doped Methanol Synthesis Catalysts in Conventional and Sustainable Methanol Synthesis Duties.

***Pauline Glen**, Norman Macleod, Monica Garcia-Dieguez, Martin Jendrlin, Mark Kent, Graham Lightfoot, and Michael Nicholson*
R&D, Johnson Matthey, Stockton-on-Tees, United Kingdom

The use of effective accelerated ageing testing protocols has allowed the development of highly stable Si-doped catalysts for methanol synthesis. These catalysts improve productivity in conventional methanol synthesis plants, increasing the useful operating life. Optimised Si-promoted catalysts for CO_2 hydrogenation allow the sustainable production of methanol via our eMERALD^{TM} technology.

CO2 - CO2 CAPTURE AND UPGRADING

CO2 - DUAL FUNCTIONAL MATERIALS FOR CO_2 CAPTURE AND CONVERSION

Wednesday, June 11, 2025 1:00 PM - 3:20 PM
Regency Ballroom VII

Chair: Marc Porosoff, University of Rochester

Co-Chair: Takashi Toyao, Hokkaido University

Self-Regenerative Ni/$CaTiO_3$/CaO Catalyst for Simultaneous CO_2 Capture and Methane Dry Reforming.

*Seongbin Jo[1] and **Kandis Leslie Gilliard-Abdulaziz**[2]*
(1)Chemical Engineering, University of Southern California, Los Angeles, CA, (2)Sonny Astani Civil and Environmental Engineering Department, University of Southern California, Los Angeles, CA

Integrated CO2 capture and utilization (ICCU) utilizes dual functional materials to convert CO2 into valuable fuels. A promising approach involves developing self-regenerative Ni/CaTiO3/CaO materials, enhancing multicycle stability and CO2 uptake in the Integrated CO2 Capture and Dry Reforming of Methane (ICCDRM) process, overcoming challenges like sintering and deactivation.

Bifunctional Catalysts for Sorption-Enhanced Reaction Processes.

Johannis AZ Pieterse
Energy Engineering, TNO, Petten, Netherlands

Sorption-enhanced reaction integrates adsorption with catalytic reactions to convert reactants such as CO_2, CH_3OH, and DME into fuels and chemicals within a single reactor, operating under mild conditions with high conversion. Material approaches to integrate the sorption and reaction functionalities avoid the challenging physically mixing of sorbents and catalysts.

Dual Function Materials Beyond the Lab: Industrial Applications and Material Improvements for Working with Real CO_2 Emissions.

Angie Merkouri[1], Soudabeh B. Gharamaleki[1], Luis. F Bobadilla[2], Maila Danielis[3], Juan L.

Martin-Espejo[2], Anna Penkova[2], Guillermo Torres-Sempere[2], Michael Short[1], Andrea Braga[4], Alessandro Trovarelli[5], José A. Odriozola[6], Tomas Ramirez Reina[2], Sara Colussi[3], and ***Melis Duyar****[7]*
(1)Chemical and Process Engineering, University of Surrey, Guildford, United Kingdom, (2)Inorganic Chemistry Department, Materials Science Institute of Seville-University of Seville-CSIC, Sevilla, Spain, (3)Polytechnic Department, University of Udine, Udine, Italy, (4)Università di Udine, Udine, Italy, (5)Polytechnic Department, Università di Udine, Udine, Italy, (6)Inorganic Chemistry Departmentnt, Materials Science Institute of Seville-University of Seville-CSIC, Sevilla, Spain, (7)Chemical Engineering, University of Surrey, Guildford, Surrey, United Kingdom

We have developed methods to collect emissions from industry sites in sealed gas bags and use these directly for our ICCU testing in the lab. We demonstrated cyclic testing with a real industrial off-gas stream, which constitutes an advancement of DFM technology readiness level to TRL 5.

Behavior of Rh-Based Dual Function Materials (DFMs) for Integrated CO_2 Capture and Methanation at Simulated Flue Gas Conditions.

Giuseppe Nava*, Alessandro Porta, Roberto Matarrese, Carlo Giorgio Visconti, and Luca Lietti*
Dipartimento di Energia, Politecnico di Milano, Milan, Italy

This work addresses DFMs behavior for CO2 capture and methanation from flue gases by operando FT-IR spectroscopy, providing insights on reaction and deactivation mechanisms, as well as guidelines for improved DFM formulations.

Metallic Phase–Free Zn-Al Mixed Oxide Dual Function Materials Enable High CO Selectivity in Reactive Carbon Capture from Dilute CO_2 Streams.

Wilson McNeary*, Alexander Hill, Chae Jeong-Potter, Martha A. Arellano-Treviño, Daniel Ruddy, and Anh To*
Catalytic Carbon Transformation and Scale-Up Center, National Renewable Energy Laboratory, Golden, CO

This work developed K-modified Zn-Al mixed oxides for reactive carbon capture (RCC) to CO with > 97% selectivity and yields up to 53% of captured CO_2 at 400 °C. *In situ* spectroscopy to elucidate the role of K-modification in improving RCC performance.

Reactive Capture and Conversion of CO_2:Catalyst and Process Development for Power-to-Gas Energy Storage.

Matthew Yung*[1], Mathew Rasmussen[2], Sawyer Halingstad[1], Nathan C. Ellebracht[3], Melinda Jue[3], Alvina Aui[4], and Simon H. Pang[3]*
(1)National Renewable Energy Laboratory, Golden, CO, (2)Bioenergy Science and Technology Department, National Renewable Energy Laboratory, Golden, CO, (3)Materials Science

Division, Lawrence Livermore National Laboratory, Livermore, CA, (4)Lawrence Livermore National Laboratory, Livermore, CA

Reactive capture and conversion of CO2 to methane on TiO2-supported dual-functional materials is presented, as well as a mechanism supported by DRIFTS and control experiments and correlation between support oxygen vacancy formation and desorbed product selectivity.

Understanding Zeolitic Adsorption Sites in Which CO_2 Outcompetes Water Under Thermodynamic Control.

Hwangho Lee[1]*, Alexander Katz*[2]*, Dan Xie*[3]*, Stacey I. Zones*[3]*, Ryohji Ohnishi*[4]*, Takahiko Takewaki*[4]*, and Shu Hikima*[4]
(1)Department of Chemical and Biomolecular Engineering, University of California - Berkeley, Berkeley, CA, (2)Chemical and Biomolecular Engineering, University of California, Berkeley, Berkeley, CA, (3)Chevron Energy Technology Company, Richmond, CA, (4)Mitsubishi Chemical Corporation, Yokohama, Japan

We demonstrate K^+-exchanged double-eight-ring secondary building units in zeolites as water tolerant CO_2 adsorption sites, in which CO_2 outcompetes water under thermodynamic control. Such sites have remained a grand challenge both for combining capture & catalysis as well as enabling practical CO_2 capture from post-combustion & point-source applications.

ENVIRO AUTO - ENVIRONMENTAL AND AUTOMOTIVE CATALYSIS

ENVIRO AUTO - N_2O CONTROL USING ZEOLITE CATALYSTS

Wednesday, June 11, 2025 1:00 PM - 3:20 PM
Centennial Ballroom I

Chair: Enrico Tronconi, Politecnico di Milano

Co-Chair: Yuejin Li, BASF

Transient Response Methods for the Investigation of N_2o Decomposition on Fe/CHA Catalysts.

Maria Elena Azzoni[1]*, Nicola Usberti*[1]*, Andrea Gjetja*[1]*,* ***Isabella Maria Nova***[1]*, Enrico Tronconi*[2]*, Roberta Villamaina*[3]*, Maria Pia Ruggeri*[3]*, Veselina Georgieva*[3]*, Loredana Mantarosie*[3]*, and Jillian Collier*[3]
(1)Dipartimento di Energia, Politecnico di Milano, Milan, Italy, (2)Politecnico di Milano, Milan, Italy, (3)Johnson Matthey Technology Centre, Sonning Common, United Kingdom

The decomposition of N_2O, a strong greenhouse gas, is investigated on Fe/CHA catalysts using Transient Response Methods. Transient kinetic analysis of the collected data provides useful information for clarifying the nature of the Fe active sites, understanding the auto-reduction of Fe and assessing the role of the associated redox chemistry.

Interrogating the Kinetic and Mechanistic Origins of N_2o Formation during NH_3 Selective Catalytic Reduction of NO_x on Cu-CHA Zeolites.

Bryan Cruz Delgado[1], *Raghav Saxena*[2], *Matthew T. Caudle*[3], *Vivek Vattipalli*[4], *Ahmad Moini*[4], *Subramanian Prasad*[3], *William Schneider*[2], *and Rajamani Gounder*[1]
(1)Charles D. Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN, (2)Chemical and Biomolecular Engineering, University of Notre Dame, Notre Dame, IN, (3)BASF Corporation, Iselin, NJ, (4)BASF Environmental Catalyst and Metal Solutions, Iselin, NJ

Experimental steady-state and transient kinetic measurements were combined with *in situ* and *operando* X-ray absorption spectroscopy and Density Functional Theory to provide evidence for N_2O formation pathways originating from NO_2-assisted reduction events of Cu(II) sites during low temperature ammonia-selective catalytic reduction of nitrogen oxides on Cu-exchanged zeolites.

DFT Evaluation of N_2/N_2o Selectivity during NH_3-NO_x SCR over Cu-SSZ-13 Zeolite Catalyst.

Raghav Saxena[1], *Bryan Cruz Delgado*[2], *Matthew T. Caudle*[3], *Anthony Debellis*[4], *Subramanian Prasad*[5], *Ahmad Moini*[3], *Rajamani Gounder*[2], *and William Schneider*[1]
(1)Chemical and Biomolecular Engineering, University of Notre Dame, Notre Dame, IN, (2)Charles D. Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN, (3)BASF Environmental Catalyst and Metal Solutions, Iselin, NJ, (4)Quantum Chemistry and Hybrid Modeling Research, BASF Corporation, Tarrytown, NY, (5)BASF Corporation, Iselin, NJ

We investigate N_2O formation, a potent greenhouse gas, during NH_3-NO_x SCR over Cu-CHA catalysts. DFT and microkinetic modeling reveal NO_2 pathways on NH_3-solvated ZCuOH sites as key contributors. Reducing NO_2 and these sites provides strategies to limit N_2O emissions, advancing cleaner technologies for heavy-duty diesel engines.

Iron-Catalyzed Cooperative Red-Ox Mechanism for the Simultaneous Conversion of Nitrous Oxide and Nitric Oxide.

Filippo Buttignol[1], *Jörg W.A. Fischer*[2], *Alberto Garbujo*[3], *Pierdomenico Biasi*[4], *Gunnar Jeschke*[2], *Oliver Kröcher*[5], *Davide Ferri*[5], *and* ***Gabriela-Teodora Dutca***[6]
(1)Paul Scherrer Institute, Villingen, Switzerland, (2)ETH Zurich, Zurich, Switzerland, (3)CASALE SA, Lugano, Switzerland, (4)Basic Research Department, CASALE SA, Lugano, Switzerland, (5)Paul Scherrer Institute, Villigen, Switzerland, (6)EPFL, Lausanne, Switzerland

This work demonstrates that i) the N_2O-NO-SCR reaction is a promising strategy for simultaneous conversion of N_2O and NO, ii) dynamic O*perando* spectroscopic experiments are essential to extract valuable molecular insights and iii) the reactivity of Fe centers in Fe-exchanged zeolites can be disentangled.

Intrinsic Kinetics of Disparate Redox Pathways for Nitrous Oxide Selective Catalytic Reduction over Fe-Zeolites.

***Elizabeth Brungardt**, Vaishnav Sunkireddy, and Siddarth Krishna*
Chemical and Biological Engineering, University of Wisconsin-Madison, Madison, WI

We investigated the selective catalytic reduction (SCR) of N_2O by NH_3 and NO over Fe-zeolites, which occurs via Fe^{II}-Fe^{III} redox cycle. Net rates are limited by Fe^{II} oxidation by N_2O, while reduction pathway selectivity is governed by the relative intrinsic rates of Fe^{III} reduction by NO+NH_3 versus NH_3 alone.

KEYNOTE: Catalysis for Green Hydrogen - Industry Perspective.

Aleksey Yezerets
Cummins Inc., Columbus, IN

This keynote presentation will cover various catalytic processes and applications, that are relevant to green hydrogen, ranging from its production via water electrolysis to its consumption in industrial and transportation applications.

FUNDAMENTALS - FUNDAMENTALS OF CATALYSIS AND SURFACE SCIENCE

FUNDAMENTALS - ZEOLITES AND ACID-BASE CATALYSIS 2

Wednesday, June 11, 2025 1:00 PM - 3:20 PM
Centennial Ballroom II

Chair: Rajat Subhra Ghosh, Cummins, Inc.

Co-Chair: Siddarth Krishna, University of Wisconsin-Madison

Electrically-Driven Proton Transfer Promotes Brønsted Acid Catalysis By Orders of Magnitude.

***Karl Westendorff**[1], Max J. Hülsey[1], Thejas Wesley[1], Yogesh Surendranath[2], and Yuriy Roman[1]*
(1)Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, MA, (2)Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA

This work probes the influence of catalyst potential on heterogeneous Brønsted acid catalysis. Differences in applied potential of ~380 mV yield a 100,000-fold rate enhancement for alcohol dehydrations. Mechanistic studies indicate that the interfacial field increases the effective catalyst acidity and activity. This effect extends across acid catalysts and reactions.

First Principles Analysis of Coke Formation on Pt-Based Catalysts during Propane Dehydrogenation.

***Yu-Hsiang Cheng** and Jeffrey Greeley*
Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN

Coke formation deactivates heterogeneous catalysts during hydrocarbon conversion, particularly in non-oxidative alkane dehydrogenation reactions. Here, we use DFT simulations to explore

structure-sensitive coke growth on Pt surfaces, revealing higher nucleation barriers on terraces than steps. Insights from graphene nucleation models highlight strategies to develop more coke-tolerant catalysts for industrial applications.

Cattesthub: Experimental Heterogeneous Catalytic Database and Fundamental Insights.

Atharva Burte[1]*, Lars Grabow*[1]*, Paul J. Dauenhauer*[2]*, Susannah Scott*[3]*, and Omar Abdelrahman*[1]
(1)William A. Brookshire Department of Chemical and Biomolecular Engineering, University of Houston, Houston, TX, (2)Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN, (3)Department of Chemical Engineering, University of California, Santa Barbara, Santa Barbara, CA

CatTestHub is a valuable tool for chemical catalysis research, enabling a more community-wide benchmarking effort. The growth of the database promises to deepen understanding of catalytic behavior and improve the precision of experimental investigations, ultimately expediting the discovery of new, efficient catalytic materials.

Shedding Light on Catalyst Restructuring in Nitic Acid Production.

Matthew Wilson[1]*, Feng Wang*[2]*, and Jay Yan*[3]
(1)JOHNSON MATTHEY, Billingham, United Kingdom, (2)Department of Chemical Engineering, University College London, London, United Kingdom, (3)Chemical Engineering, University College London, London, United Kingdom

Platinum-based gauzes for the nitric acid industry have been studied using state of the art characterization techniques, combined with catalyst testing under industrially relevant conditions to shed light on their structural evolution. Fundamental understanding of gauze catalysts supports improved plant operation, reduced emissions and better catalyst selection.

Impact of Zeolite Pore Size on the Kinetics of Liquid-Phase Epichlorohydrin Methanolysis.

Huston Locht*, Zahra Rangoonwala, and David Flaherty*
School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA

Structural confinement within zeolites alters the organization of solvent molecules around active sites, influencing catalytic activity through both van der Waals interactions with pore walls and hydrogen-bonding interactions within the reorganized solvent network. Here, we examine the effects of zeolite pore size on the rates and regioselectivities of epichlorohydrin methanolysis.

Atomically Precise Subnanometer Cu, Pd and Cupd Cluster-Based Oxidative Dehydrogenation Catalysts: Knobs for Controlling Activity & Selectivity at the Subnanometer Scale.

Stefan Vajda

Department of Nanocatalysis, J. Heyrovsky Institute of Physical Chemistry of the Czech Academy of Sciences, Prague, Czech Republic

Results demonstrating high-fidelity control of activity (by orders of magnitude) and selectivity (switching between products) in oxidative dehydrogenation of cyclohexene on Cu, Pd and CuPd clusters, will be discussed, using tuning knobs of atomic-precision size and composition of the clusters and leveraging oxide- and carbon-based supports and optimized reaction conditions.

Interrogating the Catalytic Consequences of Extra-Framework Aluminum Species in Acid Zeolites Using Protolytic Alkane Activation.

Bereket Bekele *and Rajamani Gounder*
Charles D. Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN

Chabazite zeolites containing one T-site are interrogated to assess the catalytic consequences of extra-framework aluminum (Al_{ex}) species co-occluded within zeolitic voids near H^+ sites. Measurements of entropy-enthalpy trade-offs upon confining neutral alkanes and carbocationic alkane activation transition states indicate Al_{ex} species strengthen attractive van der Waals interactions within zeolite voids.

HYDRO ECON - CATALYSIS FOR THE HYDROGEN ECONOMY

HYDRO ECON - NH3 DECOMPOSITION

Wednesday, June 11, 2025 1:00 PM - 3:20 PM
Centennial Ballroom III

Chair: Yuanyuan Zhu, University of Connecticut

Co-Chair: Yizhi Xiang, University of Missouri Columbia

The Effect of Water Impurities on Ba-Promoted Cobalt Catalysts for the Ammonia Decomposition Reaction.

Zahra Almisbaa[1] *and Philippe Sautet*[2]
(1)Research & Development Center, Saudi Aramco, Dhahran, Saudi Arabia, (2)Chemical and Biomolecular Engineering, University of California, Los Angeles, Los Angeles, CA

DFT-based microkinetic simulations of the ammonia decomposition reaction and water dissociation were used in this study to understand oxygen poisoning on promoted and unpromoted surfaces. Our results indicate that binding energy alone does not suffice in evaluating catalytic poisoning, as a thorough understanding requires incorporating the kinetics of the reaction.

Electrified Catalytic Processes of Ammonia Decomposition for Distributed H_2 Production.

Jiachun Wu[1]*, Anthony Griffin*[2]*, Paul Smith*[2]*, Zhe Qiang*[2]*, and* ***Yizhi Xiang***[1]
(1)Department of Chemical and Biomedical Engineering, University of Missouri Columbia, Columbia, MO, (2)The University of Southern Mississippi, Hattiesburg, MS

Efficient NH_3 decomposition was achieved through Joule heating catalysis with 3D printed carbon as the heating element and catalyst support. The conversion of NH_3 in Joule-heating catalysis was higher than conventional thermal catalysis, in addition to exhibiting accelerated startup and shutdown for dynamic operations using intermittent renewable electricity.

Highly Active Cobalt Catalysts for Low-Temperature Ammonia Decomposition.

Monica Pazos Urrea[1] *and Magnus Rønning*[2]
(1)Chemical Engineering, Norwegian University of Science and Technology, Trondheim, Trøndelag, Norway, (2)Department of Chemical Engineering, NTNU, Trondheim, Norway

Bimetallic cobalt-based catalysts derived from layered double hydroxides were studied for low-temperature ammonia decomposition, focusing on the effect of the second metal on reducibility and activity. In-situ X-ray absorption spectroscopy revealed the local environment and characteristics of the metal species, supporting the development of cost-effective alternatives to ruthenium-based catalysts.

Activation of Fe, Co, and Mo Based Metal Oxides for Ammonia Decomposition.

Sahra Louise Guldahl-Ibouder[1]*, Monica Pazos Urrea*[1]*, Ingeborg-Helene Svenum*[1,2]*, and Magnus Rønning*[1]
(1)Chemical Engineering, Norwegian University of Science and Technology, Trondheim, Trøndelag, Norway, (2)SINTEF Materials and Nanotechnology, Trondheim, Norway

In situ activation of Fe, Co, and Mo based oxide catalysts in ammonia was studied by XAS-XRD. The ammonia decomposition performance of the catalysts is discussed in light of their activation, the nature of the active phase, and their low-temperature activity for ammonia decomposition.

High Throughput Testing of Ru-Based Catalysts for Ammonia Cracking.

Ingo Graef*, Konrad Krois, Christian Breuer, Hans-Joerg Woelk, and Santiago Casu*
Heraeus Precious Metals GmbH & Co. KG, Hanau, Germany

For Ru-based catalysts used in the ammonia cracking reaction, low temperature activity and stability are essential. A high throughput test campaign was performed in a single-pellet string reactor, resulting in significant performance improvements by applying the right impregnation technique and appropriate dopants.

Molybdenum Carbonitride Mxene in Catalysis of Ammonia Synthesis and Decomposition.

Evgenia Kountoupi[1]*, Diana Piankova*[1]*, Mikhail Agrachev*[2]*, Zixuan Chen*[1]*, Alberto Garbujo*[3]*, Paula M. Abdala*[1]*, Christoph R. Müller*[1]*, and Alexey Fedorov*[1]
(1)Department of Mechanical and Process Engineering, ETH Zurich, Zurich, Switzerland, (2)Department of Chemistry and Applied Biosciences, ETH Zurich, Zurich, Switzerland, (3)CASALE SA, Lugano, Switzerland

H_2 pretreatment of $Mo_2(C,N)T_x$ increases the NH_3 productivity by 4-fold relative to unpretreated $Mo_2(C,N)T_x$ or the bulk β-Mo_2N. Bulk β-Mo_2N outperforms $Mo_2(C,N)T_x$ in the NH_3 decomposition, irrespective of the H_2 pretreatment. Diffusion limitations in the narrow 2D pores of multilayered $Mo_2(C,N)T_x$ inhibit the utilization of the vast MXene surface area.

Unlocking Highly Active Metal Nanoparticles Anchored on Oxide Structures for Ammonia Decomposition.

Baris Alkan, Anh Binh Ngo, Liseth Duarte, Thomas Lunkenbein, and ***Annette Trunschke***
Inorganic Chemistry, Fritz Haber Institute of the Max Planck Society, Berlin, Berlin, Germany

Chemical storage of hydrogen in the form of ammonia could become an important component of a carbon-free hydrogen economy. We present a successful strategy for the synthesis of mixed oxides with nanoscale particles, from which highly active phases with efficient metal-promoter-support interactions for ammonia decomposition are generated by exsolution.

MICRO MESO - MICROPOROUS AND MESOPOROUS MATERIALS

MICRO MESO - METAL AND ZEOLITE CATALYSIS

Wednesday, June 11, 2025 1:00 PM - 3:20 PM
Hanover Hall FG

Chair: Bjorn Moden, Zeolyst International

Co-Chair: Juan Carlos Vega-Vila, University of Maryland

***Catalyzing Epoxide Ring Opening Using Tuned Lewis Acid Zeolite Sn-Beta*.**

Nicholas Brunelli[1]*, Aamena Parulkar*[2]*, Jiawei Guo*[3]*, and Ambarish Kulkarni*[4]
(1)William G. Lowrie Department of Chemical and Biomolecular Engineering, The Ohio State University, Columbus, OH, (2)Chemical and Biomolecular Engineering, The Ohio State University, Columbus, OH, (3)Chemical Engineering, UC Davis, Davis, CA, (4)Chemical Engineering, University of California, Davis, Davis, CA

Site quantification experiments reveal thermodynamic titration, connecting structure to reactivity. Using organo tin precursors, the structure of highly active sites is discovered.

Designing Superior Zeolites for Hydrocracking: Improved Diffusion, Stability, and Performance.

Nilson de Paula[1]*, João Monnerat*[2]*, Javier García-Martínez*[3]*, and Pedro Romano*[4]
(1)Federal University of Rio de Janeiro, Rio de Janeiro, Rio de Janeiro, Brazil, (2)Chemistry Institute, Federal University of Rio de Janeiro, Rio de Janeiro, Rio de Janeiro, Brazil, (3)Molecular Nanotechnology Lab, Department of Inorganic Chemistry, University of Alicante, Alicante, Spain, (4)Campus D. de Caxias, Federal University of Rio de Janeiro, Rio de Janeiro, Brazil

The present work highlights the enhanced performance and stability of surfactant-templated mesoporous Pt/HUSY zeolites in the hydrocracking of hexadecane. The findings are particularly relevant for industry offering improved activity efficiency and diffusion control, crucial for catalyst design, overcoming diffusion limitations and meeting the evolving demands on hydrocarbon processing.

The Isomerization of *M*-Xylene over Fe Modified ZSM-5: Chemical and Structural Effects.

*David Lennon[1], Christos Ballas[1], **Charles Kanyi**[2], Luis E. Murillo[2], Paul Collier[3], Andrew P.E. York[4], and Stewart Parker[5]*
(1)Chemistry, University of Glasgow, Glasgow, Scotland, United Kingdom, (2)Johnson Matthey, Savannah, GA, (3)Johnson Matthey, Sonning Common, United Kingdom, (4)Technology Centre, Johnson Matthey, Sonning Common, United Kingdom, (5)STFC ISIS Facility, Harwell, United Kingdom

The isomerisation of *m*-xylene over Fe modified ZSM-5 at 300°C is used as a test reaction to probe how different Fe concentrations may perturb the zeolite's surface chemistry. Low Fe concentrations lead to a reduction in *o*-xylene formation that is attributed to ion exchange at strong Brønsted acid sites.

Mechanisms of H_2 Reduction of Cu^{2+} Ions and Implications for Cu Site Distribution in Cu-Exchanged Zeolites.

***Jose Rebolledo-Oyarce**[1], Angel Santiago-Colón[2], Lauren Kilburn[2], Rajamani Gounder[3], and William Schneider[4]*
(1)Chemical Engineering, University of Notre Dame, Notre Dame, IN, (2)Chemical Engineering, Purdue University, West Lafayette, IN, (3)Charles D. Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN, (4)Chemical and Biomolecular Engineering, University of Notre Dame, Notre Dame, IN

Density functional theory, kinetic simulations, and statistical titration were combined to unravel Cu reduction mechanisms in Cu-CHA zeolites and to interpret H_2-TPR data. A general framework was established for understanding and interpreting H_2-TPR data and its variations, depending on zeolite composition, to identify active sites and their distribution.

Regioselective Active Site Control in Mo-Loaded MCM-22 and ZSM-5 Zeolites for Enhanced Regeneration in Methane Dehydroaromatization.

***Jong Hun Kang**[1], Eun Ji Choi[2], Yangho Jeong[2], Numan Muhammad[3], Do-Young Hong[3], Jangeon Roh[2], and Do Heui Kim[2]*
(1)Seoul National University, Seoul, Not US or Canada, Korea, Republic of (South), (2)Seoul National University, Seoul, Korea, Republic of (South), (3)Korea Research Institute of Chemical Technology, Daejeon, Korea, Republic of (South)

This study demonstrates the importance of controlling Al siting in 10MR zeolites through combined synthesis and post-treatment methods for highly regenerable methane

dehydroaromatization (MDA) catalysts. Enhanced catalyst performance, reduced coke formation, and improved regenerability achieved a near-record 10% BTX yield, showcasing its potential to advance sustainable MDA processes.

Pt and Sulfate Functionalized Uio-66 for Catalytic Hydrogenation.

Yinjie Ji[1]*, Libor Kovarik*[1]*, Shutthanandan Vaithiyalingam*[1]*, Jian Zhi Hu*[1,2]*, Radha Kishan Motkuri*[1]*, Sungmin Kim*[1]*, Huamin Wang*[1]*, and Johannes Lercher*[1,3]
(1)Pacific Northwest National Laboratory, Richland, WA, (2)The Gene and Linda Voiland School of Chemical Engineering and Bioengineering, Washington State University, Pullman, WA, (3)Technical University of Munich, Garching b. München, Germany

We developed heterogeneous MOF-based catalysts by functionalizing defect-containing UiO-66 with acidic sulfate groups and Pt nanoparticles, aiming to determine their catalytic consequences, with a specific focus on the synergy between the two functionalities in hydrogenation reactions.

Exploring the Structure and Function of Rare-Earth Elements Incorporated into Zeolite Catalysts.

Mingze Zheng[1]*, Shivangi Nandkumar Borate*[2]*, James W. Harris*[2]*, and Brandon C. Bukowski*[1]
(1)Department of Chemical and Biomolecular Engineering, Johns Hopkins University, Baltimore, MD, (2)Department of Chemical and Biological Engineering, The University of Alabama, Tuscaloosa, AL

We combined computational and experimental methods to identify stable structures for rare-earth elements incorporated into Beta Zeolites (REE-Beta). Electronic structure theory, reaction kinetics, pyridine adsorption, and spectroscopy were then combined to guide the design of selective and stable REE-Beta ethanol to olefins catalysts for synthesizing sustainable aviation fuel.

NEW COMP - NEW METHODS IN COMPUTATIONAL CATALYSIS

NEW COMP - MACHINE LEARNING

Wednesday, June 11, 2025 1:00 PM - 3:20 PM
Hanover Hall CDE

Chair: Alexander Mironenko, University of Illinois Urbana-Champaign

Co-Chair: Christian Sandoval Pauker, RICE University

Kinetic Consequences of Anharmonic Entropy Approximations Accelerated with Machine Learning Potentials.

Geet Gupta and ***Brandon C. Bukowski***
Department of Chemical and Biomolecular Engineering, Johns Hopkins University, Baltimore, MD

Quasi-harmonic entropy approximations of reactive intermediates in aluminosilicate zeolite catalysts were accelerated with machine learning potentials (MLPs). MLPs were found to have transferability to predict temperature-dependent quasi-harmonic entropies. We then investigated the kinetic consequences of quasi-harmonic entropies using microkinetic modeling.

Automated Efficient Computation of Coverage Dependent Kinetics Combining Quantum Chemistry Workflows with Active Learning.

Matthew S. Johnson *and Judit Zádor*
Combustion Research Facility, Sandia National Laboratories, Livermore, CA

We present an active learning framework fusing automated quantum chemistry and machine learning to efficiently automate the calculation of coverage dependent kinetic parameters. We validate our framework against an enumerated dataset for a single reaction and demonstrate the framework on a set of reactions important for ammonia decomposition on Pt111.

Global Optimization of Supported Nanoparticles Via Machine Learning Interatomic Potentials.

Tristan Maxson *and Tibor Szilvasi*
Department of Chemical and Biological Engineering, The University of Alabama, Tuscaloosa, AL

A methodology for efficient structure search of supported nanoparticles via machine learning interatomic potentials is developed to support work to understand catalytic descriptors resulting from structural changes induced by support. This methodology is verified by direct comparisons with state-of-the-art benchmark experiments, improving upon known idealized constructions.

Active Learning Accelerated Global Optimization of Atomic Structures.

Keishana Navodye S. a.[1]*, Michael Quaynor*[2]*, and Kasun Gunasooriya*[3]
(1)School of Sustainable Chemical, Biological and Materials Engineering, University of Oklahoma, Norman, OK, (2)School of Sustainable, Chemical, Biological, and Materials Engineering, University of Oklahoma, Norman, OK, (3)Chemical, Biological & Materials Engineering, University of Oklahoma, Norman, OK

A python-based software package was developed integrating DFT, genetic algorithms and on-the-fly machine learning module based on Bayesian approach to accelerate the structure optimization of surfaces and nanoclusters with different compositions and coverages. This can analyze the stable configurations of structures closely resembling the chemical environment of the real systems.

Machine Learning Perturbation Theory Makes Reference-Quality Free Energy Barriers in Catalysis Affordable.

Jérome Rey[1]*, Celine Chizallet*[2]*, Dario Rocca*[1]*, Tomáš Bučko*[3]*, and* ***Michael Badawi***[1]

(1)CNRS, Lorraine University, Nancy, France, (2)IFPEN, Lyon, France, (3)Faculty of Natural Sciences, Comenius University, Bratislava, Slovakia

Free energy barriers for catalytic reactions have been computed at an unprecendeted level of theory thanks to machine learning perturbation theory (MLPT), improving the agreement with experiments. Although MLPT is presented here for hydrocarbon conversion in zeolites, it can be directly applied to any type of chemical reaction.

Machine Learning Models for Predicting Field-Enhanced Catalysis.

Runze Zhao[1]*, Qiang Li*[1]*, Zhu Cheng*[2]*, and Fanglin Che*[1]
(1)Chemical Engineering, University of Massachusetts Lowell, Lowell, MA, (2)Lawrence Livermore National Laboratory, Livermore, CA

This study develops a machine learning framework reducing computational costs 10^5-fold, accurately predicting local electric field effects on nanoparticle catalysis. It highlights low-coordinated sites amplifying electric fields up to four times, offering insights for designing field-enhanced catalysts.

Machine Learning-Driven Dynamical Effects in Surface Chemistry of Metal Alloy Particles.

Changzhi Ai[1,2]*, Frank Abild-Pedersen*[2]*, and Johannes Voss*[2]
(1)Stanford Univerisity, Menlo Park, CA, (2)SUNCAT Center for Interface Science and Catalysis, SLAC National Accelerator Laboratory, Menlo Park, CA

We report initial results for structural evolution of complex metal alloy structures and surface reaction energetics that can be correlated with catalytic activity, where we observe a complex interplay of surface compositional and structural factors resulting in a broad distribution of binding energies across different surface sites.

POLYMER - CATALYSIS FOR POLYMER SYNTHESIS, UPCYCLING, AND RECYCLING

POLYMER - HYDROLYSIS AND PYROLYSIS

Wednesday, June 11, 2025 1:00 PM - 3:20 PM
Regency Ballroom VI

Chair: Hilal Ezgi Toraman, Pennsylvania State University

Co-Chair: Lucas Ellis, Oregon State University

Interfacial Engineering for Vapor Phase Chemical Recycling of Plastic Waste.

Xiaoshen Bai and ***Kunlun Ding***
Cain Department of Chemical Engineering, Louisiana State University, Baton Rouge, LA

In this work, we first identify the long-neglected contribution from heterogeneous catalysis in metal-salt-catalyzed liquid phase PET methanolysis. We further demonstrate that the solvent-free depolymerization of PET can be achieved with the assistance of trace amounts of zinc-based catalysts deposited by different techniques.

Tandem Methanolysis and Catalytic Transfer Hydrogenolysis of Polyethylene Terephthalate to p-Xylene over Cu/$ZnZrO_x$ Catalysts.

Siddhesh Shirish Borkar[1], *Aojie Li*[2], *Fatima Mahnaz*[1], *Jenna Vito*[1], *Ashfaq Iftakher*[1], *Faruque Hasan*[1,3], *Srinivas Rangarajan*[4], *and Manish Shetty*[1]
(1)Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX, (2)Department of Chemical and Biomolecular Engineering, Lehigh University, Bethlehem, PA, (3)Texas A&M Energy Institute, Texas A&M University, College Station, TX, (4)Chemical and Biomolecular Engineering, Lehigh University, Bethlehem, PA

The tandem catalytic transfer hydrogenolysis (CTH) of polyethylene terephthalate (PET) to p-xylene (PX) over Cu supported on reducible metal oxide $ZnZrO_x$ using methanol for (1) the methanolysis of PET to dimethyl terephthalate (DMT) and (2) as an in-situ H_2 source for the hydrogenolysis of DMT to PX is shown.

Chemical recycling of post-consumer polyester wastes using a tertiary amine organocatalyst.

Hongfei Lin[1], *Shaoqu Xie*[2], *Caiqi Wang*[1], *Wenda Hu*[1], *and Jian Zhi Hu*[3]
(1)The Gene and Linda Voiland School of Chemical Engineering and Bioengineering, Washington State University, Pullman, WA, (2)Voiland School of Chemical Engineering and Bioengineering, Washington State University, Washington State University, Pullman, WA, (3)Pacific Northwest National Laboratory, Richland, WA

This study demonstrates the effectiveness of N-methylpiperidine (NMP) as a catalyst for PET depolymerization via methanolysis, achieving over 90% monomer yield, even from mixed and post-consumer waste. Advanced MAS NMR and AIMD analyses reveal NMP's potential for efficient, sustainable polyester recycling and high-quality monomer production from various polyesters.

Polyamide Conversion to Monomer over Metal Oxide Catalysts.

Pedro Moura[1] *and Dionisios Vlachos*[2]
(1)Chemical and Biomolecular Engineering, University of Delaware, Newark, DE, (2)Delaware Energy Institute, University of Delaware, Newark, DE

This work finds alternative metal oxide catalysts for the hydrolysis of polyamides to monomers and provides insights into their stability. These catalysts can potentially improve the industrial hydrolysis of polyamides and the findings here presented help guide the selection and design of future catalysts and reaction systems.

Influence of Pyrolysis Parameters on Catalytic Co-Pyrolysis of Plastic Mixtures Using Zeolites.

Hilal Ezgi Toraman[1]*, Sean Okonsky*[1]*, and Neil Hogan*[2]
(1)Department of Chemical Engineering, Pennsylvania State University, University Park, PA, (2)Department of Chemical Engineering, Penn State University, University Park, PA

Key findings demonstrate that the co-pyrolysis of LDPE and PET with HZSM-5 resulted in increased production of C2-C4 olefins and monoaromatics. Lower catalyst-to-feedstock ratios enhanced olefins for LDPE but reduced benzene for PET, increasing benzoic acid. Optimal conditions for target circular economy products are visualized via response surface diagrams.

Catalytic Pyrolysis of Polyethylene with Microporous and Mesoporous Materials: Assessing Performance and Mechanistic Understanding.

Johan Herber van de Minkelis[1]*, Adrian H. Hergesell*[1]*, Jan C. van der Waal*[2]*, Rinke M. Altink*[2]*, Ina Vollmer*[1]*, and Bert M. Weckhuysen*[1]
(1)Inorganic Chemistry and Catalysis, Utrecht University, Utrecht, Utrecht, Netherlands, (2)Brightsite/TNO, Geleen, Limburg, Netherlands

Testing inherent catalytic properties is hampered by low pore accessibility in plastic pyrolysis. A mesoporous material improved the accessibility, thereby decoupling microkinetics from macrokinetics, and providing new mechanistic insights on catalytic pyrolysis. This enables the development of a new generation of catalyst materials tailored towards plastic recycling.

Upcycling of Additive-Containing Waste.

Jacqueline Ngu[1]*, Sean Najmi*[2]*, Esun Selvam*[3]*, Brandon Vance*[3]*, Piaoping Yang*[1]*, and* ***Dionisios Vlachos***[4]
(1)University of Delaware, Newark, DE, (2)Center for Plastics Innovation, University of Delaware, Newark, DE, (3)Chemical and Biomolecular Engineering, University of Delaware, Newark, DE, (4)Delaware Energy Institute, University of Delaware, Newark, DE

We investigate the resilience of chemical deconstruction technologies to additives. We compare hydroconversion, and melt catalytic pyrolysis using acid catalysts. Catalyst-additive surface interactions are studied thermogravimetrically, spectroscopically, and via reaction experiments. We uncover poisoning mechanisms and demonstrate that common hydroconversion catalysts are susceptible to most additives.

C1 - CATALYSIS OF C1 CHEMISTRY

C1 - METHENA CONVERSION, DRY REFORMING OF METHANE

Wednesday, June 11, 2025 3:40 PM - 5:40 PM
Centennial Ballroom IV

Chair: Felipe Polo-Garzon, Oak Ridge National Laboratory (ORNL)

Co-Chair: Kandis Leslie Gilliard-Abdulaziz, University of Southern California

Stable Dry Reforming of Methane Enabled By High-Entropy Oxides Via Synergistic Redox Exsolution and Strong Metal-Support Interaction.

Zhenzhen Yang[1]*, Qingju Wang*[2]*, and Sheng Dai*[1,2]
(1)Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN, (2)Department of Chemistry, The University of Tennessee, Knoxville, TN

Stable and coking-free dry reforming of methane (conversion of CO2/CH4 to syngas) was achieved by harnessing the restructuring behaviour of alkaline earth metal-doped high entropy oxide catalysts (BaNiMgCuZnCoOx), combining synergistic redox alloy exsolution (NiCuCo alloy) and strong metal-support interaction construction (BaOx overlayer formation).

Operando **XAS-XRD of CoPt Nanoparticles Under Dry Reforming of Methane Conditions Reveals Dynamic Order-Disorder Phase Transition.**

David Niedbalka*, Marcel Janak, Diana Piankova, Paula M. Abdala, and Christoph R. Müller*
Department of Mechanical and Process Engineering, ETH Zurich, Zurich, Switzerland

We show that alloying Co and Pt, metals with low activity for dry reforming of methane (DRM), significantly enhances catalytic performance when supported on SiO_2. *Operando* XAS-XRD reveals dynamic structural transformations and electronic interactions in CoPt alloys, highlighting how their unique electronic and local structures drive superior activity and stability.

Unraveling the Influence of Interfacial Sites on Selectivity Using a Microkinetic Model for Methane Dry Reforming on Oxide Supported Ni Catalysts.

Nirenjan Shenoy Padmanabha Naveen[1]*, Konstantinos Alexopoulos*[2]*, Michael Janik*[2]*, and Gina Noh*[3]
(1)The Pennsylvania State University, University Park, PA, (2)Chemical Engineering, The Pennsylvania State University, University Park, PA, (3)DCHAB, ETH Zurich, Zurich, CA, Switzerland

A multi-site microkinetic model is developed to explore the role of metal-support interfaces in dry reforming of methane. By quantifying the interfacial effects on activity and selectivity, this study reveals how catalyst dispersion and interfacial site tuning enhance selectivity, offering new insights for designing efficient DRM catalysts.

Improved Dry Reforming Activity, Stability, and Selectivity through Reactant Ratio Feed Tailoring.

Gabriel Otusanya*, Jonathan Lucas, and Kerry Dooley*
Cain Department of Chemical Engineering, Louisiana State University, Baton Rouge, LA

Dry Reforming of Methane (DRM) converts CH_4 and CO_2 to H_2 and CO also known as syngas. Tailoring the DRM feed by either changing the CO_2:CH_4 feed ratio or adding small partial pressures of H_2O to the feed improves the stability, selectivity and activity of DRM catalysts.

Molten Indium Alloys for CO2 and CH4 Conversion to Syngas and Carbon Fibers.

***Chester Upham**, Genpei Cai, Natascha Miederhoff, and Sawyer d'Entremont*
Chemical & Biological Engineering, University of British Columbia, Vancouver, BC, Canada

We will present on methane pyrolysis using several indium alloys to selectively produce carbon fibers. When CO_2 is also used as a co-reactant, we find that high value (2:1 H_2:CO) syngas can be also be co-produced. Kinetics, the reaction mechanism, and activity trends will be discussed.

Density Functional Theory and Raman Studies of Mo/ZSM-5 Utilizing Metal Promoters for Enhancing Methane Dehydroaromatization.

***Evgeniy M. Myshakin**[1], Duy Hien Mai[2], Swarom Kanitkar[2], Xinwei Bai[2], Wissam A. Saidi[3], and Daniel Haynes[4]*
(1)NETL Support Contractor, Pittsburgh, PA, (2)NETL Support Contractor, Morgantown, WV, (3)National Energy Technology Laboratory, Pittsburgh, PA, (4)National Energy Technology Laboratory, Morgantown, WV

The metal promoters enhance Mo/ZSM-5 performance in MDA. DFT was utilized to interpret Raman spectra of Mo/ZSM-5 with added promoters and to calculate binding energies of promoters and Mo species. The data reveal the surface modification with promoters and enhancing availability of specific locations in pores and ion-exchange sites.

CO2 - CO2 CAPTURE AND UPGRADING

CO2 - CO_2 CONVERSION TO METHANOL 1

Wednesday, June 11, 2025 3:40 PM - 5:40 PM
Regency Ballroom VII

Chair: Lun An, Ames National Laboratory

Co-Chair: Junjie Chen, Stanford University

Reactive Capture and Conversion of CO_2 to Methanol over Alkali Promoted $ZnZrO_2$-Mg_3alox Catalytic Sorbents.

***Laura Proano**[1], Katlo Galefete[1], Guanhe Rim[2], Gabriel Gusmão[2], and Christopher W. Jones[3]*
(1)School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA, (2)School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA, (3)Georgia Institute of Technology, Atlanta, GA

CO_2 reactive capture and conversion (RCC) to methanol was investigated using alkali-modified $ZnZrO_2$-Mg_3AlO_x catalytic sorbents. Na-impregnation improved CO_2 uptake and productivity. However, selectivity shifted from methanol and CO to methane under RCC conditions, revealing distinct behaviors from steady-state operation and emphasizing the interplay of material properties and dynamic reaction environments.

Insight into Structure-Activity Relationships of SiO_2 -Supported Pd-Fe Catalysts for CO_2 Hydrogenation to Methanol.

***Angelo Bellia**, Christoph R. Müller, and Paula Abdala*
Department of Mechanical and Process Engineering, ETH Zurich, Zurich, Switzerland

We focus on understanding the effect of the addition of Fe to Pd-based catalysts on their geometric and electronic structure and their catalytic activity for CO_2 hydrogenation to methanol. We observed that the addition of Fe significantly enhances the methanol yield and we characterized the catalysts via a multi-technique approach.

Tuning the Support and Metal Centers in Supported Catalysts to Boost Methanol Synthesis from CO_2 Hydrogenation.

*Yang He[1], Yuanyuan Li[2], Felipe Polo-Garzon[3], De-en Jiang[4], and **Zili Wu**[2]*
(1)Chemical Science Division, Oak Ridge National Laboratory, Oak Ridge, TN, (2)Chemical Sciences Division, Oak Ridge National Laboratory (ORNL), Oak Ridge, TN, (3)Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN, (4)Department of Chemical and Biomolecular Engineering, Vanderbilt University, Nashville, TN

This presentation will highlight two effective strategies in controlling the metal-support interactions via tuning the anion site (hydride) of the support as well as the synergy between metal centers to enhance CO_2 hydrogenation to the desired alcohol product.

Evaluation of Cu and Cuzn Exsolution for the CO_2 Hydrogenation to Methanol: Insights from an *in Situ* and *Operando* Study.

***Eleonora Cali**[1], Marco Pietro Mezzapesa[1], William Skinner[2], David J. Payne[2], Saman Khayat Noroozi[1], Enrico Sartoretti[1], Samir Bensaid[1], and Fabio A. Deorsola[1]*
(1)Department of Applied Science and Technology, Politecnico di Torino, Turin, Italy, (2)Imperial College London, London, United Kingdom

In this work, optimized catalysts for CO_2 conversion to MeOH using the novel approach of 'exsolution' have been developed. The new exsolved samples were tested for the CO_2 hydrogenation to methanol to assess their stability, activity and selectivity, and the structure-activity-selectivity correlation studied through NAP-XPS, and *operando* TEM/STEM-EDX/EELS and FTIR.

Enhancing Methanol Selectivity in CO_2 Hydrogenation through Tuning of Metal-Oxide Interfacial Sites.

***Weixin Huang**[1] and Shuxuan Feng[2]*
(1)University of North Dakota, Grand Forks, ND, (2)Chemistry, Univerisity of North Dakota, GRAND FORKS, ND

By investigating Pd-supported catalysts with uniform Pd nanocrystals, we demonstrate that metal/oxide interfaces play a crucial role in determining methanol selectivity from CO_2. These findings suggest that the design of tailored metal/oxide interfaces can lead to the development of highly effective CO_2-to-methanol catalysts

Physics-Informed Techno-Economic Assessment Shows a Path to Economical CO_2 Reduction.

Shashwati da Cunha *and Joaquin Resasco*
McKetta Department of Chemical Engineering, The University of Texas at Austin, Austin, TX

Our physics-informed techno-economic assessment highlights research priorities for electrochemical CO_2 reduction. Moving away from a plug flow reactor design lowers the levelized cost from \$1.22/kg_{CO} to \$0.97/kg_{CO}. Cheap renewable electricity cannot directly drive CO_2R if it is intermittent. Intermediate current densities are optimal, even with cheap electricity.

DYNAMICS - DYNAMIC CATALYSIS

DYNAMICS - DRIVING CATALYSIS THROUGH EXTERNAL MODULATION

Wednesday, June 11, 2025 3:40 PM - 5:40 PM
Hanover Hall FG

Chair: Ming Yang, Clemson University

Co-Chair: Omar Abdelrahman, University of Houston

Making Catalysts Dance – Dynamic Stress Boosts Hydrogen Evolution on Metals.

Xiang Yu[1], Hui Wang[1], Sander Deelen[2], and ***Matteo Monai***[1]
(1)Inorganic Chemistry and Catalysis, Institute for Sustainable and Circular Chemistry, Utrecht University, Utrecht, Netherlands, (2)Utrecht University, Utrecht, Netherlands

Better catalysts are needed for a more sustainable chemical industry. Dynamically straining a catalyst can theoretically boost catalytic performance, but approaches to induce strain at high frequency are lacking. Here, we demonstrate a method to dynamically strain catalysts up to 1000 Hz, boosting hydrogen evolution reaction on metal electrodes.

Enhancing the Activity and Selectivity of Pd-Based NH_3 Oxidation Catalysts By Forced Dynamic Reactor Operation.

Thomas Häber[1], Camilo Cárdenas[2], Olaf Deutschmann[2], and ***Patrick Lott***[2]
(1)Institute of Catalysis Research and Technology, Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, Germany, (2)Institute for Chemical Technology and Polymer Chemistry, Karlsruhe Institute of Technology, Karlsruhe, Germany

Spatiotemporal investigations demonstrate that forced dynamic reactor operation promotes both the activity and selectivity of Pd-based NH_3 oxidation catalysts operated in lean conditions and

uncover gradients evolving in dynamic operation. The findings of this work are relevant whenever NH_3 is used as carbon-free energy carrier, i.e. during combustion or decomposition.

Tuning Non-Equilibrium Surface Coverages for Enhanced Methane Activation during Forced Periodic Oscillations.

Fatou Baka Diop*, Cameron Armstrong, Felipe de Faria Teixeira, and Andrew R Teixeira*
Chemical Engineering, Worcester Polytechnic Institute, Worcester, MA

We herein found that feed modulation during methane oxidation enhances conversion with pre-adsorbed oxygen activating methane and promotes hydrogen production in the methane-rich cycle, with sufficiently fast pulses to optimize surface coverage. This study presents limits and conditions for optimizing activity, selectivity and catalyst lifetime beyond equilibrium using dynamic catalysis.

Dynamic Catalytic Ammonia Decomposition: A Strong Coupling between Localized Transient Heating and Reaction Kinetics.

Korawich Trangwachirachai *and Jimmy A. Faria*
Catalytic Processes and Materials, MESA+ Institute for Nanotechnology, Faculty of Science and Technology, University of Twente, Enschede, Overijssel, Netherlands

The dynamic reaction result shows the possibility in utilizing a Joule heating technique to localize heat specifically at the catalyst and enhance the reaction kinetics.

Introducing *Stimulando* Time-Resolved IR Spectroscopy to Study Resonant Catalysis in Pulsed Light-Stimulated CO_2 Hydrogenation.

Florentien Brzesowsky*, Mees R. Emond, Bert M. Weckhuysen, and Matteo Monai*
Inorganic Chemistry and Catalysis group, Institute for Sustainable and Circular Chemistry, Utrecht University, Utrecht, Netherlands

Development of high time-resolution IR spectra to study CO_2 hydrogenation under intermittent light stimulation. *Stimulando* involves delivering the stimulus to the catalyst, observing the area affected by the stimulus and correlating with performance to determine how much of the catalysis is affected by the stimulus.

Dynamic-Magnetic-Field-Enhanced Thermal Catalysis: Beyond Temperature Control for Hydrogen Production from Ammonia.

Alexander Adogwa[1] *and Ming Yang*[2]
(1)Chemical Engineering, Clemson University, Clemson, SC, (2)Chemical and Biomolecular Engineering, Clemson University, Clemson, SC

We demonstrate the far-reaching catalytic implication of dynamic-magnetic-field-enhanced thermal catalysis. Although standard thermocatalytic hydrogen recovery from ammonia is often

held back by the initial *N-H scission and associative *N desorption, by inducing catalyst spin (de)magnetization under MIH, we create a favorable pathway for both steps, surpassing limitations of standard thermocatalysis.

Unveiling Dynamics of Cu/ZIF-8 Catalyst: Operando and Forced Dynamic Reactor Studies for CO_2 Hydrogenation to Methanol.

Pia Dally[1] *and Pedro Castaño*[2]
(1)KAUST, Thuwal, -, Saudi Arabia, (2)KAUST Catalysis Center, King Abdullah University of Science and Technology, Thuwal, Saudi Arabia

Our work develops an advanced workflow using forced dynamic operando reactors and high-pressure pulsing, combined with in-situ and operando techniques. This approach aims to thoroughly analyze the dynamic behavior of Cu/ZIF-8 catalyst during CO_2 hydrogenation, offering insights beyond those possible with kinetic modeling alone.

ELECTRO PHOTO - ELECTROCATALYSIS AND PHOTOCATALYSIS

ELECTRO PHOTO - MODELING ELECTROCATALYTIC SYSTEMS

Wednesday, June 11, 2025 3:40 PM - 5:40 PM
Centennial Ballroom I

Chair: Tej Choksi, Nanyang Technological University

Co-Chair: Carine Michel, ENS Lyon

Challenges in Modeling Adsorption Processes in (electro)Catalysis.

Nitish Govindarajan
School of Chemistry, Chemical Engineering, and Biotechnology, Nanyang Technological University, Singapore, Singapore

This talk will discuss the challenges in the accurate estimation of adsorption energies and the description of adsorption isotherms at (electro)catalytic interfaces. Examples of using atomistic simulations to study the impact of the various molecular interactions at interfaces on adsorption energies will be highlighted.

Understanding the Difference between Thermal and Electro-Catalysis for CH_x Species on Transition Metals.

Anwin John[1] *and Jeffrey Greeley*[2]
(1)Chemical Engineering, Purdue University, West Lafayette, IN, (2)Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN

This study compares activation barriers for hydrogenation reactions catalyzed by surfaces and proton-coupled electron transfer (PCET) processes. We use DFT simulations to establish that PCET reactions exhibit a clear Brønsted-Evans-Polanyi (BEP) relationship, while surface-

mediated responses do not. These findings highlight critical thermodynamic and kinetic differences between thermal and electrocatalytic processes.

Multi-Scale Modeling Guided CO Electroreduction to Acetate.

Yuting Xu[1]*, Wanyu Deng*[2]*, Ahryeon Lee*[3]*, Hefei Li*[3]*, Yilang Liu*[1]*, Jiaqi Yang*[1]*, Feng Jiao*[2,3]*, and Fanglin Che*[1]
(1)Chemical Engineering, University of Massachusetts Lowell, Lowell, MA, (2)Energy, Environmental, and Chemical Engineering, Washington University in St. Louis, St. Louis, MO, (3)Washington University in St. Louis, St. Louis, MO

This study integrates GC-DFT and MKM simulations to identify the reaction mechanism for CORR-to-acetate under various operando conditions. The selectivity of acetate can be specifically enhanced over the catalyst with optimal binding energy of CH*. A synergetic loop between experiment and theory can allow us to make reliable predictions.

Electrolyte Effects on Electrocatalytic Reactions through Multiscale Modeling of the Electrochemical Double Layer.

Derek Zhu*, Soumya Chatterjee, Scott T. Milner, and Michael Janik*
Chemical Engineering, The Pennsylvania State University, University Park, PA

The DFT/FF-MD multiscale approach enables modeling of both the reaction process using DFT and the local field within the EDL environment through classical MD. This facilitates the study of how surface charge density, ion concentration, and ion identity influence the stability of adsorbates in ways that were previously inaccessible.

Understanding Acid Electrolyte Adsorption and pH Effects in Oxygen Electrocatalysis.

Kasun Gunasooriya
Chemical, Biological & Materials Engineering, University of Oklahoma, Norman, OK

Understanding the solid-liquid interface, especially the effects due to acid electrolyte anions and pH is crucial in designing and optimizing existing electrocatalysts under diverse electrochemical microenvironments. We provided critical insights into the non-innocent role of acid electrolyte anions and developed new microkinetic models that can capture pH effects.

Generalized Bulk Descriptors for Predicting O and OH Adsorption Energies on Metal Oxides on Non-Octahedral Metal Oxides.

Hyeonjung Jung *and Michal Bajdich*
SUNCAT Center for Interface Science and Catalysis, SLAC National Accelerator Laboratory, Menlo Park, CA

In the search for active and stable catalysts, density functional theory (DFT) and machine learning (ML)-based models can accelerate the screening of materials, aiming to derive more accurate and useful outputs from simpler inputs.

FUNDAMENTALS - FUNDAMENTALS OF CATALYSIS AND SURFACE SCIENCE

FUNDAMENTALS - CATALYST DESIGN AND SURFACE SCIENCE 2

Wednesday, June 11, 2025 3:40 PM - 5:40 PM
Centennial Ballroom II

Chair: Rajat Subhra Ghosh, Cummins, Inc.

Co-Chair: Ari Fischer, School of Chemistry, Chemical Engineering and Biotechnology, Nanyang Technological University

KEYNOTE: Heterogeneous Atomic Catalysts: Isolated Atoms, Ensembles, Dimers.

Hyunjoo Lee
Department of Chemical & Biomolecular Engineering, Korea Advanced Institute of Science and Technology (KAIST), Daejeon, Korea, Republic of (South)

Heterogeneous atomic catalysts, whose structure is elaborately controlled and the surface reaction is better understood, can be a new paradigm with higher catalytic activity, selectivity, and durability, and used in industrial applications.

Experimental and Modeling Studies on the Impact of Promoters on Surface Oxygen Species in Ethylene Epoxidation on Ag/α-Al2O3 Catalysts.

Shiuan-Bai Ann[1]*, Shawn Lu*[1]*, Jin-Xun Liu*[1]*, and Suljo Linic*[2]
(1)Department of Chemical Engineering, University of Michigan, Ann Arbor, MI, (2)Chemical Engineering, University of Michigan, Ann Arbor, MI

We deployed first-principles density functional theory, *in operando* surface-enhanced Raman spectroscopy, kinetic measurements, and experiment-guided microkinetic modeling to investigate how Cs and Cl promoters influence oxygen intermediates and the properties of Ag/α-Al_2O_3 arriving to a picture that depicts the intricate interplay between different mechanisms of promotion depending on reactions conditions.

Ultrathin Tungstate Films on MgO(100): Model Catalysts for Chemical-Looping Oxidative Dehydrogenation (CL-ODH) of Alkanes.

Andrew Pedersen[1]*, Fanxing Li*[2]*, and H. Henry Lamb*[2]
(1)Chemical & Biomolecular Engineering, North Carolina State University, Raleigh, NC, (2)Department of Chemical and Biomolecular Engineering, North Carolina State University, Raleigh, NC

We report the growth of ultrathin WO3 films and the synthesis of monolayer Na2[W2O7] films on MgO(100). The resultant films were characterized by X-ray photoelectron spectroscopy (XPS), grazing-incidence X-ray diffraction (GI-XRD), and Raman spectroscopy to determine film composition and W oxidation state(s), crystallographic phase(s), and local structure and bonding, respectively.

Decyphering Facet-Dependent Water Impact on Alkanol Dehydration on TiO_2.

Wenda Hu[1,2], *Jinshu Tian*[3], *Anthony Savoy*[2], *Fan Lin*[1], *Zihao Zhang*[1], *Yiqing Wu*[1], *Junming Sun*[2], *Huamin Wang*[1], *Jian Zhi Hu*[1,2], *and Yong Wang*[1,2]
(1)Pacific Northwest National Laboratory, Richland, WA, (2)Washington State University, Pullman, WA, (3)Zhejiang University of Technology, Hangzhou, Zhejiang, China

We revealed that water inhibits alkanol dehydration on TiO2(001) four times more than on TiO2(101). On TiO2(001), isopropoxide-H2O complexes raise activation barriers by 49 kJ/mol, while weakly bonded IPA-H2O on TiO2(101) increases it by 23 kJ/mol. These findings provide valuable guidance for designing catalysts for water-containing environments.

Modulation of Metal Oxide Surface Basicity Using Ppm Levels of Single Atoms of Pt on FeO_x.

Shiva Murali[1], *Honghong Shi*[2], *Fan Lin*[2], *Oliver Gutiérrez-Tinoco*[2], *Johannes Lercher*[2], *Huamin Wang*[2], *and Yong Wang*[1,2]
(1)The Gene and Linda Voiland School of Chemical Engineering and Bioengineering, Washington State University, Pullman, WA, (2)Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA

Small ppm loadings of reduction stable single atom Pt/FeO_x introduces new Lewis acid-base site pairs for acetone aldol condensation with greater tunability and control of individual elementary reaction steps. Base catalyzed α-H enolation activation barrier is lowered, which changes rate determining step to C-C coupling and enhances activity.

HYDRO ECON - CATALYSIS FOR THE HYDROGEN ECONOMY

HYDRO ECON - METHANE PYROLYSIS

Wednesday, June 11, 2025 3:40 PM - 5:40 PM
Centennial Ballroom III

Chair: Aayush Singh, SandboxAQ

Co-Chair: Zahra Almisbaa, Saudi Aramco

Induction Heating Impact on Catalytic Methane Decomposition to Hydrogen Beyond Thermal Effect.

Ben Ko[1], *Erdem Sasmaz*[1], *Henry Moise*[2], *and Matteo Cargnello*[2]
(1)Chemical and Biomolecular Engineering, University of California, Irvine, Irvine, CA, (2)Chemical Engineering, Stanford University, Stanford, CA

This study explores catalytic methane decomposition (CMD) using induction heating (IH) to examine magnetic field effects on catalyst behavior. Results show IH enhances methane conversion by 24% at 750 ºC and stability of Fe/Al_2O_3 compared to conventional heating. The magnetic field effect on surface properties and reaction mechanisms is discussed.

Using Operando TEM to Clarify the Effect of (Earth) Alkali Additives on Ni/C Catalysts for Catalytic Methane Pyrolysis.

Daan van Eck[1]*, Suzan E. Schoemaker*[1]*, Stefan Bismeijer*[1]*, Erik Betz-Güttner*[1]*, Tom A. J. Welling*[2]*, and Petra E. de Jongh*[1]
(1)Materials Chemistry and Catalysis, Utrecht University, Utrecht, Netherlands, (2)Frontier Research Institute for Interdisciplinary Sciences, Tohoku University, Sendai, Japan

In this study, operando transmission electron microscopy is used alongside macroscopic catalytic testing to understand the influence of alkali (earth) additives to Ni/C catalysts on a microscopic scale. Slower growth of individual nanofibers in Mg-promoted catalysts contributes to a higher carbon yield and a longer lifetime on the macroscopic scale.

The Role of Hydrogen on the Kinetics of Methane Pyrolysis.

Caleb Bavlnka*, Laura Alejandra Gomez Gomez, Phuong Nguyen Thi, Daniel E. Resasco, and Steven Crossley*
School of Sustainable Chemical, Biological and Materials Engineering, University of Oklahoma, Norman, OK

Catalytic methane pyrolysis could produce industrial scale CO_2-free hydrogen by also producing base growth carbon nanotubes with in situ separation. We show hydrogen significantly impacts methane conversion rates, and utilize a kinetic model, measured barriers, and reaction orders for methane and hydrogen to explain the reaction mechanism.

Exsolution-Driven Catalytic Decomposition of Methane Via. $SrFe_xAl_{12-x}O_{19}$ Hexaaluminates for CO_x-Free Hydrogen and Carbon Nanotubes.

Samuel Portillo[1]*, Mohammadreza Kosari*[1]*, Kunran Yang*[2]*, Andrew Pedersen*[1]*, Elizabeth Nguyen*[1]*, and Fanxing Li*[1]
(1)Chemical & Biomolecular Engineering, North Carolina State University, Raleigh, NC, (2)Department of Chemical and Biomolecular Engineering, North Carolina State University, Raleigh, NC

Study demonstrates that $SrFe_xAl_{12-x}O_{19}$ hexaaluminates are active for CDM. Activity of the material is attributed to structure collapse to α-Fe supported on $SrAl_2O_4/FeAl_2O_4$. Differences in activity and carbon morphology depend on iron loading. Fragmentation of Fe nanoparticles causes deactivation. The roles of α-Fe and Fe_3C in iron-based CDM are explored.

Cerium-Assisted Iron Oxidation in Nickel-Catalyzed Chemical Looping Dry Reforming.

Minjung Kim[1] *and Shang Zhai*[2]
(1)Mechanical and Aerospace Engineering, The Ohio State University, Columbus, OH, (2)Department of Mechanical and Aerospace Engineering, The Ohio State University, Columbus, OH

This study explores iron-nickel oxide supported on CeO_2 for chemical looping dry reforming of methane, converting CH_4 and CO_2 into syngas. Ni facilitates CH4 pyrolysis and Fe-Ce acts as oxygen carriers. Optimal Ni loading and CeFeO3 formation ensure high methane and CO2 conversion, stability, and minimal carbon accumulation.

Turquoise Hydrogen and Carbon Nanotubes Generation By Catalytic Decomposition of Methane and Toluene.

Qian Huang*, Biswajit Saha, Sathyapal Churipard R., and Ajay Dalai*
Chemical and Biological Engineering, University of Saskatchewan, Saskatoon, SK, Canada

This study highlights that ferrocene-catalyzed decomposition of methane and toluene results in a higher quality of carbon products. This study emphasizes the dual role of toluene as both a solvent for catalyst delivery and an additional carbon source, contributing positively to the overall production of hydrogen and carbon.

NEW COMP - NEW METHODS IN COMPUTATIONAL CATALYSIS

NEW COMP - DYNAMIC SAMPLING

Wednesday, June 11, 2025 3:40 PM - 5:40 PM
Hanover Hall CDE

Chair: Judit Zádor, Sandia National Laboratories

Co-Chair: Wenshuo Hu, Texas Tech University

Data-Efficient Modeling of Catalytic Reactions Via Enhanced Sampling and on-the-Fly Learning of Machine Learning Potentials.

Simone Perego*, Luigi Bonati, and Michele Parrinello*
Atomistic Simulations, Istituto Italiano di Tecnologia, Genova, Italy

We developed a workflow combining enhanced sampling and active learning to construct machine learning potentials requiring only ~1,000 DFT calculations per reaction. Applied to ammonia decomposition on FeCo catalysts, this approach accurately captured reaction mechanisms, free energy profiles, and dynamic surface behavior under operando conditions, enabling efficient catalytic modeling.

Unraveling Competing Catalytic Reactions Sharing a Common Transition State through Blue Moon Sampling with Path-Based Reaction Coordinate.

Monika Gešvandtnerová[1,2]*, Pascal Raybaud*[3]*, Céline Chizallet*[3]*, and Tomáš Bučko*[2,4]
(1)Université de Lorraine, Metz, France, (2)Faculty of Natural Sciences, Comenius University,

Bratislava, Slovakia, (3)IFP Energies Nouvelles, Solaize, France, (4)Institute of Inorganic Chemistry, Slovak Academy of Sciences, Bratislava, Slovakia

Blue moon ab initio molecular dynamics with a path-based reaction coordinate combined with Bennett-Chandler theory quantified temperature-dependent pathway preferences in isobutanol dehydration. Competing pathways with a shared dynamic transition state (TS) were identified, revealing a post-TS bifurcation. This work advances the accurate determination of rates for key alcohol dehydration reactions.

A Molecular View of Methane Activation on Nickel Surfaces through Enhanced Sampling and Machine Learning Potentials.

Yinan Xu[1]*, Yezhi Jin*[1]*, Jireh García Sánchez*[1]*, Gustavo Perez Lemus*[1]*, Pablo Zubieta*[1]*, Massimiliano Delferro*[2]*, and Juan De Pablo*[3]
(1)Pritzker School of Molecular Engineering, University of Chicago, Chicago, IL, (2)Chemical Sciences and Engineering Division, Argonne National Laboratory, Lemont, IL, (3)Tandon School of Engineering, NYU, New York, NY

Machine-learned potentials (MLPs) combined with enhanced sampling enable detailed molecular view of methane activation on Ni surfaces at experimental conditions. Iteratively refined MLPs, incorporating adaptive biasing forces and key collective variables, predict density functional theory-level energies and forces, revealing temperature-dependent thermodynamics, dynamics, and reactant-surface interactions with unprecedented efficiency and accuracy.

Integrating ML-Accelerated Estimation of Coverage Dependent Thermodynamics in Reaction Mechanism Generator (RMG) for CO Methanation.

Chao Xu *and* ***Richard West***
Department of Chemical Engineering, Northeastern University, Boston, MA

Using an ML model to reduce DFT workload for coverage-dependent microkinetic modeling, we examined how CO coverage influences CO/H binding energies on Ni(111) surfaces. We extended Reaction Mechsnism Generator to incorporate coverage-dependent thermodynamics, enabling construction of a predictive CO/H2 methanation mechanism on Ni(111) for improved heterogeneous catalysis predictions.

KEYNOTE: Bridging Length and Time Scales in Catalysis for C1 Chemistry : From the Molecule to the Catalyst Particle Level.

Veronique Van Speybroeck
Ghent University, Ghent, Belgium

C1 catalysis over zeolites involves multi-scale processes like reactions, transport, and surface barriers. New methods, leveraging machine learning and enhanced sampling molecular dynamics open perspective to understand the dynamics from the molecule to the crystal particle level. Key steps in C1 conversion will be illustrated.

POLYMER - CATALYSIS FOR POLYMER SYNTHESIS, UPCYCLING, AND RECYCLING

POLYMER - C-H ACTIVATION AND OXIDATION

Wednesday, June 11, 2025 3:40 PM - 5:40 PM
Regency Ballroom VI

Chair: Hongfei Lin, Northeastern University

Co-Chair: Hyunjin Moon, National Renewable Energy Laboratory

Upcycling Polyolefin Waste to Light Olefins with Ethylene and Base-Metal Heterogeneous Catalysts.

Alexis Bell
Department of Chemical and Biomolecular Engineering, University of California-Berkeley, Berkeley, CA

Polyethylene and polypropylene comprise 57% of polymer waste in landfills. This work demonstrates the feasibility of deconstructing PE and PP, individually or in a mixture to form propylene and isobutylene, important feedstocks for the chemical industry, using inexpensive heterogeneous catalysts in a semi-batch reactor.

Oxidative Upcycling of Polyolefins, with and without Chain Cleavage.

Costanza Leonardi[1] and ***Susannah Scott***[2]
(1)Chemical Engineering, University of California, Santa Barbara, Santa Barbara, CA, (2)Department of Chemical Engineering, University of California, Santa Barbara, Santa Barbara, CA

Selective catalytic oxidation of polyethylene without chain cleavage was achieved in aqueous tBuOOH in the presence of $MnBr_2$, leading to polyketone materials. Changing the reaction conditions led to oxidative chain cleavage, resulting in polar waxes.

Effect of Dehydrogenation Catalyst and Solvent on Hydrogen-Free Tandem Heterogeneous Catalysis for Polyethylene Depolymerization Via an Olefin-Intermediate Approach.

Andrew Tran[1], Selena Moore[1], Andreas Palmateer[1], Jose Naranjo-Mendez[1], Dimitri Gatzios[2], and ***Lucas Ellis***[1]
(1)School of Chemical, Biological, and Environmental Engineering, Oregon State University, Corvallis, OR, (2)Chemical, Biological, and Environmental Engineering, Oregon State University, Corvallis, OR

This study examines hydrogen-free tandem catalysis for polyethylene depolymerization, focusing on the dehydrogenation catalyst and solvent effects. A Pd-based catalyst achieved the highest overall rates. Key findings reveal structure-property relationships and the crucial role of solvent thermodynamics in enhancing reaction efficiency and selectivity at low temperatures.

Mechanistic Insights in the Oxidative Conversion of Polyethylene Towards Di-Carboxylic Acids with O_2/NO.

Thomas Jan Smak[1]*, Rinke M. Altink*[2]*, Jan C. van der Waal*[2]*, Ina Vollmer*[1]*, and Bert M. Weckhuysen*[1]
(1)Inorganic Chemistry and Catalysis, Utrecht University, Utrecht, Utrecht, Netherlands, (2)Brightsite/TNO, Geleen, Limburg, Netherlands

The conversion of polyethylene towards di-carboxylic acids using O_2/NO has been studied. It is observed that the addition of NO increases the di-carboxylic acid yield from 7 up to 32 mol%. The reactions were followed over time using a combination of GC, IR and NMR, leading to new mechanistic insights.

Hydroformylation of Plastic Oil Model Compounds into Aldehydes Catalyzed By Unmodified Cobalt Carbonyl Under Mild Conditions.

Houqian Li[1]*, Clark Landis*[2]*, and George Huber*[3]
(1)Department of Chemical and Materials Engineering, New Mexico State University, Las Cruces, NM, (2)Department of Chemistry, University of Wisconsin-Madison, Madison, WI, (3)Department of Chemical and Biological Engineering, University of Wisconsin-Madison, Madison, WI

This study examines hydroformylation kinetics of plastic pyrolysis oils under mild conditions (<80 bar, <453 K), focusing on isomerization-hydroformylation tandem reactions. A mechanistic model quantitatively describes aldehyde selectivity and formation rates, providing insights to enhance the conversion of waste plastics into value-added chemicals.

One-Pot Conversion of Poly(lactic acid) to 1,2-Propanediol on Cu Catalysts.

Yiqi Xu[1]*, Damilola Akinneye*[2]*, and J. Will Medlin*[3]
(1)Chemical and Biological Engineering, University of Colorado-Boulder, Boulder, CO, (2)Chemical & Biological Engineering, University of Colorado, Boulder, Boulder, CO, (3)Department of Chemical and Biological Engineering, University of Colorado Boulder, Boulder, CO

We developed a one-pot tandem reaction of Poly (lactic acid)(PLA) ethanolysis and ethyl lactate (EL) hydrogenation on a bifunctional Cu-based catalyst to produce 1,2-propanediol (PDO), which is widely used as a plasticizer, surfactant, and resin. The PLA can be completely depolymerized with PDO selectivity as high as ~99%.

OTHER EVENTS

WEDNESDAY POSTER SESSION

Wednesday, June 11, 2025 6:00 PM - 8:00 PM
Grand Hall

Novel Green Method for the Preparation of Supported Sub-10 Nm Non-Noble Metal (Cu, Sn and Ga) Nanoparticles.

Abdennour Benabbas, Catherine Especel, and ***Florence Epron***
CNRS, Université de Poitiers, Institut de Chimie des Milieux et Matériaux de Poitiers-IC2MP, Poitiers, France

Abundant non-noble metals such as copper, tin, and gallium are alternatives for tomorrow's sustainable industries. Herein, we have successfully developed a general, efficient, and inexpensive green method that gives rise to some fascinating physico-chemical properties of these metals, triggered at the nanoscale in both liquid and solid states.

Regulating Lattice Oxygen Property of TiO_2 Redox Catalyst for Enhanced Oxidative Dehydrogenation of Ethane.

Xiaoqiao Zhang*, Jianhong Gong, Lingtao Liu, and Xiaoli Wei*
Sinopec Research Institute of Petroleum Processing, Beijing, China

A systematic set of machine-learning designed catalysts were applied in ethane oxidative dehydrogenation reaction, aiming to achieve accurate regulation of catalytic performance and product distribution through the regulation of molecular oxygen on the catalyst surface.

In – Flow Catalytic Production of Levoglucosenone from Levoglucosan over Propylsulfonic Acid Functionalized SBA-15 Using γ – Valerolactone.

Alexa Gonzalez-Rosario*[1,2], Oscar Oyola-Rivera[3], and Nelson Cardona Martinez[4]*
(1)Chemical Engineering, University of Puerto Rico - Mayagüez, Mayaguez, PR, (2)Department of Natural Sciences, University of Puerto Rico - Carolina, Carolina, PR, (3)Ketjen Corp, Pasadena, TX, (4)Department of Chemical Engineering, University of Puerto Rico - Mayagüez, Mayagüez, PR

We studied the reaction kinetics and catalytic performance of propylsulfonic acid functionalized SBA-15 for levoglucosan (LGA) conversion into levoglucosenone (LGO) in a flow reactor. We obtained a selectivity of 67% towards LGO at 57% LGA conversion. The reaction is second-order reaction for LGA with an activation energy of 37.6 kJ/mol.

Microwave-Assisted Catalytic Gasification of Various Biomass with Mixed Plastic Wastes for Clean H2 Production.

Ashraf Abedin*, Duy Hien Mai, and Pranjali Muley*
NETL Support Contractor, Morgantown, WV

Catalytic gasification of biomass with plastics has been a challenge since it requires an optimal catalyst to simultaneously activate these materials with complex chemical compositions. This study highlights the roles of Fe-oxide catalyst and biochar produced in-situ during in microwave gasification of plastic-biomass to maximize product selectively towards clean H_2.

Opportunities and Challenges in Utilization of Unrefined Methanol Synthesized from Waste Methane.

Hsiang-Sheng Chen *and Paul Yelvington*
M2X Energy Inc., Rockledge, FL

M2X Energy explores hydrogen production via electrolysis using crude methanol derived from waste methane sources. While impurities increase energy consumption compared to purified methanol, potential solutions include optimizing synthesis operations or developing impurity-tolerant processes, promoting direct use of unrefined feedstock while reducing energy use and emissions from waste methane utilization.

Pretreatment and Catalyst Effects on Biocrude Production Via Hydrothermal Liquefaction of Canadian Lignocellulosic Residues for Renewable Transportation Fuels.

John Churchill, Venu B. Borugadda, and ***Ajay Dalai***
Chemical and Biological Engineering, University of Saskatchewan, Saskatoon, SK, Canada

Mild pretreatment and catalysts significantly influence biocrude yield and quality from lignocellulosic residues during HTL. Despite ineffective washing and steam explosion, alkaline pretreatment with Fe enhanced yields from high-lignin, while acid pretreatment with K_2CO_3 and Fe reduced biocrude oxygen in low-lignin feedstocks. Further methods to improve HTL were also identified.

Hydrodeoxygenation of Lignocellulosic Model Compound Using Nickel Phosphide Catalyst Supported on Mesoporous Geopolymer.

Suraj P[1] *and Sonali Sengupta*[2]
(1)Chemical Engineering, Indian Institute of Technology, Kharagpur, Kharagpur, India,
(2)Chemical Engineering, IIT Kharagpur, Kharagpur, India

Catalytic hydrodeoxygenation is an effective route to upgrade highly oxygenated bio-oils. Herein, nickel deposited (Ni/H-GP) and nickel phosphide (Ni_2P/H-GP) deposited on mesoporous and acidic geopolymer were prepared and tested for anisole hydrodeoxygenation to cyclohexane. Ni_2P/H-GP showed high anisole conversion and selectivity to cyclohexane because of presence of moderate acid sites.

Development and Enhancement of Iron-Based Catalysts to Boost the Conversion of CO_2 to Liquid Hydrocarbons.

Florian Mai
Chair of Chemical Process Engineering, Faculty of Engineering, University of Bayreuth, Bayreuth, Germany

The focus of this research is the development of new catalysts capable of performing both reactions (RWGS + FTS) simultaneously in a single step, thereby increasing the overall efficiency.

Therefore, this study specifically investigated the effects of promoters Cu, Zn and K on sintered iron catalysts for CO_2 hydrogenation.

Utilization of Waste Biomass and Sewage Sludge for CO_2 Capture.

Sarah Stofik, *Thossaporn Onsree, Patton Courie, and Jochen Lauterbach*
Department of Chemical Engineering, University of South Carolina, Columbia, SC

Direct air capture is an emerging field that could counteract the negative impact of rising CO_2 emissions. This work utilizes waste biomass to optimize a material that can capture CO_2 from the air. Initial studies determined that wood-based biomass can capture over 8 wt% in CO_2.

Zeolites and Its Active Cations: Direct Air Capture of CO_2.

Do Yeong Kim[1], *Kyeong-Hun Ryu*[2], *Sungjoon Kweon*[3], *Min Bum Park*[3], *and Sung Bong Kang*[2]
(1)School of Environment and Energy Engineering, Gwangju Institute of Science and Technology, Gwangju, Korea, Republic of (South), (2)Department of Environment and Energy Engineering, Gwangju Institute of Science and Technology, Gwangju, Korea, Republic of (South), (3)Department of Energy and Chemical Engineering, Incheon National University, Incheon, Korea, Republic of (South)

Major findings in this study—including the DAC performance of ZSM-5 with respect to the kind of cation in real atmospheric air and the effect of humidity for DAC performance and behavior on ZSM-5—can be further explored for practical application of zeolite ZSM-5 as a feasible DAC adsorbent.

Advancing Molybdenum Carbide Catalysts for Sustainable Syngas Production in the Reverse Water-Gas Shift.

Wijnand Marquart, Michael Claeys, and ***Nico Fischer***
Department of Chemical Engineering, Catalysis Institute, University of Cape Town, Cape Town, Western Cape, South Africa

Thermodynamics of the rWGS confirm that an effective catalyst kinetically suppresses CO_x methanation and the Boudouard reaction. Mo_2C based catalysts have shown to be highly selective but at elevated pressures these side reactions are more prominent. Transient flow experiments using $^{13}CO_2$ suggest that CH_4 is predominantly formed via CO methanation.

Alkali Activated Carbons from Melamine-Resorcinol-Formaldehyde Resin: Activation Mechanism.

Shailza Sharma[1], *Selvakannan Periasamy*[2], *and Suresh Bhargava*[3]

(1)School of Science, RMIT University, Melbourne, VIC, Australia, (2)Applied Chemistry, RMIT University, Melbourne, Australia, (3)CAMIC, RMIT, Melbourne, VIC, Australia

The escalating CO_2 emissions necessitate advanced mitigation strategies. This study developed nitrogen-rich activated carbons derived from melamine-based resins via a template-assisted approach, enhancing microporosity and achieving a high surface area (2465 m^2/g) with tunable pore diameter (20.4 Å). Comprehensive characterization demonstrates their potential for efficient CO_2 capture and utilization.

Direct CO_2 Hydrogenation to *E-Crude* over a Promoted Fe-Based Catalyst.

***Mattia Piacentini**, Beda Rolandi, Alessandro Porta, Luca Lietti, and Carlo Giorgio Visconti*
Dipartimento di Energia, Politecnico di Milano, Milan, Italy

A promoted iron-based catalyst was tested under conditions favoring high selectivity towards e-crude, primarily in the C_8-C_{16} range, with CH_4 and C_2-C_4 paraffins accounting for less than 15% of the products. The catalyst exhibited reversible deactivation, primarily driven by the water partial pressure.

Novel Sputtered ITO/TiO_2 Catalyst for Highly Efficient Reverse Water-Gas Shift Reaction.

***Luis F. Bordini**[1], Camila P. Ferraz[2], João Monnerat[3], and **Pedro Romano**[4]*
(1)School of Chemistry, Federal University of Rio de Janeiro, Rio de janeiro, Rio de janeiro, Brazil, (2)Chemistry Institute, Federal University of Rio de Janeiro, Rio de Janeiro, Rio de Janeiro, Brazil, (3)Chemistry Institute, Federal University of Rio de Janeiro, Rio de Janeiro, Brazil, (4)Campus D. de Caxias, Federal University of Rio de Janeiro, Rio de Janeiro, Brazil

The study highlights the industrial significance of the Reverse Water Gas Shift (RWGS) reaction for carbon capture and utilization. By employing sputtering for synthesizing ITO/TiO_2 catalysts, the research achieved near-equilibrium conversion and ~100% CO selectivity, advancing CO_2 utilization and supporting sustainable synthetic fuel production through innovative catalytic processes.

Tailoring Catalyst for CO_2 Hydrogenation: Synthesis and Characterization of NH_2-MIL-125 Frameworks.

***Leidy Patricia Figueroa Quintero**[1], Tomás Cordero[2], Enrique V. Ramos Fernandez[1], Unni Olsbye[2], and Javier Narciso[1]*
(1)University Institute of Materials (IUMA), Inorganic Chemistry Department, University of Alicante, Alicante, Spain, (2)Department of Chemistry, University of Oslo, Oslo, Norway

This work details the innovative modification of NH2-MIL-125 with Zr, Ce, and Cu, enhancing its stability and catalytic efficiency. These advanced catalysts offer a sustainable approach to CO_2 valorization, paving the way for methanol production while contributing to environmental impact reduction.

CO_2 Hydrogenation over Cu on Early Transition Metal Carbides and Nitrides on Alumina Supports.

Siobhan Brown[1]*, Justin Notestein*[2]*, and Neil Schweitzer*[3]
(1)Center for Catalysis and Surface Science, Northwestern University, Evanston, IL,
(2)Department of Chemical & Biological Engineering, Northwestern University, Evanston, IL,
(3)Department of Chemical and Biological Engineering, Northwestern University, Evanston, IL

The goal of our work is to study the dynamic nature of supported early transition metal carbides and nitrides (TMNC) by varying their local environment by careful synthesis of the TMNC layer. We present a study of the impact of TMNC phases on supported-Cu for CO_2 hydrogenation to C1 products.

Cu-ZnO Bimetallic Catalyst for Industrial Relevant Production of C_{2+} Alcohols in the Alkaline CO_2 Electrolyzer.

Taha Baghban-Ronaghi[1]*, Seyed Parsa Amouzesh*[1]*, Sina Fazlifard*[1]*, Praveen Raju*[1]*, and Mohammad Asadi*[2]
(1)Chemical and Biological Engineering, Illinois Institute of Technology, Chicago, IL,
(2)Chemical and Biological Engineering, Illinois Tech, Chicago, IL

Electrocatalytic CO_2 reduction in alkaline media shows promise for carbon mitigation and sustainable alcohol production at industrial rates. However, achieving high alcohol selectivity with copper catalysts in moderate environments proves challenging. Advancing efficient catalysts to maintain high current densities and selectivity for alcohols remains a key challenge.

Direct CO_2 Hydrogenation to C_{2+} carboxylic Acids Via Heterogenous Thermo-Catalysis in Liquid Phase.

Satya Sireesha Rameswarapu[1]*, Rajan Lakshman*[1]*, Paul Webley*[1]*, and Akshat Tanksale*[2]
(1)Chemical and Biological Engineering, Monash University, Clayton, VIC, Australia,
(2)Chemical Engineering, Monash University, Clayton, VIC, Australia

This research tackles the challenges of direct CO_2 hydrogenation to C_{2+} carboxylic acids, including low yields and high energy barriers, by employing metal organic frame work-derived catalysts. It establishes sustainable route for acetic acid production, reducing CO_2 emissions, decreasing fossil fuel dependence, and promoting green chemical synthesis for industrial applications.

Advancing CO_2 Methanation Catalysts.

Shubham Sharma and ***Sagar Sourav***
Chemical Engineering, Indian Institute of Technology Madras, Chennai, Tamil Nadu, India

A novel catalyst was designed and demonstrated for highly exothermic CO_2 methanation reaction. The core of the catalyst has a highly conductive material for effective heat dissipation, where as the surface layers have chemical functionalities to efficiently carry out the reaction.

Probing the Effects of Potassium on the Structural Properties and Reactivity of Iron-Based CO_2 Hydrogenation Catalysts.

Sinqobile Vuyisile Lusanda Mahlaba[1], *Alisa Govender*[2], *Jaco Olivier*[3], *and Eric van Steen*[1,4]
(1)Catalysis Institute, Dpt. Chemical Engineering, University of Cape Town, Rondebosch, Western Cape, South Africa, (2)Energy Operations, R&T, SASOL, Sasolburg, Free State, South Africa, (3)Centre for High Resolution Transmission Electron Microscopy, Nelson Mandela University, Gqeberha, Eastern Cape, South Africa, (4)Catalysis Institute, Dpt. Chemical Engineering, University of Cape Town, Cape Town, South Africa

The role of potassium on the performance of pre-carbided hematite in the hydrogenation of CO2 shows that the activity is hardly affected, whereas the selectivity is strongly affected by potassium. This is linked to the phase composition, and the CO2 and CO adsorptive properties.

Thermocatalytic Hydrogenation CO_2 to Methanol over Medium and High-Entropy Oxides.

Amy Knorpp[1], *Monika Mielniczuk*[1,2], *and Michael Stuer*[1]
(1)Empa, Duebendorf, Switzerland, (2)AGH University of Science and Technology, Krakow, Poland

Mesoporous high-entropy oxides (HEOs) were synthesized with 5 to 7 cations (Al, Cr, Fe, Co, In, Ga, Ce) using a solvothermal technique. Synthesized materials were active for the thermocatalytic hydrogenation of CO_2 to methanol, and differences in the selectivities were observed between samples, showing HEOs are potential tailorable hydrogenation catalysts.

Toward Understanding the Mechanism of Selective Hydrogenation of CO_2 on Rh-Based Catalysts.

Yifeng Zhu, ***Honghong Shi****, Libor Kovarik, John L. Fulton, Oliver Gutiérrez-Tinoco, and Johannes Lercher*
Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA

The multifunctional sites at the FeO_x−Rh interface exhibit significantly stronger interactions with CO_2 compared to Rh-only surfaces, presenting higher energy barriers for C−O bond cleavage while providing a barrierless pathway for the stabilization and facile-hydrogenation of methoxy species, therefore enabling the selective CO_2-to-methanol conversion process.

First-Principles Aided Understanding of Oxidative Degradation of Amines Supported on Silica during CO_2 Capture.

Neha Mehra[1], *Wilson McNeary*[1], *Gabrielle Kliegle*[1], *Wade Braunecker*[2], *and Carrie Farberow*[1]
(1)Catalytic Carbon Transformation and Scale-Up Center, National Renewable Energy

Laboratory, Golden, CO, (2)Chemistry and Nanoscience Center, National Renewable Energy Laboratory, Golden, CO

Stability of amine-based adsorbents against degradation by oxygen is critical for sustained performance over multiple regenerative CO_2 capture cycles. We perform density functional theory calculations on *N*-methyl-3-aminopropyl (MAPS), a secondary amine, to examine CO_2 binding to silica-grafted MAPS and evaluate the energetics of oxidative pathways yielding amide and imine products.

Molten Salt Upcycling of CO_2 to Diverse Carbon Architectures for Energy Storage Applications.

Shannon Mahurin[1]*, Bishnu Prasad Thapaliya*[1]*, Siyuan Gao*[1]*, Dylan Weber*[2]*, Aye Meyer*[2]*, Eric Wolfe*[3]*, and Sheng Dai*[4]
(1)Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN, (2)Manufacturing Science Division, Oak Ridge National Laboratory, Oak Ridge, TN, (3)Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN, (4)Chemical Sciences Division, Oak Ridge National Laboratory (ORNL), Oak Ridge, TN

The electrocatalytic upcycling of CO_2 into value-added carbon materials with controlled microstructure in a carbonate molten salt system as a means to utilize waste CO_2 and reduce carbon emissions is reported. The effect of reaction conditions on the carbon product and a preliminary techno-economic analysis will be presented.

Zeolites-Based Dual Function Materials (DFMs) for CO_2 Capture and in-Situ Methanation: Effect of Zeolite Framework.

Galal Nasser, Shaza Yousef, and ***Jan Kopyscinski***
Catalytic & Plasma Process Engineering, Department of Chemical Engineering, McGill University, Montreal, QC, Canada

This study explores zeolites as potential Dual-Function Materials (DFMs) for integrated CO_2 capture and in-situ methanation. The synthesized cost-effective zeolites demonstrated high CO_2 adsorption. The research contributes to the advancement of efficient carbon management technologies and achieving the goal of net-zero emissions by enhancing the utilization of CO_2 and energy.

Mo-Modified Zeolites for Methane Aromatization: A Study on Metal Speciation, Distribution, and Control.

Emanuele J Hiennadi[1]*, Fateme Molajafari*[2]*, Rachita Rana*[3]*, Adam Hoffman*[4]*, Simon Bare*[4]*, Joshua D. Howe*[2]*, and* ***Sheima Khatib***[1]
(1)Chemical Engineering, Virginia Tech, Blacksburg, VA, (2)Chemical Engineering, Texas Tech University, Lubbock, TX, (3)Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, MA, (4)Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, Menlo Park, CA

Through combined experimental and computational endeavors, this work investigates what factors may govern the speciation, distribution, and evolution of Mo species supported on H-ZSM-5 for methane aromatization. Preparation technique and/or metal loading can influence the distribution of precatalytic Mo-oxide structures (MoO_2^{2+}, MoO_2OH^+, $Mo_2O_5^{2+}$) existing simultaneously.

Surface Carbon Formation and Its Impact on Methane Dry Reforming Kinetics on Rh-Based Catalysts By Operando Raman Spectroscopy.

*Riccardo Colombo[1], Gianluca Moroni[1], Chiara Negri[1], Matteo Monai[2], Bert M. Weckhuysen[2], and **Matteo Maestri**[1]*
(1)Laboratory of Catalysis and Catalytic Processes - Dipartimento di Energia, Politecnico di Milano, Milano, Italy, (2)Inorganic Chemistry and Catalysis, Institute for Sustainable and Circular Chemistry, Utrecht University, Utrecht, Netherlands

A mechanism for carbon deposition and its impact on Methane Dry Reforming kinetics using rhodium-based catalysts is presented. Coupling operando Raman spectroscopy and kinetic analysis, we discovered that carbon deposition on $Rh/\alpha\text{-}Al_2O_3$ catalyst follows a nucleation-growth mechanism strongly influenced by the CO_2/CH_4 ratio and the CH_4 inlet concentration.

Enhancing Surface Activity through in-Situ Exsolution of Co-Fe Nanoparticles on Co-Doped (La,Sr)FeO_3 Perovskite for Electrocatalytic Oxidative Coupling of Methane (OCM).

Serra Yesilata[1], *Jaesung Kim[1], Yu Jin Kim[2], Matthew Ferree[1], Seval Gunduz[1], Anne Co[3], Minkyu Kim[2], and Umit Ozkan[1]*
(1)William G. Lowrie Department of Chemical & Biomolecular Engineering, The Ohio State University, Columbus, OH, (2)Yeungnam University, Gyeongsan, Geongbuk, Korea, Republic of (South), (3)Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH

Performing oxidative coupling of methane (OCM) reactions in solid oxide cells is a promising approach for converting methane into olefins. This study focuses on modifying the surface properties of Co-doped (La,Sr)FeO_3 via in-situ exsolution of CoFe alloy nanoparticles to enhance its activity for electrochemical OCM reactions.

Support Effects in Fischer-Tropsch Synthesis.

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New developed generation of Fischer-Tropsch catalysts that optimizes the C_{5+} selectivity under ambient pressure condition by leveraging the electronic metal-support interaction. Our hypothesis is that by using basic oxide supports, electron can be injected into metal nanoparticles, strengthening binding of CO to the surface and driving the selectivity toward C_{5+}.

Autothermal Dry Reforming of Methane at Kg-Lab Scale Using Ni-Ugso Catalyst Pellets at Elevated Pressures: A Parametric Study.

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This work presents the experimental evaluation of pelletized Ni-UGSO catalyst applied to dry catalytic reforming of methane at elevated pressures. A kg-lab scale setup was used and the reported results show that the pellets have better performances than the powder used at g-lab scale. The optimal operating conditions are presented.

Microkinetic Modeling of the Fischer-Tropsch Synthesis over Co: Pushing Boundaries through Automated Mechanism Generation.

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The Reaction Mechanism Generator (RMG) is extended to automatically develop detailed chemical kinetic models for the Co-catalyzed Fischer-Tropsch synthesis. RMG explores a chemical reaction space of over 170k possible reactions. Microkinetic modeling with detailed chemical kinetics provides insights into the chain growth mechanism and the role of abstraction reactions.

In-Situ **XAS Investigation of Co-Based Model Catalysts for FTS.**

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This *in-situ/operando* XAS study provides valuable insights into catalyst reduction behavior during FTS. By preparing model catalysts with two different methods, this study promotes to accelerate the identification of key parameters influencing the catalytic performance and especially, by metal-support-interaction, helping optimize catalyst design for improved efficiency and stability in FTS.

Iron Silicalite-1 for Oxidative Dehydrogenation of Ethane.

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Evanston, IL, (2)X-ray Science Division, Advanced Photon Source, Argonne National Laboratory, Lemont, IL, (3)Department of Chemical and Materials Engineering, University of Alabama in Huntsville, Huntsville, AL

This work investigates the selective oxidation of ethane using silicalite-supported iron oxide catalysts. Framework iron species enhance selectivity by modulating acidity, while extra-framework species improve activity. Incorporating nickel facilitates ethane oxidative dehydrogenation with CO_2 as an oxidant, offering an environmentally friendly route to value-added chemicals.

Mechanism in Ethanol Upgrading to 1-Butanol over MgO Catalyst: Insights from Synchrotron Irradiation-Based Nanospectroscopy.

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Synchrotron Irradiation-based Nanospectroscopy (SINS) was employed to investigate ethanol upgrading to 1-butanol over MgO catalysts. By integrating Ex situ Ethanol Temperature-Programmed Desorption and SINS, local reaction intermediates were identified. Results reveal magnesium hydride's role as a surface intermediate, advancing mechanistic understanding of the Guerbet reaction pathway for new catalysts design.

Exploiting Mo-V Catalysts in Non-Oxidative and Oxidative (CO_2- and O_2-Assisted) Propane Dehydrogenation.

Letícia Rasteiro[1]*, Victor Brandão*[2]*, Carsten Sievers*[2]*, and Leandro Martins*[3]
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This study investigates catalysts for propane dehydrogenation (DHP) and oxidative dehydrogenation (ODHP) using CO_2 and O_2. V_MoO_3 showed high stability and selectivity, while MoV-N_2 exhibited higher propane conversion but rapid deactivation in CO_2-ODHP. The findings highlight the importance of reaction conditions in influencing catalyst behavior and coke formation.

Enhancing the Carbon and Energy Efficiency in SAF Production: Converting Alkenes to Aromatics and Hydrogen.

Yang He*, Udishnu Sanyal, Junxia Wang, and Karthikeyan Ramasamy*
Pacific Northwest National Laboratory, Richland, WA

Ga- and Zn-promoted ZSM-5 catalysts boost SAF-range aromatic yields and hydrogen production from olefins, addressing by-product inefficiencies in Fischer-Tropsch synthesis. This scalable approach enhances carbon and energy efficiency in SAF production, optimizing reaction pathways via tailored zeolite acidity and metal sites to support aviation decarbonization and sustainable fuel goals.

Support Effects in Butadiene Hydrogenation over Cu and PtCu Dilute-Limit Alloys.

Ho Yi Lam[1] *and Nathaniel Eagan*[2]
(1)Chemical and Biological Engineering, Tufts University, Medford, MA, (2)Department of Chemical and Biological Engineering, Tufts University, Medford, MA

Selective hydrogenation of 1,3-butadiene to butene was studied using Cu-based catalysts supported on SiO_2, TiO_2, and CeO_2. CeO_2 showed the highest activity but reduced selectivity to form butane. Alloying Cu with Pt improved activity but reduced selectivity, especially on CeO_2, attributed to interfacial site effects and possible Pt aggregation.

Understanding the Effects of Organic Coatings on 4-Nitrostyrene Hydrogenation Selectivity over Pt Catalysts.

Jesús Meléndez Gil*, Wilson A. Smith, and J. Will Medlin*
Department of Chemical and Biological Engineering, University of Colorado Boulder, Boulder, CO

The effects of different organic coatings (thiols, phosphonic acids (PAs), and ionomers) on 1wt%Pt/TiO_2 were studied for the hydrogenation of 4-nitrostyrene. Thiol coatings shifted product selectivity towards 4-aminostyrene, while PAs and ionomers shifted towards 1-ethylnitrobenzene. These changes were attributed to the identity of adsorption sites modified by the different coatings.

Identifying and Solving the Catalytic Deactivation Problem to Improve Process Performance.

Steve Wainwright[1] *and* ***Shane Chen***[2]
(1)Johnson Matthey, Royston, United Kingdom, (2)Johnson Matthey, West Deptford, NJ

A key consideration in catalyst and process design is expected lifetime of the catalyst and the acceptable loss over time of catalytic activity and/or selectivity. By more effectively identifying the root cause of the deactivation in a process the correct mitigation can be implemented in a timely and cost-efficient manner.

Investigating the Kinetics of Ethane Hydrogenolysis over Supported Liquid Metal Catalysts.

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(1)Chemical Engineering, The Pennsylvania State University, University Park, PA, (2)Chemical

and Biomedical Engineering, The Pennsylvania State University, University Park, PA, (3)Department of Chemical Engineering, The Pennsylvania State University, University Park, PA, (4)Department of Chemistry, The Pennsylvania State University, University Park, PA

Ethane hydrogenolysis is studied over Ni-Ga liquid metal catalysts to evaluate the influence of H_2 absorption by Ga. Determination of the surface ensemble sizes and bulk partitioning of the catalytically active metals due to H_2 would allow for the application of these catalysts in combined catalytic reaction/separations.

Mesoporous Organosilica As Catalyst Support for Aqueous Phase Hydrogenation of Phenol: The Effect of Aromatic Content and Amine Loading of the Support.

Snehal Patil[1]*, James N. Gyamfi*[1]*, Anagha Hunoor*[2]*, Luke Gillespie*[1]*, Paul Edmiston*[3]*, and Umit Ozkan*[1]
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ABPS, a silica-based hybrid material, was used as support for Pd catalysts for aqueous phase phenol hydrogenation. Pd catalysts supported on ABPS-type supports performed significantly better than conventional Pd/SBA-15 and Pd/AC. Aromatic groups of ABPS imparted thermal stability to the support and improved Pd dispersion. Amine incorporation enhanced cyclohexanone yield.

Insights into Solvation Thermodynamics Under Different Pores and Solvent Environments in Zeolite Catalysts.

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To clarify the influence of solvent mixtures on the stability of adsorbates, we study their solvation thermodynamics in solvent mixtures and compare them to pure water solvent. Increases (becoming more positive) of solvation entropies are observed in methanol/water mixtures compared to pure water.

Calorimetric Study of Acid-Base Interactions in Solvated Zeolite Voids.

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Calorimetric analysis of base molecule adsorption on acidic zeolites in gas and liquid phases helps build a Born-Haber cycle to assess solvation effects. This study aims to deepen understanding of solvent impacts on acid-base interactions in zeolites, crucial for designing liquid-phase catalytic reactions.

Mechanistic Approaches to Solvent Design for Acid-Catalyzed Biorenewable Chemical Processes.

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(1)Chemical Engineering, Indian Institute of Technology Delhi, New Delhi, India,
(2)Department of Chemistry, Technische Universität München, Garching, Germany

This study explores mechanistic insights into acid-catalyzed lactone dehydration in various solvents, highlighting how solvent nature and polarity influence reaction environments. Optimizing solvent-reactant interactions, including those with Brønsted acidic protons, the study proposes solvent recipes to enhance biomass-derived oxygenate conversions, improving conversion, product selectivity, and reducing reaction free energy barriers.

O_2-Cofeed Demonstrates the Potential of Surface H-Scavenging to Boost Ammonia Decomposition on Ru-Based Catalysts.

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(2)Politecnico di Milano, Dipartimento di Energia, Via La Masa, Milan, Italy

This work reveals that a significant improvement of NH_3 decomposition kinetics lies in the elimination of the H*-saturation. This concept (demonstrated by O_2-cofeed tests) paves the way for designing multifunctional reactors where H_2 is removed from the Ru sites by varying methods, creating an expansive field for chemical reaction engineering.

Highly Efficient Low Metal Content Ni/CeO_2 Catalysts Prepared Bymagnetron Sputtering Deposition for Ethanol Steam Reforming.

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(1)LIPCAT, UFRJ, Rio de Janeiro, Brazil, (2)UFRJ, Rio de Janeiro, Brazil, (3)INMETRO, Rio de Janeiro, RJ, Brazil, (4)Bluenano group, Porto Alegre, RS, Brazil, (5)CNPEM, Campinas, SP, Brazil, (6)Chemistry Institute, Federal University of Rio de Janeiro, Rio de Janeiro, Brazil, (7)Campus D. de Caxias, Federal University of Rio de Janeiro, Rio de Janeiro, Brazil

This study compares synthesis methods (sputtering deposition, SP, and incipient wetness impregnation, IWI) for Ni/CeO_2 catalysts in ethanol steam reforming. The SP catalyst exhibited superior hydrogen production, attributed to uniform Ni nanoparticle distribution, enhanced metal-support interactions, and increased oxygen vacancies, optimizing catalytic performance.

Experimental and CFD Study of CH_4 Pyrolysis over Fe-Al_2O_3 Catalyst: The Challenge of C Build-up for the Kinetic and the Reactor Studies.

*Davide Cafaro, Marco Orsenigo, **Veronica Piazza**, Chiara Negri, Lidia Castoldi, Gianpiero Groppi, Matteo Maestri, and Alessanda Beretta*
Laboratory of Catalysis and Catalytic Processes - Dipartimento di Energia, Politecnico di Milano, Milano, Italy

Thermo-catalytic methane pyrolysis is explored for CO_2-free hydrogen using Fe-Al_2O_3 catalysts. In this work, iron-based catalysts with Al_2O_3 as textural promoter were prepared and tested for CH_4 pyrolysis at different scales and reactor configurations, integrating experiments with a comprehensive reactor and kinetic modeling to guide process optimization and scale-up.

Highly Active Ru/CeO_2 Catalysts Prepared By Conventional Iwi and Novel Mechanochemistry Methods for Ammonia Cracking.

*Yi Qiu[1], Ivan Conti[1], Nicole Bendazzoli[1], Rudy Calligaro[2], Alessandro Trovarelli[2], Enzo Alessio[3], Elisabetta Iengo[3], and **Alessanda Beretta**[1]*
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Ru is the preferred catalyst for NH_3 cracking, but its reaction rate is limited by Ru–H* interaction, especially at higher temperatures. The support plays a crucial role: CeO_2 offers outstanding performance and minimizes H* poisoning, and both factors are highlighted over the catalyst obtained by milling.

Electrified Ammonia Cracking Via Indirect Joule Heating of Thermally Conductive Packed Pocs.

***Federico Sascha Franchi**[1], Matteo Ambrosetti[1], Alessandra Beretta[1], Gianpiero Groppi[1], Enrico Tronconi[1], Giovanna Massobrio[2], and Matteo Lualdi[2]*
(1)Laboratory of Catalysis and Catalytic Processes - Dipartimento di Energia, Politecnico di Milano, Milano, Italy, (2)SNAM, Milano, Italy

A NH_3 cracking reactor which uses a thermally conductive aluminium POCS, packed with Ru-based catalyst and heated internally by a resistive heater in thermal contact with the POCS, enables high conversion and thermal efficiency in a compact reactor with reduced temperature gradients, while enabling fast heat up and excellent scalability.

Finding the Needle in the Haystack: Material Discovery and Design for Oxygen Electrocatalysis.

Kasun Gunasooriya
Chemical, Biological & Materials Engineering, University of Oklahoma, Norman, OK

Discovering acid-stable and active catalysts for oxygen electrocatalysis remains a challenging task. Based on our extensive theoretical work, we discuss strategies to improve the OER catalytic activity, stability, and the remaining challenges.

Enhancement of Ce^{3+} in Reduced CeO_2 Via U-Ce Charge Transfer. Implications on Hydrogen Production By the Thermochemical Water Splitting Reaction..

Carlos Morales[1], Rudi Tschammer[1], Ingo Flege[1], Thomas Gouder[2], and ***Hicham Idriss***[3]
(1)Brandenburg University of Technology, Cottbus, Germany, (2)European Commission, Karlsruhe, Germany, (3)Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

Hydrogen production via thermochemical water splitting over polycrystalline $Ce_{1-x}U_xO_2$ and single crystalline is investigated. Test reactions indicated that a small % of U (<10 %) is optimal for production hydrogen production. This is tracked down to the increase in Ce^{4+} reduction to Ce^{3+} because of the presence of U^{4+} cations.

Ni Atomically Dispersed in CeO_2 Aerogels for Unprecedented Selectivity in the Water-Gas Shift Reaction.

Travis Novak[1], *Austin Herzog[2], Matthew Buck[3], Kyle Sendgikoski[2], Ryan DeBlock[1], Todd H. Brintlinger[4], Paul A. DeSario[5], and Debra Rolison[1]*
(1)Chemistry, Surface Chemistry Branch, U.S. Naval Research Laboratory, Washington, DC, (2)NRC Postdoc, Naval Research Laboratory, Washington, DC, (3)Chemistry, US Naval Academy, Annapolis, MD, (4)Materials Science and Technology Division, U. S. Naval Research Laboratory, Washington, DC, (5)Office of Naval Research, Arlington, VA

Atomically dispersing Ni in CeO_2 aerogels solves a key selectivity problem present in traditional Ni-based water-gas shift (WGS) catalysts. The 2.5% at.% Ni in CeO_2 aerogel catalyst (2.5NiCeO) combines unprecedented selectivity (< 2 ppm CH_4) with excellent activity and stability, marking a notable advance in WGS catalysts.

Novel Ni-Co/$Ca_{12}Al_{14}O_{33}$ Bimetallic Catalyst for Hydrogen Production Via Sorption-Enhanced Steam Methane Reforming Process.

Ahmad Farooqi, Muhammad Zubair Shahid, and ***Medhat Nemitallah***
King Fahd University of Petroleum & Minerals, Dhahran, Saudi Arabia

SE-SMR is the emerging technology to produce clean hydrogen and has the potential to replace the conventional SMR process. The present study has proposed an efficient catalyst/bifunctional material (Ni-Co/$Ca_{12}Al_{14}O_{33}$) that has proven excellent performance to achieve high methane conversion and low CO_2 emissions.

Mechanism of Electrochemical C=O Hydrogenation and Electroreductive C-C Coupling on Cu Cathodes.

Rachit Khare[1], *Hongwen Chen[1], and Johannes A. Lercher[1,2]*

(1)Department of Chemistry, Technische Universität München, Garching, Germany, (2)Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA

Aqueous-phase electrochemical hydrogenation of benzaldehyde on Cu leads to the formation of both benzyl alcohol and hydrobenzoin. By combining kinetic studies with molecular simulations, we present the mechanism of benzaldehyde conversion and describe the mechanistic conditions that facilitate C-C coupling between conjugated aromatic aldehyde molecules on metal surfaces.

Oxide Supported Single-Atom Catalysts for Oxygen Electrocatalysis.

Keishana Navodye S. a.[1] *and Kasun Gunasooriya*[2]
(1)School of Sustainable Chemical, Biological and Materials Engineering, University of Oklahoma, Norman, OK, (2)Chemical, Biological & Materials Engineering, University of Oklahoma, Norman, OK

Single atom catalysts (SAC) supported on acid stable SnO_2 were evaluated for the stability and activity under oxygen electrochemical conditions. We further used machine learning to identify descriptors and to predict adsorption energies. Based on these theoretical findings, rational catalyst design principles for next-generation SACs based oxygen electrocatalysts are established.

Modeling Electron-Hole Recombination in Promising Photocatalytic Magnetic Materials.

Nicholas Harmon *and David Kumi*
Physics and Engineering Science, Coastal Carolina University, Conway, SC

We develop a set of rate equations for carrier charge and spin in order to calculate electron-hole recombination in magnetically doped perovskites and other materials. Our results show that carrier decay times can be optimized by engineering the electronic structure.

Hierarchical Analysis of Transport Limitations in Gas-Diffusion Electrode Based CO_2 Electroreduction.

Kaustav Niyogi*, Mauro Bracconi, and Matteo Maestri*
Laboratory of Catalysis and Catalytic Processes - Dipartimento di Energia, Politecnico di Milano, Milano, Italy

This work explains the experimentally observed gas-diffusion electrode based CO_2 electrolyzer under-performance at high current densities, using a continuum modeling approach. Our analysis shows that the GDE diffusional resistance significantly influences the experimentally measured reaction rates, highlighting the importance of considering such limitations when benchmarking the electrolyzer performance.

Synthesis of High Efficiency and More Durable Pt-Ni Nanocatalysts.

Shutang Chen
Honda Research Institute USA Inc., San Jose, CA

Pt-Ni nanocatalysts demonstrated the best durability performance in acid electrolyte when compare with the state of the art.

Conductive Polymer-Coated Hydrophobic Membrane with Electrocatalyst As Robust Gas Diffusion Electrode for Long-Term Operation.

Hwiyoon Noh and ***Brian M. Tackett***
Charles D. Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN

This first-of-its-kind gas diffusion layer (GDL) consisting of conductive polymer and hydrophobic membrane shows remarkably enhanced long-term stability at commercially relevant current regime compared to current carbon-based GDL, and represents the next generation GDL technology for various electrocatalytic reactions making the implementation of electrochemical conversion commercially viable.

V-Fe Based Photocatalysts for Oxidative Desulfurization of Dibenzothiophenes.

Luis Cedeño-Caero*, Marco A. Alvarez-Amparan, and Uriel Chacon-Argaez*
ING. QUIMICA, FAC. QUIMICA, UNAM, CDMX, DF, Mexico

Several V oxides formulations on alumina modified with Fe were evaluated on the photocatalytic oxidative desulfurization (PODS) of dibenzothiophene compounds. The structural and optical properties, and surface species of the catalysts were determined by SEM-EDS, TPR, XRD, Raman, ATR-FTIR, photoluminescence, UV-Vis diffuse reflectance, and XPS spectroscopy.

First-Principles Study of Hybrid Structure Containing Pt Clusters inside CNTs: Application As ORR Catalysts.

Hyeong Kyu Park
Department of Chemistry and Chemical Engineering, Inha University, Incheon, Korea, Republic of (South)

The overuse of fossil fuels drives global warming. PEMFCs offer clean energy but face commercialization challenges due to expensive Pt catalysts. Using DFT, we designed Pt@CNT hybrids to reduce Pt usage while enhancing ORR activity. PtM alloys further improve performance, analyzed via electronic structure studies.

Cu_2O-Pd Photocatalysts for Carbon-Carbon Coupling Reactions in Ambient Conditions.

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(2)School of Chemical, Biological, and Materials Engineering, University of South Florida,

Tampa, FL, (3)Department of Chemical, Biological and Materials Engineering, University of South Florida, Tampa, FL

This work demonstrates the potential of Cu_2O-Pd hybrid photocatalysts for efficient, visible light-driven oxidative C-C coupling reactions under ambient conditions, offering a sustainable pathway for producing high-value chemicals in pharmaceutical, agrochemical, and fine chemical industries. This approach demonstrates an eco-friendly, energy-efficient method for solar-driven chemical transformations under ambient, base-free conditions.

Effects of Pt:Pd Ratios on the Activity and Stability of Pt:Pd/γ-Al_2O_3 Catalysts for Lean Methane Oxidation.

*Min Wang[1], **Haiying Chen**[2], Yuliana Lugo-Jose[3], Melissa Hess[3], Joseph M. Fedeyko[3], Todd Toops[1], and Jacqueline Fidler[4]*
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Addition of Pt to PdO/γ-Al_2O_3 catalyst has been recognized to enhance the on-stream stability of the catalyst in methane oxidation reactions. In this study, we systematically vary the Pt:Pd ratios from 1:0 to 0:1 with total (Pt+Pd) loading at 3 wt.% to investigate the effects of Pt in PtPd/γ-Al_2O_3 system.

Catalysts Based on Pt Clusters and Nanoparticles on CeO_2: Influence of the Noble Metal Size and Support Morphology in the Oxidation of CO.

***Nicola Da Roit**[1], Christian Schmitt[1], Joachim Czechowsky[2], Omar Bettini[3], Ajai Lakshmi Nilayam[4], Marco Neumaier[4], Christian Kübel[4], Silvia Gross[3], Manfred Kappes[4], Maria Casapu[2], and Silke Behrens[1]*
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Powder model catalysts for emission control catalysis were prepared using the "precursor" concept, where atom-precise Pt clusters and monodisperse nanoparticles were supported on ceria. We show the influence of the Pt particle size, their surface noble metal concentration and support morphology on the catalytic performance in the oxidation of CO.

Effect of CO on Alcohol Oxidation over PGM-Based Commercial Oxidation Catalysts for Control of Emissions from Lean-Burn Engines.

***Md Masudur Rahman**, Sreshtha Sinha Majumdar, and Josh A. Pihl*
Oak Ridge National Laboratory, Oak Ridge, TN

Methanol oxidation was inhibited by CO on Pt DOC, Pd+Pt DOC, and MOC catalysts at temperatures below 150 °C. Ethanol formed acetate species as a partial oxidation product on the catalyst surface. Strongly adsorbed acetate species delayed CO oxidation on the Pt DOC and MOC catalysts until 200 °C.

Influence of Zirconia Loading on Pd–Pt/SBA-15 Catalysts for Methane Oxidation.

Gianni Caravaggio
CanmetENERGY-Ottawa, Natural Resources Canada (NRCan), Ottawa, ON, Canada

To address methane slip (with high GHG potential) in lean burn natural gas (LBNG) engines, where water vapor and sulfur in the exhaust deactivate conventional catalysts, Pd–Pt/SBA-15 catalysts doped with zirconia (5–15 wt%) were developed. These catalysts showed excellent methane oxidation activity under simulated LBNG exhaust

Automatically Generated Exhaust Gas Conversion Mechanism over Pt(111) Explores Chemistry between C and N Containing Adsorbates.

***Kirk Badger**, C Franklin Goldsmith, and Bjarne Kreitz*
School of Engineering, Brown University, Providence, RI

Experimental data suggests that reactions between adsorbates with N and C play an important role in the conversion of exhaust gas over Pt. The open-source software RMG is extended and used to automatically generate a microkinetic model that considers such reactions in the conversion of exhaust gas over Pt(111).

Origins of the Photocatalytic NO_x Oxidation and Storage Selectivity of Mixed Metal Oxide Photocatalysts: Prevalence of Electron-Mediated Routes, Surface Area, and Basicity.

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(1)Chemistry, Bilkent University, Ankara, Turkey, (2)Sabanci University, Istanbul, Turkey

CaO-promoted TiO_2/Al_2O_3 were utilized in photocatalytic NOx oxidation and storage reaction. An e^--scavenger suppressing the e^--mediated route, attenuated the photocatalytic selectivity by triggering NO_2(g). Superior NO_x storage selectivity was attributed to presence of e^- trapped at oxygen vacancies and superoxide species allowing direct NO oxidation to NO_3^- species.

Impact of Water on Ammonia Oxidation Performance of Coinage Metals and Their Comparison to Platinum.

***Amish Chovatiya**, Hanyu Ma, and William Schneider*
Chemical and Biomolecular Engineering, University of Notre Dame, Notre Dame, IN

We use a conversion dependent mean field microkinetic model to compare ammonia oxidation activity and selectivity of coinage metals with Pt and show that the choice of catalyst is

dependent on whether the feed gas is dry or wet. We then test sensitivity of our conclusions to model assumptions.

Highly Efficient Ag Single-Atom Catalyst for Selective Catalytic Oxidation of NH_3.

Kailong Ye[1]*, Shaohua Xie*[2]*, and* ***Fudong Liu***[3]
(1)University of California, Riverside, Riverside, CA, (2)Department of Civil, Environmental, and Construction Engineering, University of Central Florida, Orlando, FL, (3)Department of Chemical and Environmental Engineering, University of California, Riverside, Riverside, CA

Ag single-atom catalysts (SACs) with enhanced catalytic activity for the selective catalytic oxidation of NH_3 reaction were successfully developed by tailoring the Ag coordination environment and optimizing the surface density of Ag atoms within the catalysts.

Restructuring of Au-Pd Nanoparticles in the Presence of Adsorbates: Insights into Catalysis and Selectivity.

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The interaction of surface restructuring, adsorbate binding energy, and local atomic environments is crucial for stabilizing and forming intermediates during H_2O_2 production. It is essential to understand this restructuring and its impact on catalytic behavior to optimize AuPd single atom alloys for efficient and selective H_2O_2 synthesis.

Mechanistic Insights into PFOA Degradation on Covalent Organic Framework Photo-Catalysts.

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We demonstrate that COF materials can photo-oxidize PFOA through defluorination. DFT calculations show PFOA binding to the –C≡C– fragment induces critical structural and electronic changes in the COF. Electron density localized around the carboxylate group facilitates PFOA photooxidation. This insight provides guidance for designing COFs for photo-catalytic PFAS removal

Identifying and Quantifying Carbon in Municipal Solid Waste Ash & Implications for Ash's Performance As a Heterogeneous Catalyst.

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This study explores waste-to-energy (WTE) ash as a low-cost NO_X reduction catalyst by characterizing its carbon forms using FTIR, TGA, and "smart" combustion. Performance testing showed promising NO conversion rates, suggesting ash's potential viability in treatment of harsh flue gases and thus, advancing circular economy practices in emissions control.

The Application of Spaci-MS on Cucha SCR Monolith Catalysts.

Aldo Lanza[1]*, Pietro De Angeli*[2]*, Nicola Usberti*[2]*, Isabella Maria Nova*[2]*,* ***Enrico Tronconi***[2]*, Tomas Hlavaty*[3]*, Petr Koci*[3]*, Djamela Bounechada*[1]*, Roberta Villamaina*[1]*, and Andrew P.E. York*[1]
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The development of a fast, simple and 'easy to use' analytical model represents a useful simplification in the evaluation of the probe intrusion effects when dealing with spatially resolved data. CFD validated the effectiveness of the use of this technique.

Homogeneously Distributed Heterostructure Energizes and Replenishes Oxygen Species for Boosting Toluene Degradation on Pharmaceutical Industry Park.

Bin Wang[1]*, Sunwen Xia*[1]*,* ***Bo Ning***[2]*, Kaihang Zhang*[3]*, Qiaowan Chang*[4]*, and* ***Dong Wang***[1]
(1)Shandong University, Jinan, Shandong Province, China, (2)Wenzhou Medical University, Wenzhou, China, (3)Georgia Institute of Technology, Atlanta, GA, (4)Columbia University, New York, NY

We present a scalable one-pot strategy for the in situ fabrication of a homogeneously distributed heterostructure, which brings La_2CuO_4 perovskite a 58-fold activity enhancement and robust anti-sintering/water/coke in toluene oxidation, superior to currently reported perovskite catalysts.

Advancing Pt Catalysts for the Selective Catalytic Reduction of Nitrogen Oxides with Hydrogen.

Shaohua Xie[1]*, Liping Liu*[2]*, Yuejin Li*[3]*, Hongliang Xin*[4]*, and* ***Fudong Liu***[5]
(1)Department of Civil, Environmental, and Construction Engineering, University of Central Florida, Orlando, FL, (2)Department of Chemical Engineering, Virginia Polytechnic Institute and State University, Blacksburg, VA, (3)BASF, Iselin, NJ, (4)Department of Chemical Engineering, Virginia Tech, Blacksburg, VA, (5)Department of Chemical and Environmental Engineering, University of California, Riverside, Riverside, CA

Unlike conventional strategies that focus on modifying active sites, we present a simple and versatile approach using the physical mixing of Pt catalysts with zeolites to fine-tune the

surrounding environment of active sites, thereby significantly enhancing catalytic performance in the selective catalytic reduction of NO_x using H_2.

Effect of Ions on the Aqueous-Phase Adsorption of Organics on Ag.

Ankit Mathanker[1]*, Gyan Sharma*[1]*, Bolton Tran*[1]*, Nirala Singh*[1]*, and Bryan Goldsmith*[2]
(1)Department of Chemical Engineering, University of Michigan, Ann Arbor, MI, (2)Chemical Engineering, University of Michigan, Ann Arbor, MI

Ions can change the aqueous-phase adsorption strength of organics. Our main findings suggest ions can vary the adsorption of organics on Ag by up to ±10 kJ mol^{-1}. The change in adsorption is mainly attributed to the change in the adhesion of water in the presence of ions.

Kinetic Analysis Reveals Active Sites in Heterogeneous Metathesis Catalysts: Insights from the *Cis-Trans* Isomerization of 2-Butenes.

Maria Rikaela Ilagan[1]*, James Rawlings*[2]*, and Susannah Scott*[3]
(1)Chemical Engineering, University of California, Santa Barbara, Santa Barbara, CA, (2)University of California, Santa Barbara, Santa Barbara, CA, (3)Department of Chemical Engineering, University of California, Santa Barbara, Santa Barbara, CA

A kinetic analysis of the *cis-trans* isomerization of 2-butene was performed using Re_2O_7/Al_2O_3, revealing active sites in heterogeneous olefin metathesis. Global curvefit analysis identified the Re ethylidene as the most abundant surface intermediate, advancing our understanding of elementary rate constants and the relative abundances of key surface intermediates.

Resolving Coverage Dependent CO and H Co-Adsorption on Pt(111).

Sifat Hossain *and Rachel Getman*
Department of Chemical and Biomolecular Engineering, The Ohio State University, Columbus, OH

The investigation of the CO*-H* system on Pt(111) using cluster expansions show H* having a 2-fold effect on CO*, evident through changes in co-adsorption saturation coverage. GCMC models connect reaction conditions to adsorbate configurations and CH_4 selectivity, providing insights to enhance selectivity for industrial CO hydrogenation processes.

Impact of Pd Single Atoms during CO Oxidation over Ceria-Supported Ni and Pt Single Atom Catalysts: Are Synergistic Effects Present?.

Kayla Eudy[1]*, Shyam Deo*[2]*, Michael Janik*[1]*, and Robert Rioux*[3,4]
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Ceria-supported Pd single atoms demonstrate ‘synergy’, arising from non-bonding influences between metal atoms mediated through the reducible support. The addition of Pd single atoms to CeO_2-supported Ni and Pt single atoms does not influence the behavior of Ni or Pt nor influence intra-atom communication between Pd atoms during CO oxidation.

Taming Complexity in Catalysis Using Transient Methods.

Christopher R. O'Connor[1], *Eric A. High*[1,2], *Taek-Seung Kim*[3,4], *and Christian Reece*[1]
(1)Harvard University, Cambridge, MA, (2)Tufts University, Medford, MA, (3)Rowland Institute at Harvard, Harvard University, Cambridge, MA, (4)Korea Institute of Energy Research, Daejeon, Korea, Republic of (South)

We combine ambient pressure transient flow and spectroscopy CO oxidation experiments to probe the state of a powdered Pd/γ-Al_2O_3 catalyst and find that the kinetics and coverage dependencies measured quantitatively agree with those measured in ultra-high vacuum over model Pd/Al_2O_3/NiAl(110) and Pd(111) systems.

Sintering Resistance in Dilute-Alloy Catalysts Is Described By Decreased Surface Mobility Due to Metal Hybridization.

Audrey Dannar[1,2], *Jordan Finzel*[3], *Phillip Christopher*[4], *and E Charles Sykes*[5]
(1)Rowland Institute at Harvard, Harvard University, Cambridge, MA, (2)Rowland Institute, Harvard University, Cambridge, MA, (3)Chemical Engineering, University of California Santa Barbara, Santa Barbara, CA, (4)Department of Chemical Engineering, University of California, Santa Barbara, Santa Barbara, CA, (5)Department of Chemistry, Tufts Univ, Medford, MA

Single-atom alloy (SAA) catalysts have demonstrated an unexpected and previously unexplained resistance to sintering, a major catalyst deactivation pathway. We reveal the atomic-scale processes behind sintering and SAA sintering resistance using results from supported SAA catalyst samples under high pressure environments, single crystals in UHV conditions, and computational models.

Electronic and Geometric Features Controlling the Reactivity of C_1–C_3 Alkanes on Mg-Vanadate Catalysts—a DFT+U Study.

Hansel Montalvo-Castro[1], *Alvaro Loaiza*[2], *Randall Meyer*[3], *Craig Plaisance*[2], *and David Hibbitts*[4]
(1)Department of Chemical Engineering, University of Florida, Gainesville, FL, (2)Cain Department of Chemical Engineering, Louisiana State University, Baton Rouge, LA, (3)Exxonmobil, Annandale, NJ, (4)Charles D. Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN

This work employs density functional theory (DFT) and constrained orbital (CO-DFT) to elucidate geometric and electronic features that govern initial C–H activation of C_1–C_3 alkanes on Mg-vanadate catalysts during oxidative dehydrogenation reaction.

In-Situ Computational Design of Ni-Supported Metal Nitride Interfaces for Mild Temperature Ammonia Synthesis.

***Pranav Roy**, Weiye Qu, Chao Wang, and Brandon C. Bukowski*
Department of Chemical and Biomolecular Engineering, Johns Hopkins University, Baltimore, MD

We performed a mechanistic study of the associative Mars-van Krevelen mechanism in metal nitrides for ammonia synthesis using combined DFT and AIMD. We developed a Ni-MnN nanowire model to facilitate hydrogen adsorption on MnN. A computational workflow is presented for kinetic modeling of nanowire-metal nitride interfaces at reaction conditions.

Role of Water in the Dynamics of Active Sites in Pt-MoO_x Catalysts during Liquid-Phase Reactions.

***Samir Castilla Acevedo Sr.**[1], Ben Auer[1], John Styers[1], and Alan Allgeier[2]*
(1)Chemical and Petroleum Engineering, University of Kansas, Lawrence, KS, (2)Center for Environmentally Beneficial Catalysis (CEBC), University of Kansas, Lawrence, KS

The density of the active sites is strongly influenced by the presence of water in the system and ignoring these influences may lead to invalid TOF assessments.

Thermochemical Interconnectivities of Redox, Brønsted, and Lewis Sites on Metal Oxide Surfaces and Their Kinetic Consequences in C−H Scission and C−O Formation of Alkanols.

***Guangming Cai** and Ya-Huei (Cathy) Chin*
Department of Chemical Engineering and Applied Chemistry, University of Toronto, Toronto, ON, Canada

The knowledge on the interconnectivities among diverse active sites on metal oxides, encompassing their thermochemical, electronic, and kinetic properties, establishes a foundation for rationalizing turnover rate couplings across multi-functional catalysts and aid in design and optimization of catalysts for alkanol ODH and DEH catalysis.

Kinetic Consequences of Surface Segregation Processes in Catalysis By Metal Alloys.

***Samiha Bhat**[1], Rong (rocky) Ye[1], Jared Arkfeld[1], Chenggong Jiang[1], Bryan Goldsmith[2], Nirala Singh[1], Eranda Nikolla[1], and Suljo Linic[1]*
(1)Department of Chemical Engineering, University of Michigan, Ann Arbor, MI, (2)Chemical Engineering, University of Michigan, Ann Arbor, MI

Reaction kinetics on heterogeneous bimetallic catalysts is influenced by *in situ* structural transformations, including surface segregation. This phenomenon of adsorbate-induced alloy restructuring on exposure to reaction environments is not thoroughly investigated. This study

highlights the restructuring potential of Pt-Cu alloys under CO oxidation, and its effect on observed kinetics.

Unveiling the Catalytic Potential of Extra-Large Pores Zeo-1 Zeolite.

Nourrdine Chaouati[1], *Mohammad Fahda*[2], *Svetlana Mintova*[1], *Ludovic Pinard*[3], *and Valentin Valtchev*[4]
(1)Laboratoire de Catalyse et Spectrochimie, Caen, No State, France, (2)Laboratoire de Catalyse et Spectrochimie, Caen, France, (3)CNRS-ENSICaen-UniCaen, Caen, France, (4)CNRS-ENSICaen-UniCaen, Caen, Calvados, France

Our contribution focuses on the study of the fundamental catalytic properties of the recent extra-large pore zeolite ZEO-1. Results indicate that ZEO-1 has a cracking ability comparable to that of a USY, its shape selectivity is imposed by the 12 MR channels while its 16 MR channels enhance its stability.

Sterically Encumbered [(3,3'-dimethyl-2,2'-bipyridine)Ir(Cl)COE$_2$] Catalyst for Aromatic and Heteroaromatic Borylation.

Eric Slack*, Douglas Hartline, and Samantha Grosslight*
Life Science Technologies, Johnson Matthey, Magnolia, NJ

Experimental and computational study of iridium borylation of heteroaromatic and aromatic substrates using a sterically encumbered 3,3'-dimethyl-2,2'-bipyridine ligand for improved scope and efficiency compared to the standard process using [Ir(OMe)COD]$_2$ with 3,4,7,8-tetramethyl-1,10-phenanthroline.

Impact of Ceria Support Morphology on the Electronic Properties and Catalytic Behavior of Rh Single Atoms during CO Oxidation.

Mohamed Eisa Omar[1], *Sean Evans*[1], *Kai Shen*[2], *Raymond Gorte*[2], *John Vohs*[2], *Dionisios Vlachos*[3], *and Ayman M. Karim*[1]
(1)Department of Chemical Engineering, Virginia Polytechnic Institute and State University, Blacksburg, VA, (2)Department of Chemical and Biomolecular Engineering, University of Pennsylvania, Philadelphia, PA, (3)Delaware Energy Institute, University of Delaware, Newark, DE

The study demonstrates how ceria morphology influences the electronic properties and catalytic behavior of Rh single atoms during CO oxidation. By correlating oxygen vacancy dynamics with Rh's electronic environment and performance, the findings provide critical insights for designing optimized single-atom catalysts for CO emissions control and beyond.

Transition Metal-Triazine Electrocatalysts for Carbon Dioxide Transformation and Hydrogen Storage.

***Phong Huynh**, Manuel Quiroz, and Krista Kulesa*
PNNL, Richland, WA

Mitigating CO_2 emissions requires carbon capture and recycling into green energy carrier molecules. For the first time, we synthesize and characterize three transition metal-triazine (TMT) complexes. These TMT platforms are evaluated for CO2 reduction selectivity, efficiency and mechanism, introducing a promising class of molecular electrocatalysts for closing the carbon cycle.

Ambient Pretreatment Effect on Low Temperature CO Oxidation over Ni Doped Co_3 O_4 Nanocatalysts.

Zichen Wang
University of Connecticut, Storrs, CT

This study reveals that pretreatment temperature significantly impacts Ni-doped Co_3O_4 catalysts' performance in CO oxidation. Moderate pretreatment (300–600°C) enhances activity by optimizing spinel structure, while high-temperature treatment (900°C) induces phase separation, reducing effectiveness. Insights provide valuable guidance for catalyst design and environmental applications.

Synthetic Methods to Control the Siting of Trivalent Heteroatoms in MFI Zeolite Channels for Selective Toluene Methylation to p-Xylene.

***Bereket Bekele**, Andrew Norfleet, and Rajamani Gounder*
Charles D. Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN

Synthetic strategies that bias active (H^+) sites towards smaller MFI channel voids are generalizable to any trivalent heteroatoms, evidenced by regioselective toluene methylation towards less bulky para-xylene isomers. Variations in acid strength, by changing heteroatom identity, enable independent control over methylation rates while maintaining high confinement-driven selectivity in MFI zeolites.

Interplay of Local Structure and Spin State on the ORR and Oer Performance of M-N-C Catalysts.

***Hyeonjung Jung** and Michal Bajdich*
SUNCAT Center for Interface Science and Catalysis, SLAC National Accelerator Laboratory, Menlo Park, CA

This study investigates the effects of z-displacement and spin states on ORR and OER performance in M-N-C catalysts using DFT. By analyzing 22 transition metals across 3d, 4d, and 5d rows, it identifies spin stability, adsorption energy trends, and dual-ligand interactions, providing insights for optimizing single-atom catalysts in energy conversion.

Toward Understanding of Oxygen Depletion Effects on Chemical Looping Propane Oxidative Dehydrogenation Using Strontium Ferrites.

Kun Wang[1]*, Sophie Liu*[2]*, Randall Meyer*[3]*, and Jonathan Mitchell*[1]
(1)ExxonMobil Technology and Engineering, Annandale, NJ, (2)ExxonMobil Research and Engineering Company, Annandale, NJ, (3)Exxonmobil, Annandale, NJ

Using strontium ferrites with perovskite and Ruddlesden-Popper structures as oxygen carriers for propane chemical looping oxidative dehydrogenation, we show the surfaces maintain high levels of O population and are insensitive to O depletion during the reaction. The surface reaction is limiting and the ODH performance is little impacted.

Microkinetic Modelling for Electrochemical C-N Coupling By Metal-Organic Materials.

Yuting Xu[1]*, Jiaqi Yang*[1]*, Gregory Foley*[2]*, Sophia Mac*[2]*, Lan On*[2]*, Sara Thoi*[2]*, and Fanglin Che*[1]
(1)Chemical Engineering, University of Massachusetts Lowell, Lowell, MA, (2)Chemistry, Johns Hopkins University, Baltimore, MD

BIFs' discrete active sites and atomic precision provide an excellent platform for advancing single-atom catalysis. This project deepens understanding of structure-reactivity relationships in single-atom electrocatalysis within cage frameworks. Integrating DFT, MKM with AI enables a fundamental approach to catalyst design, moving beyond trial-and-error.

Isomerization of Epoxides By Tris(Pentafluorophenyl)Borane (BCF): Investigation of Solvent Effects and Induction Period.

Hiyab Mekonnen[1]*, Guanhua Wang*[2]*, Linda Broadbelt*[3]*, and Justin Notestein*[4]
(1)Northwestern University, Evanston, IL, (2)Chemical Engineering, Northwestern University, EVANSTON, IL, (3)Department of Chemical and Biological Engineering, Northwestern University, Evanston, IL, (4)Department of Chemical & Biological Engineering, Northwestern University, Evanston, IL

This study investigates tris(pentafluorophenyl)borane (BCF) as a Lewis acid catalyst for epoxide isomerization. It examines how solvent properties, such as hydrogen bonding and coordination strength, influence reaction rates and selectivity. Kinetic experiments, in situ NMR, and DFT calculations offer insights into solvent interactions in BCF-catalyzed reactions.

Designing Strategies for the Modification of ZIF-8 for Its Optimization As an Adsorbent.

David Villalgordo Hernández *and Javier Narciso*
University of Alicante, Alicante, Spain

ZIF-8 has been post-synthetically modified with four different Triazoles aiming to tune its adsorption capacity and affinity towards CO_2 by adding a series of N sites. Incorporation of these exchanging ligands generate new coordinative systems leaving available N sites which act as anchoring points enhancing its aptitude for CO_2 capture.

Surface Brønsted Acidity Characterization of Phosphotungstic Acid.

Hyunju Lee[1] *and Brent H. Shanks*[2]
(1)Chemical and Biological Engineering, Iowa State Univeristy, Ames, IA, (2)Department of Chemical and Biological Engineering, Iowa State University, Ames, IA

Surface proton concentration and acid strength of heteropoly acid catalysts were measured by means of temperature-programmed desorption of 2,6-di-tert-butylpyridine. Also, it was found that medium level of hydration of phosphotungstic acid resulted in the highest surface proton density, as [H_3O^+] showed higher mobility than H^+ and $H_5O_2^+$.

A Simple Ligand Exchange Strategy to Functionalize ZIF-8 to Improve Mercury Adsorption from Water.

Maria Karla Lopez González[1] *and Javier Narciso*[1,2]
(1)University of Alicante, Alicante, Spain, (2)Alicante Institute for Health and Biomedical Research, Alicante, Spain

This study demonstrates the power of post-synthetic modification (PSM) of ZIF-8 to enhance material functionality, offering innovative pathways for designing efficient adsorbents. The successful functionalization with 3-mercapto-1,2,4-triazole resulted in materials with high Hg^{2+} adsorption, with Int.Z2.1-0.5 excelling due to its high sulfur content.

Conversion of Low-Density Polyethylene and Waste Plastic Bottles to Fuel Grade Hydrocarbons Using Metal-Supported KIT-6 Catalysts.

Maliheh Heravi[1]*, Sathyapal Churipard R.*[1]*, Sundaramurthy Vedachalam*[1]*, Saumitra Saxena*[2]*, and Ajay Dalai*[1]
(1)Chemical and Biological Engineering, University of Saskatchewan, Saskatoon, SK, Canada, (2)CCRC, KAUST, Thuwal, Jeddah, Saudi Arabia

Efficient catalyst design enables high liquid yield and selective cracking of LDPE and plastic bottles to fuel-range hydrocarbons. Transition metals enhance KIT-6 performance by tuning pore size and creating active sites. This study highlights the potential of heteroatom introduction in KIT-6 for sustainable plastic waste conversion, advancing the circular economy.

Automation Tools As an Enabler for Zeolite Discovery and Optimization.

Joel Schmidt*, Marat Orazov, Kurt Jensen, Nan Chen, Jilei Liu, Howard S. Lacheen, and Axel Brait*
Chevron, Richmond, CA

The use of automation tools is a necessity in a competitive R&D environment to improve on the catalyst development/commercialization cycle. This talk will give an overview of our efforts to implement these tools in Chevron's Catalytic Materials team.

Mg-MOF-74 As a Promising Precursor for Synthesizing Highly Active and Porous MgO Catalyst Towards Knoevenagel Reaction.

Mehdi Niknam[1] *and Thomas U. Schwartz*[2]
(1)The University of Maine, Orono, ME, (2)Biology, Massachusetts Institute of Technology, Cambridge, MA

MgO catalyst can be effectively synthesized from Mg-MOF-74, with several advantages over conventional MgO. One of the key benefits is its high site density as the result of increased surface area. This enhanced surface area is critical for improving catalytic performance, as it provides more active sites for reactions.

Achieving Controllable Distribution of M Cations (Pd, Pt, Ni, Cr, Cu) As $[M\text{-}OH]^{+1}$/1Al or M^{2+}/2Al in a Zeolite Gives Mechanistic Insights for Adsorptive, Catalytic Reactions.

Nicholas Jaegers[1]*, Hristiyan A. Aleksandrov*[2]*, Eric D. Walter*[3]*, Georgi Vayssilov*[2]*, Dhruba Jyoti Deka*[3]*, Janos Szanyi*[3]*, Garam Lee*[3]*, and* ***Konstantin Khivantsev***[4]
(1)University of California at Berkeley, Berkeley, CA, (2)Faculty of Chemistry, University of Sofia, 1126 Sofia, Bulgaria, (3)Pacific Northwest National Laboratory, Richland, WA, (4)Physical and Computational Sciences Directorate and Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA

We show the first synthetic pathway for selective placement of divalent metal cations in a zeolite with the same Si/Al ratio wither as M(II)-OH/1Al or M(II)/2Al species and their divergent reactivity for important industrial catalytic and adsorption chemistries.

Metal Nanoparticle Encapsulation Strategies in MOF for Enhanced and Stabilized CO_2 Hydrogenation to Methanol.

Vijay Velisoju[1]*, Enrique V. Ramos Fernandez*[1,2]*, Jose Cerrillo*[3]*, Rafia Ahmad*[1]*, Hend Omar Mohamed*[1]*, Luigi Cavallo*[4]*, and* ***Pedro Castaño***[1]
(1)KAUST Catalysis Center, King Abdullah University of Science and Technology, Thuwal, Saudi Arabia, (2)Inorganic Chemistry Department, University of Alicante, Alicante, Spain, (3)King Abdullah University of Science and Technology, Thuwal, Saudi Arabia, (4)KAUST, Thuwal, Saudi Arabia

This study demonstrates Cu and Pd catalysts embedded in ZIF-8, achieving superior activity and stability for CO_2 hydrogenation to methanol under industrial conditions. The catalysts' performance is driven by highly dispersed metal nanoparticles and metal-Zn interfaces within ZIF-8, highlighting the potential for efficient, sustainable CO_2-to-methanol conversion.

Unraveling Solvent Effects on n-Butane Cracking and Dehydrogenation in H-MFI Zeolites: A Hybrid QM/MM Approach.

Muhammad Zeeshan*, Subrata Kumar Kundu, and Andreas Heyden*
Department of Chemical Engineering, University of South Carolina, Columbia, SC

Developed an explicit solvation scheme for porous zeolites (called eSZS), which was subsequently used to study solvent effects during cracking in H-MFI.

Synthesis of a Nickel Based Nanostructured Hierarchical ZSM-5 Zeolite for Enhanced Dry Reforming of Methane to Syngas.

*Yahuza Nantomah Abdulai[1], **Khalid Alhooshani**[2,3], and Saheed Ganiyu[2]*
(1)Chemistry, King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia, (2)Chemistry, King Fahd University of Petroleum and Minerals, Dhahran, Dammam, Saudi Arabia, (3)Chemistry, Interdisciplinary Research Center for Refining & Advanced Chemicals, King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia

This study assesses the catalytic performance of a Ni/ZSM-5-S catalyst in dry reforming of CH4 (DRM), converting CH4 and CO2 into syngas. Hierarchical ZSM-5 was synthesized hydrothermally, and Ni/ZSM-5-S via wet impregnation. The catalyst showed high syngas production (82.5% CO2,78.0% CH4 conversion) and stability for 22 hours at 700°C.

SiO_2-Coated Cu-Based Catalysts for Efficient CH_3oh Production from CO_2.

*Marco A. Rossi[1], Letícia Rasteiro[2], Jose Assaf[3], Elisabete Assaf[1], and **Luiz Vieira**[1]*
(1)Sao Carlos Institute of Chemistry (IQSC), University of Sao Paulo (USP), Sao Carlos, Sao Paulo, Brazil, (2)Institute of Chemistry, Sao Paulo State University, Araraquara, Sao Paulo, Brazil, (3)Chemical Engineering Department, Federal University of São Carlos, São Carlos, Brazil

This work presents a mesoporous SiO_2 coating strategy for $Cu/In_2O_3/CeO_2$ and $Cu/In_2O_3/ZrO_2$ catalysts. This approach limited the nanoparticle size, increased metal dispersion, and resulted in higher activity and selectivity in the hydrogenation of CO_2 to methanol, with methanol yields up to 4 times higher.

Essential Insights into Electronic and Crystal Structure Modulation of Co-Catalysts By Iridium for Enhanced Fischer-Tropsch Synthesis.

***Ji Won Lee**, Ji Woo Son, Seung Ju Han, Yunjo Lee, and Yang Sik Yun*
Hydrogen & C1 Gas Research Center, Korea Research Institute of Chemical Technology (KRICT), Daejeon, Korea, Republic of (South)

This work establishes Iridium as a highly effective promoter for optimizing Co-based catalysts, providing a strategic framework for the development of advanced catalysts for FTS applications.

The Effect of Buffer Electrolyte on Proton-Coupled Electron Transfer Kinetics in Electrochemical Hydrogenation Reactions.

Zhiqin Liang
School of Physical Science and Engineering, Beijing Jiaotong University, Beijing, China

Special caution must be taken when interpreting the intrinsic pH dependence in the presence of buffer species because of its potential role as a proton or oxygen carrier, which is easily overlooked in current research. We show how buffer electrolytes steer the interfacial kinetics of electrochemical hydrogenation reactions.

Molecular Catalysts Design with Massively Parallel Physics-Based Computational Workflow.

Croix Laconsay[1]*, Mathew D. Halls*[2]*, and Pavel Dub*[3]
(1)Schrödinger, Portland, OR, (2)Materials Science, Schrödinger, Inc., San Diego, CA, (3)Schrödinger, Inc., San Diego, CA

Molecular catalysts have traditionally been designed through experimental trial-and-error. We present Schrödinger's Reaction Network Enumeration Profiler module, the first fully automated computational framework capable of predicting both selectivity and turnover frequency (TOF) for dynamically generated libraries of virtual molecular catalysts, leveraging quantum mechanics.

Machine Learning-Assisted Design of Integrated Single-Atom Electrodes for Enhanced Water Oxidation.

Lingxi Zhou *and Ruitao Lv*
Tsinghua University, Asian (Including Pacific Islander), Beijing, China

The activity-stability dilemma of electrocatalysts limits their practical use, especially in OER for hydrogen production. We introduce a 'chemical steam deposition' strategy with machine learning to synthesize a Ru-Ti-Mn electrode with self-healing mechanisms, achieving high activity and stability across all pH levels. ML identified the optimal atomic metal-support ratio.

DBD Plasma Treatment on Ni/γ-Al_2O_3 for Catalytic Methane Decomposition: Effects of Pure Argon and Pure Hydrogen.

Bella -[1]*, Xun Cao*[2]*, Kang Hui Lim*[3]*, Chee Kok Poh*[1]*, Luwei Chen*[1]*, Jie Chang*[1]*, and Sibudjing Kawi*[3]
(1)Carbon Conversion and Future Energy Carriers, Institute of Sustainability for Chemicals, Energy and Environment (ISCE2), Singapore, Singapore, (2)Advanced Characterization and Instrumentation, Institute of Sustainability for Chemicals, Energy and Environment (ISCE2), Singapore, Singapore, (3)Department of Chemical and Biomolecular Engineering, National University of Singapore, Singapore, Singapore

DBD plasma was used to decompose Ni precursor on γ-Al_2O_3 where the effects of using different pure gases (Ar and H2) were studied on low temperature catalytic methane decomposition reaction to co-produce hydrogen and carbon nanotubes. Surface characterizations were conducted to understand the effects of different gases on the catalysts.

Machine Learning Driven Catalyst Optimization for Biomass to H_2

-Rich Syngas with Experimental Validation.

Kaushik Kundu[1]*, Avan Kumar*[2]*, Hariprasad Kodamana*[1]*, and Kamal Pant*[3]
(1)Chemical Engineering Department, Indian Institute of Technology Delhi, New Delhi, India, (2)School of Sustainability, Arizona state university, Tempe, AZ, (3)Chemical Engineering, Indian Institute of Technology Roorkee, Roorkee, India

Transforming biomass into hydrogen-rich syngas tackles fossil fuel depletion and environmental harm. Machine learning optimization, validated experimentally, ensures reliable, scalable industrial applications. This research supports the shift to a low-carbon economy, promoting sustainability and energy independence while addressing critical global energy and environmental challenges.

***Immobilization of Endoxylanase Onto Functionalized SBA-15 for Xylooligosaccharides Production*.**

Parasuraman Selvam
Department of Chemistry & NCCR, IIT-Madras, CHENNAI, India

Enzymatic methods are eco-friendly while the immobilization of the enzyme enhances stability, rigidity and reusability, therefore the immobilized enzymes are more suitable as catalysts for the industrial production of xylooligosaccharides from xylan.

Step-Wise Activation of CH_4 and CO_2 over Partially Oxidized Surfaces of MoO_xC_y.

Nurul Farhana Binti Abd Ghaffar[1]*, Tej Choksi*[1]*, Wen Liu*[1]*, and Mingwu Tan*[2]
(1)School of Chemistry, Chemical Engineering and Biotechnology, Nanyang Technological University, Singapore, Singapore, (2)4Agency for Science, Technology and Research (A∗STAR), Singapore, Singapore

We study the evolution of Mo_2C surface structure upon exposure to different reactive environments, viz., 1) CO_2; 2) H_2 and (3) CH_4. We demonstrate 20 cycles of chemical looping DRM with a steady increase of methane conversion from 74 % to 93 % with no obvious sign of deactivation.

The Influence of Strong Metal Support Interaction Phenomena on the Rates and Selectivity of Formic Acid Decomposition.

Luan Q. Le[1]*, Chuhong Lin*[1]*, Hui Ling Tan*[1]*, Lavie Rekhi*[1]*, Renhong Li*[2]*, Wen Liu*[1]*, and* ***Tej Choksi***[1]
(1)School of Chemistry, Chemical Engineering and Biotechnology, Nanyang Technological University, Singapore, Singapore, (2)National Engineering Lab for Textile Fiber Materials and Processing Technology, Zhejiang Sci-Tech University, Hangzhou, China

Noble metals like Pd supported on TiB_2 exhibit a first-of-its-kind strong metal support interaction phenomena, that yields sinter-resistant metal catalysts. Using first principles microkinetic modelling and experimental characterization, we elucidate how dynamically formed

TiB_2 overlayers on Pd nanoparticles modify the reaction mechanism, rates, and selectivity, for formic acid decomposition.

Modeling Dynamic Activation of Single Atom Catalysts: Conversion of Formic Acid on Rh/Fe3O4 (001).

Benjamin Jackson[1], *Christopher Lee*[1], *Marcus Sharp*[1], *Mausumi Mahapatra*[1], *Simone Raugei*[1], *Liney Arnadottir*[1,2], *Mal Soon Lee*[1], *Bruce D. Kay*[1], *and Zdenek Dohnalek*[1]
(1)Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA, (2)School of Chemical, Biological and Environmental Engineering, Oregon State University, Corvallis, OR

Supported single-atom catalysts (SACs) have emerged as a frontier in fundamental catalytic research. This study demonstrates how thermally stable octahedral Rh single atoms incorporated in the Fe_3O_4(001) surface are dynamically released to form Rh adatoms catalytically active Rh adatoms due to surface hydroxyl recombination to water during reaction conditions.

Conversion of Bio-Ethanol into Olefins and Other Products for the Production of Sustainable Aviation Fuel.

Svetlana Tungatarova
Chemistry and Chemical Technology faculty, al-Farabi Kazakh National University, Almaty, Kazakhstan

Integrated technology for the catalytic conversion of bioalcohols is a solution to the growing global energy needs and ensures the creation of environmentally friendly technologies.

Synthesis of a Magnetic Fe-Cu-Zn Trimetallic Catalyst for CO2 Hydrogenation to Value-Added Chemicals.

Jayalatha Robinson[1], *Tyler Davide*[1], *Sanjaya D. Senanayake*[2], *and Cheng Zhang*[1]
(1)Long Island University Post, Brookville, NY, (2)Chemistry Division, Brookhaven National Laboratory, Upton, NY

This project focuses on converting CO_2 to light olefins via hydrogenation, addressing global warming and advancing green energy. The catalyst's novelty lies in tailored Fe-Cu-Zn interactions, enabling efficient conversion and high selectivity. Preliminary results show excellent catalytic performance and structural stability under reaction conditions.

One Step Dimethyl Ether Synthesis from CO_2 Hydrogenation over Hybrid Cu-ZnO-Al_2O_3/ Desilicated ZSM-5 Catalysts.

Dominique A. DAniel[1], *Amanda Guimarães*[1,2], *Lícia Ranni F. Coelho*[1,3], *Andressa Andrade Alves da Silva*[1], *Gabriel L. CAtuzo*[4], *Elisabete Assaf*[4], *and* ***Lisiane Veiga Mattos***[1]
(1)Fluminense Federal University, Niteroi, Brazil, (2)Rio de Janeiro State University, Rio De Janeiro, Rio de Janeiro, Brazil, (3)Military Institute of Engeneering, Rio De Janeiro, Rio de

Janeiro, Brazil, (4)Instituto de Química de São Carlos/Universidade de São Paulo, São Carlos, Brazil

This work evaluates the performance Cu-ZnO-Al_2O_3/desilicated ZSM-5 catalysts for direct DME synthesis from CO_2 hydrogenation. The 6CZA/ZSM-5 catalyst achieved optimal performance (240°C, 28 bar, 2,400 mL h^{-1} g^{-1}), demonstrating high CO_2 conversion and DME selectivity, highlighting the potential of this hybrid system as an efficient solution for CO_2 utilization.
4o

A Unique Magnetic FeCo Bimetallic Catalyst for Carbon Dioxide Conversion to Value Added Chemicals.

Tyler Davide[1]*, Jayalatha Robinson*[1]*, Sanjaya D. Senanayake*[2]*, and Cheng Zhang*[1]
(1)Long Island University Post, Brookville, NY, (2)Chemistry Division, Brookhaven National Laboratory, Upton, NY

Addresses climate change by advancing CO_2 utilization through innovative catalysts. Synthesized iron and cobalt organometallic complexes, oxidized to produce magnetic Fe_3O_4 and Co_3O_4, achieved efficient CO_2 hydrogenation. The process yielded valuable chemicals, including light olefins, with high selectivity and conversion rates, showcasing potential for sustainable energy and greenhouse gas mitigation.

Role of Carbon Species in Dry Reforming and Pyrolysis of Methane: Insights from Molten in-Sn and in-Ni Alloys.

Nikil Surya R[1]*, Genpei Cai*[2]*, Chester Upham*[2]*, and* ***Vishal Agarwal***[3]
(1)Department of Chemical Engineering, Indian Institute of Technology, Kanpur, India, (2)Chemical & Biological Engineering, University of British Columbia, Vancouver, BC, Canada, (3)Department of Chemical Engineering, Indian Institute of Technology Kanpur, Kanpur, India

This study presents a comparative analysis of the impact of accumulated carbon on the surface of molten In-Sn and In-Ni alloys, emphasizing its role in modulating catalyst surface properties and altering reaction pathways during methane dry reforming and pyrolysis reaction.

Quantitative TPR for Spillover and Surface Vacancy Determination on Reducible Oxide Supported Metal Catalysts.

Greg Barber[1]*, Griffin A. Canning*[2]*, and Robert Rioux*[1,3]
(1)Department of Chemical Engineering, The Pennsylvania State University, University Park, PA, (2)Chemical Engineering, The Pennsylvania State University, University Park, PA, (3)Department of Chemistry, The Pennsylvania State University, University Park, PA

A methodology for quantifying total spilled over hydrogen and estimating surface vacancies on metal supported reducible oxide catalysts by closing the H mass balance utilizing the captured

water from temperature programmed reduction was developed and applied to a Cu/TiO_2 catalyst to demonstrate the role of spillover hydrogen in alkene hydrogenation.

Catalytic Activity of Iron-Doped Molybdenum Oxide on Cyclohexane Oxidation.

Nishamini Ruwanthika Jayasekara[1], *Inosh P. Perera*[1], *Isaac Olowookere*[1], *Yasas Wickramathilaka*[1], *Santiago T. Salamanca*[1], *Sami Dursun*[2,3], *and Steven L. Suib*[1,2]
(1)Department of Chemistry, University of Connecticut, Storrs, CT, (2)The Institute of Materials Science, University of Connecticut, Storrs, CT, (3)Department of Metallurgical and Materials Engineering, Konya Technical University, Konya, Turkey

Cyclohexane oxidation produces important key monomers which are crucial for nylon synthesis. In this study, iron-doped molybdenum oxide materials were synthesized and used as a promising candidate for the oxidation of cyclohexane due to its higher conversion and better selectivity towards desired products under ambient conditions.

The Relation between Energy Transfer and Chemical Production during Ultrasound-Induced Cavitation..

Ari Fischer, *Tej Choksi, and Robert Maligon Querimit*
School of Chemistry, Chemical Engineering and Biotechnology, Nanyang Technological University, Singapore, Singapore

Ultrasound waves drive aqueous chemical reactions through bubble cavitation. We show that the reaction energy generated during cavitation, not the total work applied on the bubble, controls chemical production. These findings rationalize the effects of acoustic (e.g., wave amplitude) and solution properties (e.g., density) on chemical yields.

Dynamic Behavior of Oxide Overlayer on Supported Metal Catalysts.

Seyeon Park, *Daeyeon Lee, Raymond Gorte, and John Vohs*
Department of Chemical and Biomolecular Engineering, University of Pennsylvania, Philadelphia, PA

We investigate the dynamics of WO_x overlayers on Pt/SBA-15 and Pt/Al_2O_3. Its impacts on Pt coverage and catalytic activity are evaluated. Characterization reveals that WO_x migrates onto Pt on SBA-15, suppressing gas adsorption, but remains on Al_2O_3, partially covering Pt. Atomically thin WO_x maintained Pt reactivity in cyclohexane dehydrogenation.

Ragchem: Unlocking Chemical Knowledge.

Damian Camilo Martinez Martinez[1] *and Hui Fang*[2]
(1)Electical and Computer Engineering, University of Delaware, Newark, DE, (2)University of Delaware, Newark, DE

RAGChem, an innovative search engine designed to provide accurate and citable answers to chemistry questions. This system integrates our proposed RAG pipeline. Additionally, it extracts property-related entities from scientific literature in the field of catalysis

Development of Pt-Based Catalysts for the Dehydrogenation of Liquid Organic Hydrogen Carriers.

Musbau Gbadamosi[1], *Kaveh Shariati*[2], *Yanjiao Yi*[3], *John Meynard Tengco*[3], *Thossaporn Onsree*[2], *Azadeh Mehrani*[2], *Jagoda M. Urban-Klaehn*[4], *John Monnier*[3], *Jochen Lauterbach*[2], *and Donna Chen*[5]
(1)Chemistry and Biochemistry, University of South Carolina, Columbia, SC, (2)Department of Chemical Engineering, University of South Carolina, Columbia, SC, (3)Chemical Engineering, University of South Carolina, Columbia, SC, (4)Idaho National Laboratory, Idaho Falls, ID, (5)Chemistry, University of South Carolina, Coulmbia, SC

Pt catalysts supported on SiO_2, Al_2O_3, TiO_2, and ZrO_2 were studied for methylcyclohexane dehydrogenation. Pt/Al_2O_3 showed highest activity and stability, while Pt/SiO_2 deactivated due to carbon fouling and pore blockage. Findings support improved hydrogen release in LOHC systems.

Chen et al., *Fuel*, 360, 130607, 2024

Direct Visualization of Metal–Support Interactions during CO_2 Hydrogenation Via in Situ Gas-Cell TEM.

Hongkui Zheng[1], *Pritam K. Chakraborty*[2], *Ronald Spruit*[3], *Yevheniy Pivak*[1,3], *Hongyu Sun*[1,3], *Shibabrata Basak*[2], *Rüdiger-A Eichel*[2], *and Hugo Pérez Garza*[1,3]
(1)DENSsolutions, Irvine, CA, (2)Forschungszentrum Jülich GmbH, Jülich, NA, Germany, (3)DENSsolutions, Delft, Netherlands

We use in situ gas-cell TEM to visualize nanoparticle exsolution from a perovskite catalyst during CO_2 hydrogenation at 800 °C. Time-resolved imaging reveals dynamic migration, nucleation, and anchoring of particles, offering nanoscale insights into metal–support interactions critical for designing stable, high-performance catalysts under realistic conditions.

Mechanistic Insights into Crotyl Alcohol Isomerization over Cu/CeO_2 Catalysts.

Haiting Cai[1], *Shiva Murali*[1,2], *Huamin Wang*[1,2], *and Yong Wang*[1,2]
(1)Pacific Northwest National Laboratory, Richland, WA, (2)The Gene and Linda Voiland School of Chemical Engineering and Bioengineering, Washington State University, Pullman, WA

Controlling isomerization of crotyl alcohol is critical for the selective crotonaldehyde hydrogenation. The finding that the reaction preferentially occurs on the Cu^0-Ce^{n+}-O^{2-} active site ensembles, with the rates limited by the α-C-H cleavage, can shed light on the rational catalyst design for improving product selectivity during the selective crotonaldehyde hydrogenation.

Comparison Study on the NH_3 Cracking Catalysts Depend on the Manufacturing Methods for Commercialization.

Noh-Hyun Park
Ceracomb Co.,LTD., Asan-Si, Korea, Republic of (South)

For commercialization, nickel-based catalysts were prepared by coating, extrusion, and tablet methods, then evaluated for ammonia decomposition. The coating catalyst exhibited the highest ammonia conversion, attributed to the abundant of active materials on the surface. This result indicated the importance of catalyst structure in enhancing ammonia conversion performance.

Can in Situ TEM Identify Dynamic Active Sites?.

Gbolagade Olajide[1]*, Tristan Maxson*[2]*, and Tibor Szilvasi*[2]
(1)Chemical and Biological Engineering, University of Alabama, Tuscaloosa, AL, (2)Department of Chemical and Biological Engineering, The University of Alabama, Tuscaloosa, AL

Using DFT-trained machine learning interatomic potentials and TEM simulations, we show that active site formation and elimination occurs too quickly to be captured by *in situ* TEM. Consequently, relying only on *in situ* TEM for active site identification risks overlooking transient structures that may be crucial for catalytic performance.

CO_2 Direct Conversion to Methanol on Novel Membrane Reactor.

Yiqing WU[1]*, Matthew Seabaugh*[1]*, Anna Lee Tonkovich*[2]*, Eric Daymo*[2]*, Yong Wang*[3]*, and Wei Liu*[4]
(1)Nexceris, Lewis Center, OH, (2)Tonkomo LLC, Gilbert, AZ, (3)The Gene and Linda Voiland School of Chemical Engineering and Bioengineering, Washington State University, Pullman, WA, (4)Molecule Works Inc., Richland, WA

In this poster, our Nexceris team will present a novel reactor design that integrates a water-removal membrane into a CO_2-to-methanol reactor. This innovative membrane reactor design addresses two major challenges in the commercial development of CO2-to-methanol techniques: low CO2 single pass conversion and limited catalyst hydrothermal stability.

Development of Testing Methodology and Characterization Methods for Chromium Getters for Solid Oxide Fuel Cells.

Melissa Hess[1]*, Kevin Doura*[1]*, Nicole Garcia*[1]*, Joseph M. Fedeyko*[1]*, and Prabhakar Singh*[2]
(1)Clean Air - SEC, Johnson Matthey, Audubon, PA, (2)Materials Science and Engineering, University of Connecticut, Storrs, CT

The development of a chromium getter can lead to extended lifetimes for SOFC components, speeding adoption of new, environmentally friendly technologies. Testing these new

technologies can be difficult, expensive, and unsafe, but the reactor systems described here allow development to occur in a safe, efficient manner.

Copper Based Nitride Nanoparticles for Efficient Electrochemical Carbon Dioxide Reduction Under Low Overpotential.

Junrui Li[1]*, Oluwaseun Olarinde*[1]*, Rihana Burciaga*[1]*, Chaochao Dun*[2]*, Uhart Bradnock*[3]*, and Kayla Crawford*[1]
(1)Department of Chemistry, Clark Atlanta University, Atlanta, GA, (2)The Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, CA, (3)Williams College, Williamstown, MA

Current catalysts for CO_2 reduction suffer from low activity, poor selectivity, or limited stability. Herein, Cu-based nitride nanoparticles were precisely synthesized. Operando XAS study revealed the co-exisiting Cu^0 and Cu^+ that are believed to be active sites for ethanol production, emphasizing the importance of precise synthesis of catalysts.

Machine Learning Assisted Design of Metal-Nitrogen-Carbon Dual-Atom Catalysts for the Oxygen Reduction Reaction.

Prajeet Oza *and Guoxiang (Emma) Hu*
Georgia Institute of Technology, Atlanta, GA

Our ML-assisted computational framework employs the percentage of catalytically active structures, a more reliable descriptor than single structural configurations, to design stable, high-performing M1M2–N–C dual atom catalysts (DACs) for oxygen reduction reaction. This approach captures experimental trends and provides actionable guidance for rational design of DACs.

Choosing the Right Computational Model for Electrochemical Interfaces: Insights from MoS_2.

Ankit Bansal[1] *and Guoxiang (Emma) Hu*[2]
(1)Material Science and Engineering, Georgia Institute of Technology, Atlanta, GA, (2)Georgia Institute of Technology, Atlanta, GA

Accurate modeling of the electrochemical interface is critical for understanding catalytic mechanisms. Three main computational approaches are commonly employed: the computational hydrogen electrode (CHE) model, capacitance-based corrections, and grand canonical density functional theory (GC-DFT). These methods are investigated in this study using molybdenum disulfide (MoS_2) as a model system.

Dynamic Electrification Steers CO_2 Hydrogenation Selectivity Via Transient Surface Intermediates.

Kewei Yu[1]*, Sagar Sourav*[2]*,* ***Weiqing Zheng***[3]*, and Dionisios Vlachos*[4]
(1)Chemical and Biomolecular Engineering, University of Delaware, Newark, DE,

(2)Department of Chemical Engineering, Indian Institute of Technology Madras, Chennai, Tamil Nadu, India, (3)Delaware Energy Institute, University of Delaware, Newark, DE, University of Delaware, Newark, DE, (4)Delaware Energy Institute, University of Delaware, Newark, DE

Rapid pulse heating of CO_2 hydrogenation over Ni/Al_2O_3 enhances CO selectivity by dynamically modulating *CO and *H surface coverages. Operando spectroscopy reveals that temperature pulsing promotes *CO desorption over hydrogenation, enabling non-equilibrium pathways. This strategy offers a low-cost route to steer selectivity without altering catalyst composition or structure.

Copper-Doping and Surface Activation in Atomically Precise Au_{42}

Nanorods for Carbon Dioxide Reduction.

Rahul Somni *and Guoxiang (Emma) Hu*
Georgia Institute of Technology, Atlanta, GA
Change in potential-determining steps operando causes copper doping to hinder catalytic activity for CO_2RR for atomically precise Au_{42} nanoclusters (APNCs), a deviation from the norm for copper-based materials. This work highlights the importance of operando characterization of structure transformation, for which APNCs offer unique advantages.

Engineering the Nature of Rh Catalyst for Integrated CO_2 Capture and Utilization Via Dry Reforming of Methane: Effect of CeO_x and FeO_x Promoters on HAP.

Aybala Topcu[1]*, Ayse D. Erdali*[2]*, Erdem Deniz*[1]*, Yusuf Kocak*[2]*, Kaan Karaca*[2]*, and Zafer Say*[1,3]
(1)Micro and Nanotechnology, TOBB University of Economics and Technology, Ankara, Turkey, (2)Chemistry, Bilkent University, Ankara, Turkey, (3)Material Science and Nanotechnology Engineering, TOBB University of Economics and Technology, Ankara, Turkey

This study develops Rh-based dual functional materials (DFMs) for integrated CO_2 capture and dry reforming of methane over HAP supports with CeO_x and FeO_x promoters. The tailored systems show enhanced stability and coke resistance, offering a promising pathway for syngas production aligned with net-zero and circular carbon strategies.

Dimensional Energy: Converting CO_2 into Chemicals Via Reverse Water Gas Shift and Fischer-Tropsch Catalysts.

Bradley Brennan *and Sam Garncarz*
Dimensional Energy, Ithaca, NY

Dimensional Energy has developed a two-step process to convert CO_2 into chemicals and fuels, providing a scalable and sustainable alternative to fossil-based feedstocks. The Reverse Water Gas Shift thermocatalyst shows thermodynamic maximum conversion and high selectivity under wide boundary conditions, and the Fischer-Tropsch catalyst designed for high liquid/wax output.

Predicting Acid Pka at Catalyst-Solution Interfaces Using O-H Vibrational Frequency.

Bolton Tran*, Dean Sweeney, Yifei Liu, Jean-Patrick Selo, Mad Lindsey, and Bryan Goldsmith*
Chemical Engineering, University of Michigan, Ann Arbor, MI

We developed a computational approach to compute the O-H vibrational frequency of acids at catalyst-solution interfaces, from which the acid pKa value can be inferred. Our results advance fundamental understanding of the relationship between acid dissociation and the hydration environment.

Enhancing Dual Reforming Via Electric Field-Assisted Nanocomposite Catalysts.

Jung-Il Yang
Clean Fuels Laboratory, Korea Institute of Energy Research, Daejeon, Korea, Republic of (South)

Electric field-assisted nanocomposite catalysts demonstrated high CH_4 and CO_2 conversions and excellent coke resistance in low-oxidant dual reforming. The observed performance is attributed to internal electric fields formed within nanopore structures. The results suggest a promising pathway toward catalytic reforming electrification at lower temperatures for stable hydrogen production.

Enhancing Durability and Activity Toward Oxygen Evolution Reaction Using Single-Site Re-Doped Nifeox Catalysts at Ampere-Level.

Xiang Lyu *and Alexey Serov*
Oak Ridge National Laboratory, Knoxville, TN

Herein, we prepared a NiFeReOx catalyst with single-site Re dopants and observed that the single-site Re dopants could significantly enhance the durability without compromising the activity. A low degradation rate is observed with NiFeReOx catalyst in anion-exchange membrane water electrolyzer, which outperforms the NiFeOx and commercial IrOx catalysts.

Nanoporous Metal Oxide-Carbon Hybrid Materials Synthesized By Biomass Pyrolysis for Carbon Dioxide Capture.

Hong Je Cho *and Md Razaul Karim*
Chemical Engineering, Oklahoma State University, Stillwater, OK

We present one-step, facile synthesis of metal oxide-carbon (MO-C) hybrid materials via metal precursor-activating pyrolysis of spent coffee grounds (SCG) as carbon precursors, and elucidate how structure and properties of MO-C materials tailored by the control of synthetic factors affect their CO_2 adsorption performance.

Catalytic $SnSe_2$@Mxene Composite Separators for Superior Polysulfide Regulation in Lithium–Sulfur Batteries.

Amirhossein Mirtaleb**, Ruigang Wang, and **Md Monir Hossain
Chemical Engineering and Materials Science, Michigan State University, East Lansing, MI

Lithium–sulfur batteries offer high energy density but face issues like polysulfide shuttling and poor cycling stability. This study introduces $SnSe_2$@MXene composites as functional interlayers to enhance LiPSs adsorption, catalysis, and conductivity, thereby improving redox kinetics and stability for high-performance lithium–sulfur batteries.

Accelerated Catalyst and Process R&D for Conversion of Bio-Based Ethanol to Green Chemical Intermediates and Products.

Matthias Stehle
R&D Solutions, hte GmbH, Heidelberg, Germany

Catalytic valorization of bio-Ethanol into target products Ethylene and Acetaldehyde was investigated in parallel using high throughput experimentation. High quality data was acquired within short time, thus providing the right tool for process optimization and increased sustainability in chemical production.

Unlocking Superior Ethylamine Electro-Oxidation and Nitrile-like Intermediates Poisoning Resistance on Pt Enabled By Electronic and Geometric Modulation (Poster).

***Yanlin Zhu**, Jinyao Tang, and Zhenmeng Peng*
Chemical Engineering, University of South Carolina, Columbia, SC

Platinum (Pt) is active for ethylamine electro-oxidation but deactivates quickly. We developed a Pt_3Ni_1@Au catalyst, utilizing electronic effects from Pt-Ni alloying and geometric modulation via Au deposition, achieving enhanced stability. After 100 CV cycles, its activity retention is 5 times higher than pure Pt, showcasing its potential for hydrogen storage.

Iron Catalysts for Methane Pyrolysis: Understanding the Effects of Carbon Build-up on Structure and Activity (Poster).

***Veronica Piazza**, Lidia Castoldi, Chiara Negri, Marco Orsenigo, Davide Cafaro, Matteo Maestri, Gianpiero Groppi, and Alessandra Beretta*
Laboratory of Catalysis and Catalytic Processes - Dipartimento di Energia, Politecnico di Milano, Milano, Italy

This work examines Fe-Al_2O_3 catalysts at high Fe load for methane pyrolysis. The compositional effects, the role of reduction, the transformations that follow the incipient and extensive growth of carbon are investigated to better elucidate C build-up chemism and obtain rational guidelines to scale-up and industrialization.

Catalysts for Nylon-6 Depolymerization to ε-Caprolactam: Understanding the Structure-Performance Relationship. (Poster).

Prabin Dhakal[1]*, Derek Creaser*[2]*, and Louise Olsson*[2]
(1)Chemistry and chemical engineering, Chalmers University Of Technology, gothenburg, Sweden, (2)Chemical Engineering, Chalmers University of Technology, Gothenburg, Sweden

We have demonstrated a heterogeneous catalytic pathway for nylon depolymerization using only hydrogen. By investigating the influence of various metal oxide support properties, we provide valuable insights for designing efficient catalysts. These findings contribute to advancing polymer recycling and upcycling, promoting more sustainable processes in a circular economy.

Sugars and Polysaccharides As Renewable Feedstocks: The Use of Microwaves and Catalytic Mechanisms for Oxygenates (Poster).

Iris Yu
Civil & Environmental Engineering, National University of Singapore, Singapore, Singapore, Singapore

Energy-efficient processing and selective production are key to biomass valorization. We explore the potential of microwave-assisted processing in offering superheating, which concentrates energy on activating target chemical bonds. Furthermore, understanding the behaviors of bio-based molecules on catalyst surfaces will guide the future catalyst design for high-throughput and selective reactions.

Catalytic Depolymerization of Polyethylene By Induction Heating: A Continuous Flow Reactor System (Poster).

Bernard Whajah*, Sharonda Angelle, James Dorman, and Kerry Dooley*
Cain Department of Chemical Engineering, Louisiana State University, Baton Rouge, LA

Our system combining induction heating, metal-exchanged zeolites and in particular those with BEA morphology offers a good chance of long-term catalyst operation for polyolefin depolymerization to gasoline-range products without added H_2. These results underscore the importance of both catalyst selection and operating conditions for the continuous depolymerization of LDPE.

Hydrodeoxygenation of Phenol with NiMo and Niw Catalysts Supported on SBA-15.

Jessica Katherine Lamus Sanguino[1]*, Carlos Eduardo Santolalla-Vargas*[2]*, Fernando Trejo-Zárraga*[1]*, Octavio Aguilar Martínez*[2]*, and Luis Antonio Ramos Huerta*[2]
(1)CICATA Legaria, Instituto Politecnico Nacioanl, Mexico City, DF, Mexico, (2)Biociencias e Ingenieria, Departamento de Biociencias e Ingeniería, Centro Interdisciplinario de Investigaciones y Estudios sobre Medio Ambiente y Desarrollo, CIIEMAD-IPN, Instituto Politécnico Nacional, Gustavo A. Madero 07340, Ciudad de México, México., Mexico City, DF, Mexico

Mesoporous silicas SBA-15 were synthesized to be impregnated by incipient wetting with Ni, Mo and W, for phenol hydrodeoxygenation. The support was characterized by X-ray diffraction, scanning electron microscopy and nitrogen physisorption, confirming the synthesis of the support. The selectivity of the catalytic evaluation favors the hydrogenation route.

Time-Dependent Synthesis of ZnS and Its Influence on Photocatalytichydrogen Generation.

Jessica Katherine Lamus Sanguino[1], *Octavio Aguilar Martínez*[2,3], *Carlos Eduardo Santolalla-Vargas*[2], *Luis Antonio Ramos Huerta*[2], *Victor Florencio Santes Hernandez*[2], *Fernando Trejo-Zárraga*[1], *and Francisco Javier Tzompantzi Morales*[4]
(1)CICATA Legaria, Instituto Politecnico Nacioanl, Mexico City, DF, Mexico, (2)Biociencias e Ingenieria, Departamento de Biociencias e Ingeniería, Centro Interdisciplinario de Investigaciones y Estudios sobre Medio Ambiente y Desarrollo, CIIEMAD-IPN, Instituto Politécnico Nacional, Gustavo A. Madero 07340, Ciudad de México, México., Mexico City, DF, Mexico, (3)Departamento de Formación Básica, Instituto Politecnico Nacional. Unidad Profesional Interdisciplinaria de Ingeniería y Ciencias Sociales y Administrativas, Ciudad de Mexico, DF, Mexico, (4)Departamento de Química, Universidad Autónoma Metropolitana, Ciudad de México, DF, Mexico

The study investigates the effect of synthesis time on ZnS properties and its photocatalytic hydrogen generation efficiency. ZnS synthesized in 0.5 hours showed the highest hydrogen production (276 µmol/g/h) due to optimal surface area and crystallite size. Prolonged synthesis decreased efficiency despite improved crystallinity, emphasizing time's critical role in optimization.

PLENARY LECTURES

2025 EUGENE J. HOUDRY AWARD PLENARY LECTURE BY JOSÉ SANTIESTEBAN

Thursday, June 12, 2025 8:00 AM - 9:00 AM
Centennial Ballroom

Chair: Enrique Iglesia, Purdue University

Zeolite-Based Catalyst Technologies at the Forefront; Tackling the pressing challenges in the energy and chemical industries today and in the future.

Jose Santiesteban
ExxonMobil Research and Engineering Company, Leander, TX

BIOMASS - BIOMASS AND WASTE VALORIZATION CATALYSIS

BIOMASS - WASTE VALORIZATION

Thursday, June 12, 2025 9:30 AM - 11:30 AM
Regency Ballroom VI

Chair: Theodore Walker, Syracuse University

Co-Chair: Houqian Li, New Mexico State University

KEYNOTE: Impact of Feedstock Contaminants on Catalysts for Waste Valorization.

Josephine Hill
Chemical & Petroleum Engineering, University of Calgary, Calgary, AB, Canada

Waste materials represent tremendous resources that are inexpensive, accessible, and abundant, but these materials contain impurities that impact catalysts, positively or negatively depending on the process. Several examples will be given that demonstrate the impacts of sulphur and silicon on activated carbon production, esterification, and gasification.

Methane Assisted Catalytic Organic Solid Wastes Valorization.

Hua Song
Chemical and Petroleum Engineering, University of Calgary, Calgary, AB, Canada

This work reports a unique methane assisted catalytic low cost carbon resources valorization technology practiced both at lab and pilot scales (up to 1 ton/day) for clean fuel and/or high value-added chemicals production with great economic, environmental, and social benefits.

Hydrolysis of Dipeptides and Nylon 6 over Acid-Base Bifunctional Zirconia Catalyst.

***Mizuho Yabushita**, Satoshi Tomita, Takuma Kawakami, Yoshinao Nakagawa, and Keiichi Tomishige*
School of Engineering, Tohoku University, Sendai, Japan

ZrO_2 was found to be a highly active catalyst for the amide-bond hydrolysis: dipeptides with acidic or basic side chain into amino acids as well as nylon 6 into ε-caprolactam and ε-aminocaproic acid. The acid-base bifunctionality of ZrO_2 was demonstrated to be the key surface property to these hydrolysis reactions.

Selective Hydrogenation of FAMEs to Fatty Alcohol over Cationic Cu^+/Cu^+-H Catalyst.

*Chanisara Nooto[1], Kittisak Choojun[1], and **Tawan Sooknoi**[1,2]*
(1)Chemistry, King Mongkut's Institute of Technology Ladkrabang, Bangkok, Thailand,
(2)Catalytic Chemistry Research Unit, King Mongkut's Institute of Technology Ladkrabang, Bangkok, 10520, Thailand

High fatty alcohol production (>90% selectivity) was achieved via selective hydrogenation of FAMEs using CuMgAlOx catalysts. Cu^+/Cu^+-H reversible interconversion, facilitated by Mg content, optimized hydrogenation by balancing Cu^0 and Cu^+ species. $CuMg_{75}Al_{25}O_x$ exhibited 49.3 h^{-1} production with high stability.

Robust Engineered Catalysts for the Conversion of Brown Grease to Renewable Diesel Via Decarboxylation/Decarbonylation.

***Great Umenweke**[1,2], Robert Pace III[2], and Eduardo Santillan-Jimenez[1,2]*

(1)Department of Chemistry, University of Kentucky, Lexington, KY, (2)Center for Applied Energy Research, University of Kentucky, Lexington, KY

Engineered Ni-Cu catalysts converted brown grease quantitatively with excellent selectivity to renewable diesel (RD), outperforming powder formulations. Notably, the engineered catalyst effectively removed heteroatoms and metals present in the feed, affording a RD stream low in contaminants. Results demonstrate outstanding performance, showcasing the potential for scalable RD production.

C1 - CATALYSIS OF C1 CHEMISTRY

C1 - C-C COUPLING FROM C1

Thursday, June 12, 2025 9:30 AM - 11:30 AM
Regency Ballroom VII

Chair: Neil Razdan, University of California Berkeley

Co-Chair: Sheima Khatib, Virginia Tech

Quantifying Rates and Active Sites in Carbon Surfaces That Catalyze Non-Oxidative Coupling of Methane.

Justin Rosa-Rojas *and Rajamani Gounder*
Charles D. Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN

Kinetic measurements show that non-oxidative coupling of methane is catalyzed by carbon deposits formed during reaction and active sites are inhibited by hydrogen. H_2 temperature-programmed desorption is applied to quantify such active sites permitting the design of carbon-based catalysts that provide alternative surfaces for various non-oxidative reactions of hydrocarbons.

A First-Principles Analysis of Carbon Materials As Catalysts for the Non-Oxidative Coupling of Methane.

Luke Pretzie[1] *and Jeffrey Greeley*[2]
(1)Charles D. Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN, (2)Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN

Non-Oxidative Coupling of Methane is studied using Density Functional Theory calculations on carbon catalyst models. Findings suggest that graphene edge models are more catalytically active than graphene basal-plane models. This may inform the development of novel carbon catalysts, such as zeolite-templated carbons, for industrial-scale carbon-neutral ethylene production.

Synthesis and Characterization of Structurally Stable Molybdenum-Zeolite Catalysts for Methane Dehydroaromatization.

Angel Santiago-Colón[1]*, Hien N. Pham*[2]*, Abhaya Datye*[2]*, and Rajamani Gounder*[3]
(1)Chemical Engineering, Purdue University, West Lafayette, IN, (2)Department of Chemical

and Biological Engineering and Center for Micro-Engineered Materials, University of New Mexico, Albuquerque, NM, (3)Charles D. Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN

Quantitative characterization data, high-resolution microscopic imaging, and kinetic measurements show that Mo supported on small-pore (e.g., CHA) and Al-free MFI zeolites retain their structural stability during methane dehydroaromatization reaction-regeneration cycles, enabling new synthetic strategies to extend catalyst lifetime and design fully regenerable catalysts for methane dehydroaromatization applications.

Investigating the Effect of Mo and Fe Proximity in Zeolites for Methane Dehydroaromatization.

Md Sifat Hossain *and Sheima Khatib*
Chemical Engineering, Virginia Tech, Blacksburg, VA

This study demonstrates how bimetallic interactions between Mo and Fe within ZSM-5 channels enhance catalytic performance and stability in methane dehydroaromatization. Characterization reveals electronic interactions and improved reducibility of Mo species, providing key insights to optimize catalyst design for efficient methane valorization and advancing the commercialization of this promising process.

Optimized Spacing of Active Sites in Ni-Mo Catalysts Enhances Ethanol Production in Syngas Conversion.

Yangbin Ren[1], Qi Sun[1], and ***Yulong Zhang***[2]
(1)Chemical Engineering, Henan Polytechnical University, Jiaozuo, China, (2)Chemical Engineering, Henan Polytechnical University, Jiaozuo, Henan, China

Leaf-derived carbon dots modified K-promoted $NiMo_2C$ catalysts were synthesized by the temperature programmed reduction. CO hydrogenation to higher alcohols were carried out. It was indicated that the atomic-level proximity between transition metals and Mo active sites improves the transfer efficiency of active species and $C_{2+}OH$ selectivity.

Investigation of Molybdenum and Iron Catalysts for Non-Oxidative Coupling of Methane..

Mihir Kulkarni[1]*, Ethan Robey*[2]*, Bryce Clutter*[2]*, and Madelyn R. Ball*[1]
(1)Chemical Engineering and Materials Science, Michigan State University, East Lansing, MI, (2)Department of Chemical and Biomedical Engineering, West Virginia University, Morgantown, WV

Mo and Fe catalysts are investigated for methane coupling towards ethylene formation. Mo and MoFe catalysts produce ethylene from methane, with Fe addition slightly enhancing activity. However, activity does not increase linearly with Fe loading, and Fe addition does not affect ethane formation.

C2+ - CATALYSIS OF C2+ CHEMISTRY

C2+ | PROPANE DEHYDROGENATION REACTIONS

Thursday, June 12, 2025 9:30 AM - 11:30 AM
Hanover Hall FG

Chair: Juan Bravo-Suarez, The University of Kansas

Co-Chair: Xianqin Wang, New Jersey Institute of Technology

XAS for Early Stage Industrial Research in Propane Dehydrogenation Catalysts.

Randall Meyer[1]*, Pedro Serna Merino*[2]*, Alyssa Love*[1]*, and Corey Kaminsky*[1]
(1)Exxonmobil, Annandale, NJ, (2)Instituto de Tecnología Química, Valencia, Spain

ExxonMobil has a history of using X-ray Absorption Spectroscopy to aid their catalyst development programs. We will detail a few examples of studies designed to improve our understanding supported metal catalysts for alkane dehydrogenation. In situ studies at the APS and NSLS-II have been used to assess potential regenerability.

Proximity Control of Active Sites to Facilitate Tandem Catalysis in Propane Oxidative Dehydrogenation.

Geunho Han[1]*, Kunmo Koo*[2]*, Selim Alayoglu*[3]*, and Justin Notestein*[3]
(1)Center of Catalysis and Surface Science, Northwestern University, Evanston, IL, (2)NUANCE Center, Northwestern University, Evanston, IL, (3)Department of Chemical & Biological Engineering, Northwestern University, Evanston, IL

Tandem catalysis often takes place with multiple active sites. For propane oxidative dehydrogenation, we used Pt and In_2O_3 for propane dehydrogenation and subsequent CO_2 reduction by using produced H_2 *via* dehydrogenation. The proximity between the active sites was controlled by structural modification, and greater proximity resulted in faster tandem kinetics.

Re, Cs, and Cl Promotion Effects on the Selective Oxidation of Ethylene at Oxygen Vacancy Sites.

Adhika Setiawan[1]*, Tiancheng Pu*[1]*, Israel Wachs*[1]*, and Srinivas Rangarajan*[2]
(1)Department of Chemical and Biomolecular Engineering, Lehigh University, Bethlehem, PA, (2)Chemical and Biomolecular Engineering, Lehigh University, Bethlehem, PA

With an extended ethylene oxidation (EO) reaction network featuring both oxometallacycle (OMC) and non-OMC pathways, Density Funcitonal Theory (DFT) and qualitative microkinetic modeling (MKM) analyses were used to expand the understanding of promoter effects (Re, Cs, Cl) on the EO system on partially oxidized silver (Ag) surfaces.

Tuning Ga-Sites and Acidity on Ga/Al_2O_3 Catalysts Via H_2 Reduction or Co-Feeding: Insights into Propane Dehydrogenation Performance.

Sebastian Amar Gil[1]*, Catherine Especel*[1]*, Francisco J. Passamonti*[2]*, Viviana M. Benítez*[2]*, and Florence Epron*[1]
(1)CNRS, Université de Poitiers, Institut de Chimie des Milieux et Matériaux de Poitiers-IC2MP, Poitiers, France, (2)Instituto de Investigaciones en Catálisis y Petroquímica – INCAPE, Santa Fe, Argentina

H_2 co-feeding decreases propane conversion on calcined Ga/Al_2O_3. Reduction pretreatment, by decreasing acidity, improves propylene yield but reduces propane conversion, in the absence or presence of H_2. Increasing H_2 in the feed minimizes deactivation by removing coke. GaH_x produced under H_2 has no significant effect on performance.

Modulating Active Cobalt Centers Confined in Zeolite Using Non-Metal Species for Enhanced Propane Dehydrogenation.

Younhwa Kim *and Christopher W. Jones*
Georgia Institute of Technology, Atlanta, GA

This work presents an effective strategy for engineering non-noble metal-confined zeolite catalysts to achieve high-performance propane dehydrogenation. The incorporation of boron species facilitates the formation of active cobalt-boron oxide clusters. This catalyst delivered markedly improved C_3H_6 productivity with exceptional selectivity (~99%) and demonstrated excellent regenerability via calcination in air.

Synthesis-Structure-Activity Relationship of Vanadium-Impregnated Small Pore Zeolite Catalysts for Non-Oxidative and Oxidative Dehydrogenation of Propane.

Iqtidar Ali Khan[1]*, Jose Alirio Mendoza Mesa*[1]*, Max Bols*[2]*, and Michiel Dusselier*[3]
(1)Center for Sustainable Catalysis and Engineering, KU Leuven, Heverlee, Belgium, (2)Laboratory for Chemical Technology, Ghent University, Ghent, Belgium, (3)Center for Sustainable Catalysis and Engineering, KU Leuven, Leuven, Belgium

Vanadium-based small-pore zeolite catalysts were optimized for CO_2-assisted propane dehydrogenation, revealing a synthesis-structure-activity relationship that contrasts with non-redox systems reported in literature. These catalysts efficiently convert CO_2 and C_3H_8, coproducing CO and C_3H_6, offering high conversion rates and providing a sustainable alternative to traditional catalysts for industrial propene production.

DYNAMICS - DYNAMIC CATALYSIS

DYNAMICS - UNDERSTANDING STRUCTURAL DYNAMICS

Thursday, June 12, 2025 9:30 AM - 11:30 AM
Centennial Ballroom III

Chair: Rajamani Gounder, Purdue University

Co-Chair: Matteo Monai, Utrecht University

Reactant-Induced Activation of Single Atom Rh/Fe_3O_4(001) Catalysts.

*Marcus Sharp[1], Benjamin Jackson[1], Christopher Lee[1], Mausumi Mahapatra[1], Simone Raugei[1], Liney Arnadottir[1,2], Mal Soon Lee[1], Bruce D. Kay[1], and **Zdenek Dohnalek**[1]*
(1)Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA, (2)School of Chemical, Biological and Environmental Engineering, Oregon State University, Corvallis, OR

The dehydration and dehydrogenation of HCOOH on Rh/Fe_3O_4 single-atom catalysts are studied. Metastable Rh adatoms efficiently shift dehydration on Fe_3O_4(001) to dehydrogenation on Rh_{ad}/Fe_3O_4(001). The activity of structurally stable substitutional Rh in Fe_3O_4 surface is found to be induced by transient conversion to Rh adatoms induced by surface hydroxyls.

Linking the Structural and Chemical State of Bimetallic Pt Alloy Catalysts to Their Activity and Stability during Hydrocarbon Oxidation.

Steven Chavez[1], *Melissa Cendejas[2], Shyama Charan Mandal[3], Pin-Hung Chung[4], Gennaro Liccardo[5], Adam Hoffman[6], Frank Abild-Pedersen[3], Simon Bare[6], and Matteo Cargnello[7]*
(1)Department of Chemical and Biomolecular Engineering, University of California, Los Angeles, Los Angeles, CA, (2)SLAC National Accelerator Laboratory, Menlo Park, CA, (3)SUNCAT Center for Interface Science and Catalysis, SLAC National Accelerator Laboratory, Menlo Park, CA, (4)Materials Science and Engineering, Stanford University, Stanford, CA, (5)Stanford University, Stanford, CA, (6)Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, Menlo Park, CA, (7)Chemical Engineering, Stanford University, Stanford, CA

We use a combination of kinetic measurements, density functional theory, and operando x-ray/infrared spectroscopy to correlate the physical and electronic structure of highly active Pt alloy nanoparticle catalysts to their activity for hydrocarbon oxidation. We find that reducible oxide supports can mitigate dynamic catalyst restructuring.

A Metastable State Facilitates Low Temperature CO Oxidation over Pt Nanoparticles.

*Samantha L. Le[1,2], Christopher O'Connor[1], Taek-Seung Kim[1,3], **Audrey Dannar**[1], and Christian Reece[1]*
(1)Rowland Institute at Harvard, Harvard University, Cambridge, MA, (2)Department of Chemistry, Stanford University, Stanford, CA, (3)Korea Institute of Energy Research, Daejeon, Korea, Republic of (South)

We report the successful isolation and characterisation of a high-activity metastable state over supported 2nm Pt nanoparticles. This state is formed after CO desorbs from well-coordinated Pt sites, and is highly localised to the surface of the nanoparticle.

Influence of Temperature, Water and Dioxygen on the Interconversion of Monomeric and Dimeric Cu Configurations in Cu-SSZ-13.

Rohil Daya[1]*, Mi-Young Kim*[1]*, Unmesh Menon*[1]*, Lai Wei*[1]*, Hongmei An*[1]*, and Christopher Paolucci*[2]
(1)Cummins Inc., Columbus, IN, (2)Chemical Engineering, University of Virginia, Charlottesville, VA

The dynamic interconversion between monomeric and dimeric Cu in Cu-SSZ-13 as a function of temperature, H_2O and O_2 pressure is described quantitatively in a mathematical framework. We synthesize findings from spectroscopic and computational studies on Cu-Zeolites with CO titration experiments to propose a hybrid kinetic model of active site transformation.

Liquid-like Pore Environments Promote Dynamic Multi-Site Oxidation Catalysis over Metal-Zeolites.

Deepak Sonawat[1]*, Mohan Shankar*[2]*, Patrick Granowski*[1]*, Matthew Edgar*[1]*, Christopher Paolucci*[2]*, and* ***Siddarth Krishna***[1]
(1)Chemical and Biological Engineering, University of Wisconsin-Madison, Madison, WI, (2)Chemical Engineering, University of Virginia, Charlottesville, VA

We combine steady-state kinetics with synchrotron XAS on PdCu/zeolites across widely varying water vapor pressures to elucidate the catalytic consequences of intrapore water condensation on the dynamic reactivity of zeolite-bound Cu and Pd ions for Wacker oxidation of olefins, guiding design of catalysts containing mobilized active sites on solid surfaces.

Millisecond Time-Resolved IR Measurements of CO Coverage on Pt/γ-Al_2O_3 during Pulsed Visible Photon Illumination.

Ryan Berry*, Phillip Christopher, and Michael Gordon*
Chemical Engineering, University of California, Santa Barbara, Santa Barbara, CA

Millisecond time-resolved IR spectroscopy was developed to study transient CO coverage on Pt/γ-Al_2O_3 during visible light pulses. CO desorption kinetics via Pt-CO photolysis was observed as a function of photon flux, temperature, and partial pressure. Measuring these timescales provides critical insights for leveraging dynamic perturbations to control photocatalytic reactions.

ELECTRO PHOTO - ELECTROCATALYSIS AND PHOTOCATALYSIS

ELECTRO PHOTO - ORGANIC ELECTROCHEMICAL TRANSFORMATIONS 3

Thursday, June 12, 2025 9:30 AM - 11:30 AM
Centennial Ballroom I

Chair: Dohyung Kim, University of Pennsylvania

Co-Chair: Fanglin Che, University of Massachusetts Lowell

Electrochemical Regeneration of Platinum: Overcoming Biogenic Impurity Poisoning for the Electrocatalytic Hydrogenation of *Cis,Cis*-Muconic Acid to Biobased Adipic Acid.

Devanshi Mistry[1,2]*, Tyler A. Bailey*[1,2]*, Macgregor S. Catanag*[1,2]*, Luke T. Roling*[1,2]*, and Jean-Philippe Tessonnier*[1,2]
(1)Department of Chemical and Biological Engineering, Iowa State University, Ames, IA, (2)Center for Biorenewable Chemicals (CBiRC), Iowa State University, Ames, IA

The activity of Pt catalysts poisoned by biogenic impurities can be fully restored through electrochemical regeneration using reductive stripping, enabling the electrocatalytic hydrogenation of biobased muconic acid to adipic acid. This work creates new opportunities for integrating fermentation and electrocatalysis while eliminating costly purification steps for sustainable chemical manufacturing.

Doping Ni-Ooh to Boost the Electrooxidation of Hyroxymethylfurfural.

Tony Ermacora[1,2]*, Laureline Treps*[1,2]*, Stephan N. Steinmann*[1,2]*, and* ***Carine Michel***[1,2]
(1)Chemistry, ENS Lyon, Lyon, France, (2)Laboratoire de Chimie, CNRS, Lyon, France

Biomass electrocatalysis allows for the combined production of chemicals and green hydrogen, but the lack of stability of the anodic material ($Ni^{III}OOH$) at a potential lower than 1.5V is a severe limitation. We explored in silico if dopants can stabilize $Ni^{III}OOH$ and generate new sites to oxidize HMF into FDCA.

Impact of Electrolyte Engineering and Modulation of the Local Catalyst/Support Environment on Bulk Electrolysis of Furfural over Platinum Catalysts.

Marc Manye Ibanez*, Joseph Hasse, Emma Hollis, J. Will Medlin, and Adam Holewinski*
Chemical and Biological Engineering, University of Colorado Boulder, Boulder, CO

Partial electrooxidation of furanic biomass derivatives are of interest for the sustainable production of commodity and fine chemicals. In this study, oxidative bulk electrolysis of furfural is studied under varying electrolyte conditions. The effects of pH, and supporting anion are studied, and selectivity trends are coupled with in situ ATR-SEIRAS.

Selective Photocatalytic Oxidation of Methanol and Ethanol with WO_3-Based Catalysts Under Visible Light.

Robert Tracy Jr. and ***Christopher Landry***
Chemistry, University of Vermont, Burlington, VT

This study explores WO_3-based photocatalysts modified with Au and Pt for the selective photooxidation of methanol and ethanol under visible light, demonstrating enhanced efficiency and selectivity. It highlights WO_3's potential in sustainable chemical synthesis and suggests avenues for optimizing catalysts.

KEYNOTE: Unraveling the Kinetics and Mechanisms of Electroorganic Reactions.

Elizabeth Biddinger
Chemical Engineering, The City College of New York, New York, NY

Electroorganic reactions offer the opportunity to produce chemicals using renewable electricity at distributed manufacturing sites. Identifying the reaction mechanisms and kinetics is vital to being able to implement the next generation of electroorganic reactions in industry.

ENERGY INPUTS - NOVEL ENERGY INPUTS FOR CATALYSIS

ENERGY INPUTS - CATALYSIS DRIVEN BY ULTRASOUND, INDUCTION HEATING, AND MICROWAVE ENERGY

Thursday, June 12, 2025 9:30 AM - 11:30 AM
Hanover Hall CDE

Chair: Siris Laursen, University of Tennessee

Co-Chair: Steven Chavez, University of California, Los Angeles

Accelerating Sonochemical Reactions through the Ultrasonic Activation of Catalytic Cavitation Agents.

Nicholas Golio *and Prince N. Amaniampong*
Institut de Chimie des Milieux et Matériaux de Poitiers, CNRS, Poitiers, France

Copper (II) oxide (CuO) catalytic cavitation agents were shown to significantly reduce the acoustic energy input required to initiate and catalyze sonochemical reactions. Engineering catalytic cavitation agents with enhanced surface features allows us to accelerate sonochemical reaction rates while providing insight into cavitation bubble dynamics.

Radical-Driven Oxidation of Benzyl Alcohol to Oxalic Acid Via Unsaturated Dicarbonyl Intermediates Using Ultrasound.

Ari Fischer[1]*, Teseer Bahry*[2]*, Zhangyue Xie*[1]*, Roberto Batista Da Silva Junior*[3]*, Kaicheng Qian*[4]*, Renhong Li*[4]*, James Kwan*[5]*, Francois Jerome*[2]*, Sabine Valange*[2]*, Wen Liu*[1]*, Prince N. Amaniampong*[2]*, and Tej Choksi*[1]
(1)School of Chemistry, Chemical Engineering and Biotechnology, Nanyang Technological University, Singapore, Singapore, (2)Institut de Chimie des Milieux et Matériaux de Poitiers, CNRS, Poitiers, France, (3)Senai Cimatec, Salvador, Brazil, (4)National Engineering Lab for Textile Fiber Materials and Processing Technology, Zhejiang Sci-Tech University, Hangzhou, China, (5)Engineering Science, University of Oxford, Oxford, United Kingdom

Ultrasound irradiation offers a sustainable method for aqueous oxidation chemistry in water using electricity. Here, we show that ultrasound irradiation is able to fragment the aromatic ring in benzyl alcohol to oxalic acid, via unsaturated carbonyl intermediates, through aqueous radical chemistry.

Directed Electromagnetic Thermocatalysis for Low-Energy Conversion of Waste Plastic to Olefins..

Mark Elvington, Kevin Enyekwe, Yanjiao Yi, John Meynard Tengco, Sirivatch Shimpalee, John Regalbuto, and ***Jay Gaillard***
Chemical Engineering, University of South Carolina, Columbia, SC

Electromagnetic (EM) reactors provide a means for precise, site-selective heat delivery to heterogeneous catalysts. This work focuses on low-energy EM heating through novel susceptor designs as a sustainable platform system leveraging microwave and radio frequency induction reactors for conversion of waste plastic to olefins.

Enhanced Catalyst Stability and Energy Efficiency in Ethanol Steam Reforming Via Induction Heating.

Letícia Sosa[1]*, André Felipe Marandino Guimarães*[2]*,* ***João Monnerat***[1]*, and Pedro Romano*[3]
(1)Chemistry Institute, Federal University of Rio de Janeiro, Rio de Janeiro, Brazil, (2)Federal University of Rio de Janeiro, Rio de Janeiro, Brazil, (3)Campus D. de Caxias, Federal University of Rio de Janeiro, Rio de Janeiro, Brazil

This work highlights the potential of induction heating for the ethanol steam reforming reaction by significantly improving energy efficiency, catalyst stability, and hydrogen selectivity using a Ni/Al_2O_3 catalyst deposited on FeCrAl monolith.

Enhanced Hydrodeoxygenation of m-Cresol Via Bifunctional Pt/HY Catalysts in Microwave-Assisted Systems: A Pathway to Efficient Bio-Oil Upgrading.

Caio Souza[1]*,* ***Pedro Romano***[2]*, Javier García-Martínez*[3]*, and João Monnerat*[4]
(1)Escola de Química, Federal University of Rio de Janeiro, Rio de Janeiro, Rio de Janeiro, Brazil, (2)Campus D. de Caxias, Federal University of Rio de Janeiro, Rio de Janeiro, Brazil, (3)Molecular Nanotechnology Lab, Department of Inorganic Chemistry, University of Alicante, Alicante, Spain, (4)Chemistry Institute, Federal University of Rio de Janeiro, Rio de Janeiro, Brazil

In this work, we report the use of a novel bifunctional catalyst (Pt/HY) that combine metal and acid properties and, for the first time, the use of microwave heating for hydrodeoxygenation under mild conditions (150°C and 10 bar of H_2) of lignin-derived compounds.

Carbon-Coated Fibrous Silica Nanospheres for Enhanced Photothermal Catalysis.

Alejandra Rendon-Patiño[1]*, Xinhuilan Wang*[1]*, Diego Mateo*[1]*, Edgar Stiven Duran-Uribe*[2]*, Antonio Sepúlveda Escribano*[2]*,* ***Enrique Vicente Ramos-Fernandez***[1,2]*, and Jorge Gascon*[1]
(1)KAUST Catalysis Center, King Abdullah University of Science and Technology, Thuwal, Saudi Arabia, (2)Inorganic Chemistry Department, University of Alicante, Alicante, Spain

This study introduces a photothermal catalyst using carbon-coated KCC-1 nanospheres with Ru nanoparticles. It excels in ammonia decomposition (17,300 mmol gRu^{-1} h^{-1}) and CO_2 hydrogenation (90% CO selectivity), leveraging light absorption and thermal retention. The

catalyst demonstrates synergy between thermal and non-thermal effects, with stable performance over 100 hours.

FUNDAMENTALS - FUNDAMENTALS OF CATALYSIS AND SURFACE SCIENCE

FUNDAMENTALS - REACTION MECHANISMS AND KINETICS 2

Thursday, June 12, 2025 9:30 AM - 11:30 AM
Centennial Ballroom II

Chair: Manuela Serban, Honeywell UOP

Co-Chair: Elizabeth Bickel Rogers, University of Minnesota

Exploring Initial Hydrocarbons Formation in Methanol to Hydrocarbons Reaction Via Synchrotron-Based Mass Spectrometry.

Teng Li[1] *and Javier Ruiz-Martinez*[2]
(1)KAUST, Thuwal, Makkah, Saudi Arabia, (2)Chemical Engineering, King Abdullah University of Science and Technology, Jeddah, Saudi Arabia

Advanced, synchrotron-based *operando* photoelectron photoion coincidence spectroscopy and photoionization mass spectrometry were applied to study the incipient chemistry of methanol-to-hydrocarbons (MTH) reaction. Combined with theoretical calculations, we provide a comprehensive understanding on initial hydrocarbons formation over H-ZSM-5 zeolite, including the first C–C bond, olefins, and aromatics.

Deciphering the Mechanism of Methanol Oxidative Dehydrogenation on MoO_3/TiO_2 Catalysts Via Operando-Drifts Transient and Isotopic Studies.

Bastián Fuentes[1]*, Gabriel Galdames*[1]*, and Alejandro Karelovic*[2]
(1)Chemical Engineering, Universidad de Concepción, Concepción, Región del Biobío, Chile, (2)Chemical Engineering, Universidad de Concepción, Concepcion, Chile

This research combines key arguments from different perspectives on the mechanism of methyl formate formation, using transient IR experiments with deuterated isotopes. It evidences distinct mechanisms on different MoO_3 domains and clarifies the role of Lewis sites, providing a deeper understanding of the process on MoO_3/TiO_2 catalysts.

Enhancing Rh Single-Atom Catalytic Activity Via Atomically Dispersed Reducible Oxides for the Reverse Water-Gas Shift Reaction.

Baraa Werghi[1]*, Benjamin Moskowitz*[2]*, Libor Kovarik*[1]*, Simon Bare*[3]*, and Janos Szanyi*[1]
(1)Pacific Northwest National Laboratory, Richland, WA, (2)Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA, (3)Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, Menlo Park, CA

Advancing the understanding of catalyst structure-activity relationships through targeted design is critical for enabling efficient CO_2-to-CO conversion. This study offers valuable insights into designing Rh catalysts supported on alumina modified with dispersed Ce and Mo oxides, demonstrating their potential to achieve highly efficient and selective CO_2 hydrogenation

Unraveling the Proton-Coupled Electron Transfer Mechanism of H_2 Activation on Au/TiO_2 Via Kinetic Isotope Effects.

Angela Pathickal Abraham
Chemistry, Penn State University, State College, PA

Kinetic isotope effects (KIE) from isotopic labeling of gas and support for H_2 adsorption on Au/TiO_2 revealed a large secondary inverse KIE, highlighting the critical role of TiO_2 hydroxyls and supporting a proton-coupled electron transfer (PCET)-like mechanism. These insights can guide tuning the activation kinetics for enhanced catalytic performance.

Highly Reactive Ceria Nanomaces for Enhanced Lattice Oxygen Kinetics for Oxidation Reactions.

Jeong Woo Han[1], Myeong Gon Jang[2], and ***Seokhyun Choung***[1]
(1)Department of Materials Science and Engineering, Research Institute of Advanced Materials, Seoul National University, Seoul, Korea, Republic of (South), (2)Seoul National University, Seoul, 08826, Korea, Republic of (South)

By combining high-resolution characterizations and multi-scale simulations using a pretrained GNN, this work provides fundamental insights into oxygen kinetics in ceria nanostructures. The findings demonstrate the critical role of morphology control in enhancing catalytic performance and establish design principles for developing advanced metal oxide catalysts.

Understanding Dilute Alloy Catalysts for Oxidation and Hydrogenation Reactions.

Jennifer Lee[1]*, Robert J. Madix*[2]*, and Cynthia M. Friend*[1,2]
(1)Chemistry and Chemical Biology, Harvard University, Cambridge, MA, (2)School of Engineering and Applied Sciences, Harvard University, Cambridge, MA

This talk aims to show how the design of dilute alloy catalysts can be used to enhance the activity and selectivity of oxidation and hydrogenation reactions, with a special focus on characterizing the evolution of the structure and composition of catalysts and their relationship to catalytic function.

LIQUID - CATALYSIS IN LIQUID, SUPERCRITICAL, AND MULTIPHASE SYSTEMS

LIQUID - ADVANCED CATALYTIC PROCESSES AND KINETIC MODELING

Thursday, June 12, 2025 9:30 AM - 11:30 AM
Centennial Ballroom IV

Chair: Bin Wang, University of Oklahoma

Co-Chair: Manish Shetty, Texas A&M University

Selective Propylene Epoxidation from Plasma-Liquid Interactions Using Water As the Oxygen Source.

*Dongho Lee[1,2], **Han-Ting Chen**[3], and Suljo Linic[3]*
(1)Department of Chemistry, University of Ulsan, Ulsan, Korea, Republic of (South), (2)CCS Research Department, Korea Institute of Energy Research, Daejeon, Korea, Republic of (South), (3)Department of Chemical Engineering, University of Michigan, Ann Arbor, MI

We designed a plasma-induced catalytic process that converts water into hydrogen peroxide in the plasma phase, which serves as an oxidizing agent to epoxidize propylene over the titanium silicate-1 catalyst dispersed in the solution. We explored reactor designs to reach a carbon-based selectivity of 98%.

Impact of Solvents on the Catalytic Hydrogenation of Benzaldehyde on Rh-Based Catalysts.

***Thuy Le**[1], Julia de Barros Dias Moreira[1,2], Allan Cardenas[3], Donald M. Camaioni[1], Oliver Gutiérrez-Tinoco[1], Abhi Karkamkar[1], and Johannes Lercher[1,4]*
(1)Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA, (2)Technische Universität München, Garching, Germany, (3)Chemistry and Biochemistry, State University of New York at Fredonia, Fredonia, NY, (4)Department of Chemistry and Catalysis Research Center, Technische Universität München, Garching, Germany

We quantitatively investigate the effect of solvent on adsorbed reactants to establish an inverse correlation between hydrogen binding and hydrogenation rate. Weaker hydrogen binding (i.e. higher chemical potential) to the metal surface causes higher rate constants of hydrogenation, in concordance with earlier research on benzaldehyde and furfural hydrogenation on Pd/C.

Non-Faradaic Promotion Effect of Cathodic Potential on Pd-Catalyzed Benzaldehyde Hydrogenation in Aqueous Phase.

***Julia de Barros Dias Moreira**[1,2], Thuy Le[1], Laura C. Meyer[1], Alexander von Rueden[1,3], Benjamin Jackson[1], Mal Soon Lee[1], John L. Fulton[1], Sungmin Kim[1], Huamin Wang[1], Donald M. Camaioni[1], Udishnu Sanyal[1], Oliver Gutiérrez-Tinoco[1], and Johannes Lercher[1,2]*
(1)Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA, (2)Department of Chemistry and Catalysis Research Center, Technische Universität München, Garching, Germany, (3)University of Wisconsin-Madison, Madison, WI

With a kinetic and mechanistic approach, our results show that the catalyst electric potential can manipulate even the non-faradaic Pd-catalyzed benzaldehyde hydrogenation reaction and highlight the importance of accounting for the effects of metal electric potential when studying fundamental aspects of catalysis in liquid phase.

Understanding Aqueous Solvent Effects on the Carbonyl Group Hydrogenation over a Pt(111) Catalyst Surface.

Paratee Komen[1] *and Andreas Heyden*[2]
(1)Chemical Engineering, University of South Carolina, Columbia, SC, (2)Department of Chemical Engineering, University of South Carolina, Columbia, SC

This study examines aqueous-phase hydrogenation of 2-butanone to 2-butanol on Pt(111). Liquid water reduces adsorption and hydrogenation rates. Carbon hydrogenation in the hydroxy pathway dominates on Pt without water as a co-catalyst, while on Ru, water accelerates oxygen hydrogenation in the alkoxy pathway, which is rate-controlling.

Modeling of the Kinetics of Tandem Chain Scission/Aromatization.

Jiankai Ge[1]*, Jiakai Sun*[2]*, Danielle Burns*[2]*, Olajide Bamidele*[3]*, Yu-Hsuan Lee*[2]*, Mahdi Abu-Omar*[4]*, Andreas Heyden*[5]*, Baron Peters*[1]*, and Susannah Scott*[4]
(1)Chemical and Biomolecular Engineering, University of Illinois at Urbana-Champaign, Urbana, IL, (2)Department of Chemistry & Biochemistry, University of California Santa Barbara, Santa Barbara, CA, (3)Chemical Engineering, University of South Carolina, Columbia, SC, (4)Department of Chemical Engineering, University of California, Santa Barbara, Santa Barbara, CA, (5)Department of Chemical Engineering, University of South Carolina, Columbia, SC

This study investigates the catalytic depolymerization of polyethylene to alkylaromatics, emphasizing the role of moderate hydrogen pressures in optimizing reaction rates and product selectivity. By integrating experimental and kinetic modeling, it provides insights for designing sustainable catalytic processes to upcycle plastic waste into valuable surfactant-range chemicals under mild conditions.

Polymer-Modified Catalysts for Improved Biomass Conversion Processes.

David Moses[1]*, Xuyang Qin*[2]*, Shikha Nangia*[2]*, and Theodore Walker*[1]
(1)Biomedical and Chemical Engineering, Syracuse University, Syracuse, NY, (2)Department of Biomedical and Chemical Engineering, Syracuse University, Syracuse, NY

We present a strategy to modify supported catalysts with densely grafted polymer moieties, creating tunable microsolvation environments that stabilize desired product molecules over undesired ones and steering reaction selectivity in liquid water. Our approach combines molecular simulations, polymer synthesis and experimental reaction kinetic investigations.

C1 - CATALYSIS OF C1 CHEMISTRY

C1 - CO TO CHEMICALS

Thursday, June 12, 2025 1:00 PM - 3:20 PM
Regency Ballroom VII

Chair: Chester Upham, University of British Columbia

Co-Chair: Musa Najimu, University of Southern California

Structure Sensitivity in CO and CO_2 Hydrogenation over Copper-Supported Catalysts: An Operando FT-IR Study at Elevated Pressures.

Jelle Kranenborg[1,2]*, Nina Genz*[2]*, Maarten Nachtegaal*[2]*, Matteo Monai*[1]*, and Bert M. Weckhuysen*[1]
(1)Inorganic Chemistry and Catalysis, Institute for Sustainable and Circular Chemistry, Utrecht University, Utrecht, Netherlands, (2)Paul Scherrer Institute, Villigen, Switzerland

This study uses high-pressure operando infrared spectroscopy to investigate structure sensitivity in CO and CO_2 hydrogenation on Cu/SiO_2, revealing that larger particles exhibit higher turnover frequencies and that formate intermediates are particle-size dependent. Findings clarify the role of formate, guiding catalyst design to improve CO_2 conversion efficiency into renewable methanol.

Advancing Fischer-Tropsch Synthesis (FTS): Development of Bimetallic Catalysts Involving TiO_2 Nanotube Arrays on 3D-Printed Substrates and Acid-Functionalized Supports.

Luis Caballero *and Michael Nigra*
Department of Chemical Engineering, University of Utah, Salt Lake City, UT

This work encompasses the development of bimetallic iron-cobalt catalysts for Fischer-Tropsch synthesis (FTS) using innovative TiO_2 nanotube arrays on 3D-printed structures and acid-functionalized TiO_2. The catalysts exhibit significant activity for FTS, producing valuable hydrocarbon products from syngas and laying the groundwork for future optimization studies to advance traditional catalyst design.

Modulating the Production of Fischer-Tropsch Synthesized Jet Fuel By Hydrogen Transfer over Co/Al_2O_3-Hβ Composite Catalysts.

Shuaishuai Lyu[1]*, Jinxu Liu*[1]*, Run Xu*[1]*, and Xingang Li*[2]
(1)Sinopec Research Institute of Petroleum Processing Co., LTD, Beijing, Beijing, China, (2)tianjin university, Tianjin, Tianjin, China

Hydrogen spillover over Hβ modulates the catalytic performance of the highly active Co/Al_2O_3-Hβ composite catalyst in jet fuel production via Fischer-Tropsch route.

The Effects of Zn and Ni Addition to Cu/BEA for a Single Reactor Syngas-to-Hydrocarbon Process.

Hyewon Lee*, Anh To, and Daniel A. Ruddy*
Catalytic Carbon Transformation and Scale-Up Center, National Renewable Energy Laboratory, Golden, CO

Modification of Cu/BEA with Ni and Zn provides an opportunity to tune the olefin content in the HC product. The olefin content can directly affect the fuel properties of high-octane gasoline product and provides precursors to aviation fuel via downstream olefin coupling reactions.

Shaping and Stabilizing the Active Phase: The Role of Carbon Surface Defects in Carbon-Supported Co Fischer-Tropsch Catalysts.

Felix Herold *and Magnus Rønning*
Chemical Engineering, Norwegian University of Science and Technology, Trondheim, Trøndelag, Norway

Carbon surface defects that are not saturated by heteroatoms such as O, are a neglected factor of influence in carbon/metal interactions. In this study, we could demonstrate the crucial impact of carbon surface defects on catalyst genesis and catalyst stability at the example of Co/C FTS catalysts.

Atomically Dispersed Cu-Ce Species for Water-Gas Shift Reaction.

Yiwei Yu[1], Tie Wang[2], Ning Yan[3], and ***Jingyue Liu[4]***
(1)School for Engineering of Matter, Transport and Energy, Arizona State University, Tempe, AZ, (2)National University of Singapore, Singapore, Singapore, (3)Chemical and Biomolecular Engineering, National University of Singapore, Singapore, Singapore, (4)Department of Physics, Arizona State University, Tempe, AZ

High-area alumina anchored Ce^{3+} species stabilize atomically dispersed Cu^{+} to form active Cu^{+}–Ce^{3+} molecular complexes and they work synergistically to enhance performance of low-temperature water-gas shift reaction.

Selective Methane Oxidation over Zeolite-Supported Catalysts in a High Pressure Flow Reactor.

Mark Berko*, A.K.M. Kazi Aurnob, James J. Spivey, and Kunlun Ding*
Cain Department of Chemical Engineering, Louisiana State University, Baton Rouge, LA

We focused on metal catalysts—gold (Au) and rhodium (Rh)—supported on zeolite (e.g., ZSM-5) for the selective oxidation of methane. A high pressure fixed-bed plug-flow reactor was constructed for this study. We observe more selective acetic acid productivity on Rh/Zeolite and a more selective methanol productivity on Au/Zeolite catalyst.

CO2 - CO2 CAPTURE AND UPGRADING

CO2 - NEW CO_2 ACTIVATION METHODS AND CATALYSTS

Thursday, June 12, 2025 1:00 PM - 3:20 PM
Centennial Ballroom IV

Chair: Madelyn Ball, Michigan State University

Co-Chair: Juliana Carneiro, Columbia University

KEYNOTE: Challenges and Opportunities in Catalytic Conversion of CO_2.

Jingguang G. Chen
Chemistry Division, Brookhaven National Laboratory, Upton, NY; Chemical Engineering, Columbia University, New York, NY

The talk discusses strategies for CO2 conversion to value-added products to reduce emissions, emphasizing net-negative CO2 emissions through energy and mass balance considerations.

Photo-Catalytic Reactive Capture and Conversion of CO2.

*Matthew Yung[1], Sawyer Halingstad[1], **Noemi Leick**[1], and Wade Braunecker[2]*
(1)National Renewable Energy Laboratory, Golden, CO, (2)Chemistry and Nanoscience Center, National Renewable Energy Laboratory, Golden, CO

Photo-based RCC offers great potential to integrate renewable energy with DAC to storage energy or manufacture chemicals. Our process is the first-of-its kind amine-based DAC/RCC process to produce methane and show feasibility of using this as a means to store renewable energy.

Converting Carbon Dioxide into Carbon Nanotubes By Reacting with Ethane.

***Yong Yuan**[1] and Jingguang G. Chen[1,2]*
(1)Chemistry Division, Brookhaven National Laboratory, Upton, NY, (2)Chemical Engineering, Columbia University, New York, NY

An efficient method has been developed to produce carbon nanotubes from CO_2 and C_2H_6 at 750 °C, utilizing earth-abundant transition metals (Fe, Co, Ni) as catalysts. The process simultaneously generates syngas as byproducts. The morphology of the carbon nanotube depends on the type of catalysts.

Hollow ZSM5 Spheres for Selective CO_2 Hydrogenation.

***Mohammadreza Kosari**[1], Abdul Majeed Seayad[1], Armando Borgna[2], and Hua Chun Zeng[3]*
(1)Chemical & Biomolecular Engineering, North Carolina State University, Raleigh, NC, (2)Institute of Chemical & Engineering Sciences, Singapore, Singapore, (3)Department of Chemical and Biomolecular Engineering, National University of Singapore, Singapore, Singapore

Zeolites and its novel class of hollowed zeolites are of mounting importance for a variety of clean catalytic applications such as catalytically converting abundant CO_2 to valued-added chemicals. Herein, uniform spherical hollow ZSM-5 (hZSM5) with two distinct morphologies as monodispersed (mhZSM5) and networked (nhZSM5) is synthesized for selective CO_2 hydrogenation.

MOF-Derived Catalysts for Aqueous Phase CO_2 Hydrogenation to Acetic Acid.

Rajan Lakshman[1]*, Swarit Dwivedi*[1]*, Sanje Mahasivam*[2]*, Satya Sireesha Rameswarapu*[1]*, Alan Chaffee*[1]*, and Akshat Tanksale*[1]
(1)Chemical and Biological Engineering, Monash University, Clayton, VIC, Australia, (2)School of Chemistry, RIMT University, Melbourne, VIC, Australia

This work demonstrates a potential green pathway for acetic acid production through direct CO_2 hydrogenation. ZIF-derived catalysts containing highly active Co-Ni metal sites catalysed CO_2 conversion to acetic acid via a formic acid intermediate, highlighting their C-C coupling activity and contributing to the challenge of CO_2 conversion into C_{2+} compounds

Novel Functionalized Porous Polymer-Based Catalyst for CO_2 Conversion to Formic Acid or Formate.

Jane Agwara[1]*, Harry M. Meyer III*[2]*, and Michelle Kidder*[3]
(1)Oak Ridge National Laboratory (ORNL), Oak Ridge, TN, (2)Chemical Sciences Division, Oak Ridge National Laboratory (ORNL), Oak Ridge, TN, (3)Oak Ridge National Laboratory, Oak Ridge, TN

Current catalytic CO_2 conversion technologies struggle with selectivity and stability. We developed a novel porous polymer-based catalyst that integrates the advantages of both heterogeneous and homogeneous systems, enabling reactive CO_2 adsorption and selective conversion to formic acid or formate at low temperatures and pressure with high turnover number, and stability.

DYNAMICS - DYNAMIC CATALYSIS

DYNAMICS - FUNDAMENTALS OF DYNAMIC CATALYSIS

Thursday, June 12, 2025 1:00 PM - 3:20 PM
Centennial Ballroom III

Chair: Max Huelsey, Technical University of Munich

Co-Chair: Audrey Dannar, Harvard University

Understanding Metal-Adsorbate Charge Transfer: H_2 on Pt.

Justin Hopkins[1]*, Shengguang Wang*[2]*, Kyung-Ryul Oh*[3]*, Benjamin Page*[4]*, Jesse Canavan*[1]*, Nondumiso Chibambo*[5]*, Lars Grabow*[6]*, James R. McKone*[7]*, Paul J. Dauenhauer*[1]*, and Omar Abdelrahman*[6]
(1)Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN, (2)Idaho National Laboratory, Idaho Falls, ID, (3)Research Center for Nanocatalysts, Korea Research Institute of Chemical Technology, Daejeon, Korea, Republic of (South), (4)Department of Chemical and Biomolecular Engineering, University of Houston, Houston, TX, (5)CEMS, University of Minnesota Twin Cities, Minneapolis, MN, (6)William A. Brookshire Department of Chemical and Biomolecular Engineering, University of Houston, Houston, TX, (7)Chemical and Petroleum Engineering, University of Pittsburgh, Pittsburgh, PA

This work develops a method to measure the charge transfer that occurs as gas species adsorb to metal catalysts, using H_2 adsorption to Pt as a test system, to predict how applied voltages manipulate the species' binding energies to catalysts and to understand how different adsorbates respond under dynamic voltages.

Recontextualizing the Energy Efficiency for Dynamic Modulation of Formic Acid Electro-Oxidation.

Soubarno Sen *and Omar Abdelrahman*
William A. Brookshire Department of Chemical and Biomolecular Engineering, University of Houston, Houston, TX

Efficiency within electrocatalysis is typically contextualized as either faradaic or thermodynamic efficiencies. But investigations within this work point towards the non-faradaic contributions to charge, while defining efficiencies, and their significant impact over dynamic modulations in potentials. Comprehending the foundations for efficiency estimations would better help us optimize the observed enhancements.

***Mechanistic Insights into the Effect of Surface Charge Oscillation on Ammonia Synthesis from First Principles Kinetic Simulations*.**

Rajat Daga*, Ulrick Gaillard, Jesse Canavan, Paul J. Dauenhauer, and Matthew Neurock*
Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN

A multiscale kinetic modeling approach is utilized to elucidate the impact of surface charge oscillations on ammonia synthesis on Ru (0001) surface. The KMC simulations revealed that the rate vs. surface charge plot exhibits a volcano-shaped trend, with dynamic oscillations around the Sabatier optimum enhancing ammonia synthesis rate by ~3x.

KEYNOTE: Opportunities and Fundamental Aspects of Dynamic and Programmable Catalysis.

Lars Grabow
Center for Programmable Energy Catalysis (CPEC), Minneapolis, MN; William A. Brookshire Department of Chemical and Biomolecular Engineering & Texas Center for Superconductivity (TcSUH), University of Houston, Houston, TX

The advent of programmable catalysis and dynamically operated, modular reactors may shatter longstanding catalyst design principles that rely on the Sabatier principle. The prerequisites to surpass limits imposed by the Sabatier principle through transient operation and opportunities for unprecedented catalytic performance and selectivity control will be discussed.

Dynamics of a Ruthenium Catalyst Revealed during NO Oxidation to NO_2 at Industrial Nitric Acid Production Conditions.

*Jithin Gopakumar[1], Bjørn Christian Enger[2], David Waller[3], and **Magnus Rønning**[1]*
(1)Chemical Engineering, Norwegian University of Science and Technology, Trondheim, Trøndelag, Norway, (2)Process Technology, SINTEF Industry, Trondheim, Norway, (3)Yara Technology Center, Porsgrunn, Norway

The results show that NO-NO_2 equilibrium in NO oxidation to NO_2 can be efficiently attained at nitric acid plant conditions using a Ru catalyst. *In-situ* characterization can be used to monitor dynamic oscillations in the catalyst surface.

Understanding the Structure and Deactivation of NiZn Alloy Catalysts in CO_2 Dry Reforming Via Forced Dynamic Operando Reactors.

*Xueqin Bai[1], Hend Omar Mohamed[1], Pia Dally[1], Vijay Velisoju[1], Bambar Davaasuren[2], and **Pedro Castaño**[1,3]*
(1)KAUST Catalysis Center(KCC), King Abdullah University of Science and Technology(KAUST), Thuwal, Saudi Arabia, (2)Imaging and Characterization Core Lab, KAUST, Thuwal, Saudi Arabia, (3)Physical Science and Engineering, King Abdullah University of Science and Technology(KAUST), Thuwal, Saudi Arabia

We introduce the forced dynamic operando method, a novel approach combining strengths of forced dynamic operation and operando characterization. This powerful technique allows us to investigate dynamic structural changes, catalyst deactivation and reaction mechanisms of NiZn alloy catalysts under relevant DRM conditions.

ENVIRO AUTO - ENVIRONMENTAL AND AUTOMOTIVE CATALYSIS

ENVIRO AUTO - DEACTIVATION OF CU-ZEOLITE SCR CATALYSTS

Thursday, June 12, 2025 1:00 PM - 3:20 PM
Centennial Ballroom I

Chair: Galen Fisher, University of Michigan

Co-Chair: Dhruba Jyoti Deka, Pacific Northwest National Laboratory

Impact of Cu Loading on NH_3 Adsorption and Oxidation Dynamics in Cu/SSZ-13 and Cu/SSZ-39 Catalysts for NOx Reduction.

*Gabriela I Hernandez-Salgado[1] and **Gustavo Fuentes**[2]*
(1)Department of Science and Engineering, IBERO-Puebla, Puebla city, Mexico, (2)Department of Process Engineering, UAM-Iztapalapa, Mexico City, Mexico

This study examines the impact of Cu loading on NH_3 adsorption and oxidation in Cu/SSZ-13 and Cu/SSZ-39 catalysts for NOx reduction. Higher Cu content enhances NH_3 storage and activation, forming key intermediates ($[Cu(NH_3)_4]^{2+}$) that improve SCR performance. These insights guide the optimization of Cu-zeolites for efficient NOx mitigation.

Atomic-Scale Origins of the Hydrothermal Stability of Copper Chabazite for the Selective Catalytic Reduction of NO_x with NH_3.

Alyssa McNarney[1], *Michael B. Schmithorst*[1], *Bryan Cruz Delgado*[2], *Vivek Vattipalli*[3], *Subramanian Prasad*[4], *Takayuki Iida*[3], *Ahmad Moini*[3], *Rajamani Gounder*[2], *and Bradley F. Chmelka*[1]
(1)Department of Chemical Engineering, University of California Santa Barbara, Santa Barbara, CA, (2)Charles D. Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN, (3)BASF Environmental Catalyst and Metal Solutions, Iselin, NJ, (4)BASF Corporation, Iselin, NJ

These findings establish the atomic-scale origins of SCR kinetics and explain the higher hydrothermal stabilities of Cu^{2+} cations located near paired Al sites within the CHA framework. The insights provide design criteria that are expected to enable the development of new Cu-chabazite catalysts with improved NO_x conversion performance.

SO_2 and SO_3 Poisoning Effect on the N_2O Formation over Cu/SSZ-13 Used for NH_3 SCR.

Joonsoo Han, Derek Creaser, and ***Louise Olsson***
Chemical Engineering, Chalmers University of Technology, Gothenburg, Sweden

We have examined how SO_2 and SO_3 influence the N_2O formation during ammonium nitrate decomposition for NH_3-SCR applications, used for emission cleaning. A large effect on the ammonium nitrate formation and decomposition was observed after sulfur poisoning of Cu/SSZ-13, especially in the presence of SO_3.

Modeling of Cu/SSZ-13 SCR Catalyst Sulfation and HTA-Induced Changes in ZCuOH and Z_2Cu Site Distribution.

Tetyana Zheleznyak[1], *Petr Koci*[1], *and William Epling*[2]
(1)University of Chemistry and Technology, Prague, Czech Republic, (2)Chemical Engineering, University of Virginia, Charlottesville, VA

A kinetic model describing Cu site transformation during hydrothermal aging was developed, revealing that Z_2Cu sites are less vulnerable to sulfur poisoning than ZCuOH sites. The model predicts catalyst performance in sulfur-containing environments, highlighting the enhanced resilience of aged catalysts due to site transformations, crucial for optimizing SCR catalyst longevity.

Investigation of NH_3-SCR over Cu-SSZ-13 in H_2-ICE Exhaust Condition.

Garam Lee[1], *Dhruba Jyoti Deka*[1], *Kenneth Rappe*[1], *Eric D. Walter*[1], *Janos Szanyi*[1], *and Yong Wang*[1,2]
(1)Pacific Northwest National Laboratory, Richland, WA, (2)Washington State University, Pullman, WA

Cu-SSZ-13, a state-of-the-art NH_3-SCR catalyst used in diesel-ICE aftertreatment, may be less efficient and durable NH_3-SCR catalyst for H_2-ICE aftertreatment. Insight from this study can

inform the development of new catalyst formulations and aftertreatment architectures tailored for H_2-ICE exhaust systems.

KEYNOTE: New Concept Catalytic Materials for Environmental Applications.

Fudong Liu
Department of Chemical and Environmental Engineering, University of California, Riverside, Riverside, CA

Supported metal single-atom catalysts (SACs) and fully exposed cluster catalysts offer remarkable advantages in catalysis, achieving nearly 100% utilization of supported metals, particularly high-cost noble metals. The intrinsic catalytic performance of SACs and cluster catalysts is highly dependent on the local coordination environment of the isolated or ensembled metal atoms.

FUNDAMENTALS - FUNDAMENTALS OF CATALYSIS AND SURFACE SCIENCE

FUNDAMENTALS - METAL-SUPPORT INTERACTIONS & ALLOY CATALYSTS

Thursday, June 12, 2025 1:00 PM - 3:20 PM
Centennial Ballroom II

Chair: Paul Kim, Shell

Co-Chair: Houqian Li, New Mexico State University

Single Atom Catalysts on Exsolved Nano-Socket for Outstanding Stability with High Metal Dispersions.

Jeong Woo Han[1]*, Tae Yong Kim*[2]*, Hyung Jun Kim*[3]*, and Taein Lee*[3]
(1)Department of Materials Science and Engineering, Research Institute of Advanced Materials, Seoul National University, Seoul, Korea, Republic of (South), (2)School of Energy, Materials and Chemical Engineering, Korea University of Technology and Education, Cheonan, Korea, Republic of (South), (3)Department of Materials Science and Engineering, Seoul National University, Seoul, Korea, Republic of (South)

We reported highly active and stable single atom catalysts, namely nano-socket single atom (NSA) catalysts, that maximize the number of exposed Pt atoms while maintaining their metallic state. NSA catalysts consist of cerium oxide with exsolved transition metal nanoparticles (nano-socket) and single Pt atoms selectively dispersed on the exsolved nanoparticles.

Integrating Earth-Abundant Iron in Metal-Ligand Single Atom Catalysts for Propane Dehydrogenation..

Wondemagegn Wanna[1] *and Steven Tait*[2]
(1)Chemistry, Indiana University, Bloomington, IN, (2)Indiana University, Bloomington, IN

This study demonstrates propane dehydrogenation (PDH) using iron-ligand coordinated single-atom catalysts (SACs) on CeO2 support. The SACs exhibit high stability, tunable performance, and unique catalytic properties, achieving 26% propane conversion and 90% propylene selectivity, comparable to conventional catalysts, while operating at moderate temperatures.

Au-Core Pd-Shell Catalysts for Selective Hydrogenation: Impact of the Shell Thickness and Exposed Crystal Facet.

Marta Perxés Perich[1], *Jan-Willem Lankman*[1], *Petra E. de Jongh*[2], *and Jessi E.S. van der Hoeven*[1]
(1)Materials Chemistry and Catalysis, Debye Institute for Nanomaterials Science, Utrecht University, Utrecht, Netherlands, (2)Materials Chemistry and Catalysis, Utrecht University, Utrecht, Netherlands

Au-Pd core-shell catalysts exhibit extraordinary catalytic performance in the selective hydrogenation of butadiene. Here, we test the effect of the Pd-shell thickness and the exposed crystal facet on the catalytic performance by combining the hydrogen-deuterium exchange reaction and selective hydrogenation of butadiene.

The Effect of Metal-Support Interactions on Nanoparticle Catalyst Structure.

Tristan Maxson and ***Tibor Szilvasi***
Department of Chemical and Biological Engineering, The University of Alabama, Tuscaloosa, AL

We show computational results in agreement with benchmark-level experiments on how metal-support interactions influence the structure of supported metal nanoparticles with 1-5 nm diameter. We find that idealized nanoparticle constructions and extended surface models are not accurate representations below ~4 nm nanoparticles for the studied systems.

Selective Chemical Substitution of Pd-Rich Intermetallic Catalysts Enhances Net Ethylene Selectivity during Competitive Acetylene Hydrogenation.

Nilanjan ROY[1], *Mustafa Eid*[2], *Jin LI*[1], *Kathryn MacIntosh*[3], *Michael Janik*[1], *and Robert Rioux*[4,5]
(1)Chemical Engineering, The Pennsylvania State University, University Park, PA, (2)Chemistry, The Pennsylvania State University, University Park, PA, (3)Chemical and Biomedical Engineering, The Pennsylvania State University, University Park, PA, (4)Department of Chemistry, The Pennsylvania State University, University Park, PA, (5)Department of Chemical Engineering, The Pennsylvania State University, University Park, PA

Selective substitution by monovalent Cu and Ag on one of the two available Pd-sites in $InPd_3$, led to the formation of new ternary intermetallics $InPd_{3-x}M_x$ (M =Cu/Ag; x =0–1). These catalysts showed high net ethylene selectivity during competitive hydrogenation of acetylene in excess propylene, governed by electronic structure alterations.

Directing Furfural Hydrogenation Using Steric Effects of Intermetallic Compounds.

Wenyu Huang, *Charles Ward, Minda Chen, Andrew Lamkins, and Da-Jiang Liu*
Chemistry, Iowa State University, Ames, IA

Intermetallic nanoparticles (iNPs) have garnered much attention as effective catalysts. Here, furfural hydrogenation catalyzed by Rh-based iNPs displays secondary metal-dependent chemoselectivity. The explored surface steric effects provide basis for further investigation into other iNP for selectively targeting products in catalytic reactions and increasing efficiency and utility of biomass-derived chemical feedstocks.

Vapor-Phase Oxidative Coupling over Bimetallic Catalysts.

Alexander Minne and ***James W. Harris***
Department of Chemical and Biological Engineering, The University of Alabama, Tuscaloosa, AL

Oxidative coupling over bimetallic catalysts is a versatile chemistry for valorization of small molecules. The reaction is structure sensitive; the kinetics, reactivity, and selectivity depending on particle size and the presence of inorganic promoters. These findings enable economical oxidative coupling without use of stoichiometric oxidants or toxic reagents.

MICRO MESO - MICROPOROUS AND MESOPOROUS MATERIALS

MICRO MESO - ACID SITE CHARACTERIZATION

Thursday, June 12, 2025 1:00 PM - 3:20 PM
Hanover Hall FG

Chair: Gina Noh, ETH Zurich

Co-Chair: Brandon Bukowski, Johns Hopkins University

The Impact of Various Zeolite Additives and Promoters on Brønsted Acid Site Quantification in MFI Zeolites Using Common Alkylamine Tprxn.

Ismaeel Alalq, *Nabihan Abdul Rahman, Ana Carolina Jerdy, Daniel Resasco, and Steven P. Crossley*
School of Sustainable Chemical, Biological and Materials Engineering, University of Oklahoma, Norman, OK

Temperature-programmed reaction (TPRxn) of alkylamines yields comparable Brønsted acid site (BAS) quantification in non-modified zeolites. However, certain zeolite additives/promotors introduce discrepancies. Our study highlights the importance of selecting suitable alkylamines for accurate BAS quantification, addressing disparities and ensuring reliable catalytic activity assessment.

Acidity Trends across Topologies and Trivalent Framework Cations Probed By Adsorption Calorimetry and Aldol Fission Chemistry.

Richard Whitfield III[1]*, Isaac Ogabiela*[1]*, Oleksiy V. Shvets*[2]*, Mykhailo M. Kurmach*[2]*, Nataliya Shcherban*[3]*, and Friederike Jentoft*[1]
(1)Department of Chemical Engineering, University of Massachusetts Amherst, Amherst, MA, (2)L.V. Pisarzhevsky Institute of Physical Chemistry, National Academy of Sciences of Ukraine, Kyiv, Ukraine, (3)Department of porous substances and materials, L.V. Pisarzhevsky Institute of Physical Chemistry, National Academy of Sciences of Ukraine, Kyiv, Ukraine

The acidity of two series of isomorphously substituted zeotypes with BEA and MFI framework and trivalent cations of B, Al, Ga and Fe is characterized by adsorption calorimetry of isopropylamine and by activity and selectivity in aldol catalysis. The acidity trend of Al>Ga>Fe>B largely holds across the two framework topologies.

Implications of Acid and Metal Siting on Accessibility and Reactivity in (Bifunctional) Zeolite Catalysts.

Cole Hullfish*, Jun Zhi Tan, and Michele Sarazen*
Department of Chemical and Biological Engineering, Princeton University, Princeton, NJ

Acid and metal site densities on surfaces and in micropores of (bifunctional) zeolite catalysts are determined via reaction-based techniques utilizing size-excluded molecules. This siting is responsible for reactivity trends when diffusion/accessibility is relevant, including higher rates of polyethylene cracking on MFI zeolites with higher external Brønsted acid site densities.

Unravelling Irreversible Adsorbate Thermodynamics through Adsorption-Assisted Desorption.

Omar Abdelrahman
William A. Brookshire Department of Chemical and Biomolecular Engineering, University of Houston, Houston, TX

We demonstrate the ability to experimentally measure the adsorption enthalpy and entropy of alkylamines on a wide range of zeolites, investigating the effect of molecular structure and spatial proximity on adsorption thermodynamics within the confines of a zeolite pore.

The Impact of Acid-Site Pairing on Adsorption and Reactivity in CHA.

Nicole Kragt[1]*, Bereket Bekele*[2]*, John Di Iorio*[2]*, Rajamani Gounder*[2]*, and David Hibbitts*[1,2]
(1)Department of Chemical Engineering, University of Florida, Gainesville, FL, (2)Charles D. Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN

Static DFT calculations suggest alkane cracking rates increase in the presence of acid-site pairing in CHA because enthalpic barriers decrease, whereas AIMD simulations of $(CH_3)_2NH$ adsorption in CHA support experimental evidence that these rate increases are entropically driven. Therefore, we believe static DFT is unsuitable for modeling high-temperature reactions.

Dialing in Acid Sites of Mesoporous USY Zeolites Via Na^+ Ion Titration.

Abraham Martinez[1], *Jinyi Han*[2], *C.Y. Chen*[2], *Son-Jong Hwang*[3], *Bi-Zeng Zhan*[2], *Alexander Kuperman*[2], *and Alexander Katz*[4]
(1)Department of Chemical and Biomolecular Engineering, University of California - Berkeley, Berkeley, CA, (2)Chevron Energy Technical Center, Richmond, CA, (3)Chemical Engineering, Caltech, Pasadena, CA, (4)Chemical and Biomolecular Engineering, University of California, Berkeley, Berkeley, CA

We have discovered a minority of highly active sites within USY zeolite catalysts that can be dialed in through sodium ion titration. These sites result in loss of isomerization selectivity, a greater amount of coking during CI test catalysis, and the onset of activity during low temperature Friedel Crafts acylation.

Strength and Distribution of Acid Sites on Amorphous Aluminosilicate Surfaces and Their Implication for Catalytic Cracking Reactions.

Kaustubh Sawant[1], *David Stockwell*[2], *Anthony DeBellis*[2], *Roel Sanchez-Carrera*[2], *and Philippe Sautet*[1]
(1)Chemical and Biomolecular Engineering, University of California, Los Angeles, Los Angeles, CA, (2)BASF, Iselin, NY

Amorphous aluminosilicates (AS) are crucial in catalysis for their stability, porosity, and acidity, though their atomic structure is challenging to characterize. This study combines DFT, machine learning, and advanced sampling techniques to model acid sites on AS and establish structure-property relationships for catalytic cracking reactions.

NEW COMP - NEW METHODS IN COMPUTATIONAL CATALYSIS

NEW COMP - ENERGY CALCULATIONS

Thursday, June 12, 2025 1:00 PM - 3:20 PM
Hanover Hall CDE

Chair: Jean-Sabin McEwen, Washington State University

Co-Chair: Matthew Sean Johnson, Sandia National Laboratories

Independent Atom Ansatz of Density Functional Theory for Low-Cost Simulations in Chemistry and Catalysis.

Alexander V. Mironenko
Chemical and Biomolecular Engineering, University of Illinois Urbana-Champaign, Urbana, IL

Computational predictions in chemistry and catalysis are hindered by the high cost of quantum mechanical methods, such as DFT. We propose a new DFT ansatz that simplifies the electronic structure problem and lowers the cost of energy calculations. Method is demonstrated for H_x, period-2 diatomics, and catalytic H_2 dissociation.

Theoretical Model for Proton-Coupled Electron Transfer Involving Polarons on Anatase TiO_2 Surfaces.

Robert Warburton
Department of Chemical and Biomolecular Engineering, Case Western Reserve University, Cleveland, OH

Vibronically nonadiabatic proton-coupled electron transfer (PCET) theory is used to model rate constants for the PCET reaction between reduced TiO_2 surfaces and a nitroxyl radical oxidant. The model elucidates kinetic differences between polaron defects, as well as the importance of excited vibronic states on PCET rate constants.

Enthalpies of Formation of Adsorbates with Chemical Accuracy from DFT through Error Cancellation.

C Franklin Goldsmith[1] and ***Bjarne Kreitz***[1,2]
(1)School of Engineering, Brown University, Providence, RI, (2)School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA

A new method is presented that uses error cancellation reactions to boost the accuracy of DFT-derived enthalpies of formation for adsorbates. The method combines single-crystal adsorption calorimetry experiments, gas-phase databases, and DFT data into a global thermochemical network that can achieve chemical accuracy for some adsorbates on Pt(111).

Multireference Wavefunction Methods for Single-Atom Catalysts.

Colin Gallagher *and Qing Zhao*
Department of Chemical Engineering, Northeastern University, Boston, MA

Despite their ubiquity, single-reference (SR) wavefunction methods i.e. DFT are limited in their ability to accurately predict electronic structure of doped-graphene SACs. In this work, we propose using multi-reference wavefunction methods to benchmark SR methods to more accurately assess principles of catalyst design for electrochemical CO_2R applications.

Understanding the Proton Source for CO_2 Electroreduction Using Many-Body Perturbation Theory.

Dongfang Cheng[1]*, Ziyang Wei*[2]*, and Philippe Sautet*[1]
(1)Chemical and Biomolecular Engineering, University of California, Los Angeles, Los Angeles, CA, (2)Department of Chemistry and Biochemistry, University of California, Los Angeles, Los Angeles, CA

We employed RPA combined with lPB equation and surface charging to incorporate the solvent effect and electrode potential. Our findings revealed that water adsorbed on the surface acts as the proton source for the protonation of *CO to *COH across a wide range of potentials through the Grotthuss mechanism.

Metal-Independent Correlations for Site-Specific Binding Energies of Relevant Catalytic Intermediates.

Shyama Charan Mandal *and Frank Abild-Pedersen*
SUNCAT Center for Interface Science and Catalysis, SLAC National Accelerator Laboratory, Menlo Park, CA

Using a recently introduced coordination-based model, we can predict site-specific metal binding energies (ΔE_M) that can be used as a descriptor for chemical reactions. We have found linear correlations between predicted ΔE_M and ΔE_{CH} and ΔE_O. Interestingly, all the metals correlate with one another under specific surface site coordination.

Predicting Competitive Anion Electrosorption on Transition Metals.

Bolton Tran[1] *and Bryan Goldsmith*[2]
(1)Department of Chemical Engineering, University of Michigan, Ann Arbor, MI, (2)Chemical Engineering, University of Michigan, Ann Arbor, MI

Electrocatalytic systems with transition metal catalysts often involve multiple anions in the electrolytes, which can competitively adsorb and alter catalytic onsets and turnovers. To provide physical insights and rapid predictions for competitive anion adsorption, we develop a theoretical framework involving grand-canonical density functional theory, machine learning, and potential-dependent Langmuir isotherms.

POLYMER - CATALYSIS FOR POLYMER SYNTHESIS, UPCYCLING, AND RECYCLING

POLYMER - CRACKING AND HYDROCRACKING

Thursday, June 12, 2025 1:00 PM - 3:20 PM
Regency Ballroom VI

Chair: Steven Crossley, University of Oklahoma

Co-Chair: Konstantinos Goulas, Oregon State University

C-H Bond Activation By Sulfated Zirconium Oxide Is Mediated By a Sulfur-Centered Lewis Superacid.

Matt Conley
University of California, Riverside, Riverside, CA

Sulfated zirconium oxide (**SZO**) reacts with polymers and activated substrates to form carbocations by reversible C-H bond activation mediated by pyrosulfate sites.

Lewis Acid-Base Pairs on Y-ZrO_2 As Active Sites for (de-)Hydrogenation Catalysis and Bifunctional Cascades for Upgrading Alkanes.

Mikalai Artsiusheuski[1]*, Nicholas Jaegers*[1]*, Carlos Lizandara-Pueyo*[2]*, and Enrique Iglesia*[3,4]

(1)University of California at Berkeley, Berkeley, CA, (2)BASF, Ludwigshafen am Rhein, Germany, (3)Department of Chemical and Biomolecular Engineering, University of California, Berkeley, Berkeley, CA, (4)Purdue University, West Lafayette, IN

Lewis acid-base pairs (LAB) on surfaces of earth-abundant Y2O3 and ZrO2 heterolitically activate strong C–H bonds in diverse hydrocarbons and catalyze their dehydrogenation and reverse hydrogenation at predictable rates. These (de)hydrogenation functions are useful in bifunctional hydrocracking cascades for alkanes valorization and, potentially, polyolefin waste upcycling

Polyolefin Hydrocracking over Intrinsically Bifunctional and PVC-Compatible Tungsten-Carbide (W_xC) Catalysts.

*Uchenna Nwachukwu[1], Matthew Moegling[1], Sinhara Mudalige Hasitha Perera[2], Marc Porosoff[2], and **Linxiao Chen**[1]*
(1)Department of Chemical, Biomolecular, and Corrosion Engineering, The University of Akron, Akron, OH, (2)Department of Chemical Engineering, University of Rochester, Rochester, NY

This work presents the hydrocracking of polyolefins over tungsten-carbide catalysts. These earth-abundant catalysts have metallic and Brønsted-acid sites required for bifunctional hydrocracking in proximity, and are compatible with poly-vinyl chloride impurities. Surface active site structure can be tuned through synthesis and treatment conditions.

Tuning the Hydrocracking Product Spectrum of Polyethylene.

***Lunhan Chen**[1], Victor Levacher[1], Philipp Wegener[1], Raoul Naumann d'Alnoncourt[1], Michael Geske[1], Michael Bender[2], Majd Dr. habil. Al-Naji[1], and Frank Rosowski[1,2]*
(1)BasCat - UniCat BASF JointLab - TU Berlin, Berlin, Germany, (2)BASF SE, Catalysis Research, Ludwigshafen, Germany

This study investigates the catalytic hydrocracking of polyethylene using platinum-loaded silica-alumina catalysts. It explores the effects of Pt particle size and acid site distribution on hydrocracking efficiency, revealing that a smaller Pt particle size distribution improves cracking rates, enhancing recycling performance and selectivity.

Carbenium Ion Initiator-Induced Isopentane Disproportionation and Its Effects on Tandem Cracking-Alkylation Polyolefins Upcycling.

***Jiande Mai**, David Ryan, Wei Zhang, Kiyoung Jo, Janos Szanyi, Huamin Wang, Sungmin Kim, and Johannes Lercher*
Pacific Northwest National Laboratory, Richland, WA

We study the disproportionation reaction of isopentane, the alkylation agent, in the polyolefin tandem cracking-alkylation process. Carbenium ion initiators induce this side reaction. Our work provides an in-depth understanding of its reaction mechanism and kinetics, offering valuable insights to improve the efficiency and selectivity of the overall LDPE upcycling process.

Catalytic Impact of Site Distributions and Pore Architecture on Zeolite Polyethylene Conversion Rates and Selectivities.

Cole Hullfish, Jun Zhi Tan, and ***Michele Sarazen***
Department of Chemical and Biological Engineering, Princeton University, Princeton, NJ

Rates, selectivities, and stabilities of polyethylene (hydro)cracking under mild conditions is contextualized on metal-free and metal-loaded (hierarchical) zeolites (MFI, BEA, FAU) to understand impacts of site accessibility and communication between functionalities.

Roles of Chain Length and Branching in Polyolefin Deconstruction.

Samantha Ausman[1] *and Susannah Scott*[2]
(1)Chemical Engineering, University of California - Santa Barbara, Santa Barbara, CA, (2)Department of Chemical Engineering, University of California, Santa Barbara, Santa Barbara, CA

Acid-catalyzed deconstruction of model compounds shows faster C-C scission for tertiary carbons than linear ones, while HDPE undergoes more scission than branched LLDPE. These findings highlight the need for careful extrapolation from small molecules and emphasize the importance of considering property differences in catalyst design for polymer upcycling.

C1 - CATALYSIS OF C1 CHEMISTRY

C1 - METHANE CONVERSION

Thursday, June 12, 2025 3:40 PM - 5:40 PM
Regency Ballroom VII

Chair: Steven Farrell, Brookhaven National Laboratory

Co-Chair: Han Chau, Idaho National Laboratory

Investigating the Evolution and Consequences of Heterogeneous Cu Sites on Stoichiometric Partial Methane Oxidation in Cu-CHA Zeolites.

Lauren Kilburn[1]*, Jose Rebolledo-Oyarce*[2]*, Angel Santiago-Colón*[3]*, William Schneider*[4]*, and Rajamani Gounder*[5]
(1)Purdue University, West Lafayette, IN, (2)Chemical Engineering, University of Notre Dame, Notre Dame, IN, (3)Chemical Engineering, Purdue University, West Lafayette, IN, (4)Chemical and Biomolecular Engineering, University of Notre Dame, Notre Dame, IN, (5)Charles D. Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN

CO reduction and H_2 TPR were combined to quantify binuclear Cu sites formed on Cu-CHA as a function of Cu density and various O_2 activation and reduction treatments. Stoichiometric PMO yields and site characterization data were used to elucidate the contribution of individual Cu species to partial and over-oxidation pathways.

Support Effects in the Platinum-Catalyzed Selective, Aerobic Oxidation of Methane to Formaldehyde.

Same Malatji, ***Sinqobile Vuyisile Lusanda Mahlaba****, and Eric van Steen*
Catalysis Institute, Dpt. Chemical Engineering, University of Cape Town, Rondebosch, Western Cape, South Africa

The selective, aerobic oxidation of methane to formaldehyde over supported platinum-based catalyst is a promising route requiring a hydrophobic support with minimum acid sites, such as BN or carbon.

C-H Bond Activation on Transition Metal Carbides: An Mlff Approach with Reactive Active Learning.

Siddarth Achar[1,2], ***Chinmay Mhatre****[3], Priyanka Bholanath Shukla[3], Caitlyn Vinger[4], Leonardo Bernasconi[5], and Karl Johnson[3]*
(1)Computational Modeling and Simulation, University of Pittsburgh, Pittsburgh, PA, (2)Pritzker School of Molecular Engineering, University of Chicago, Chicago, IL, (3)Department of Chemical and Petroleum Engineering, University of Pittsburgh, Pittsburgh, PA, (4)University of Pittsburgh, Pittsburgh, PA, (5)Center for Research Computing Department of Chemistry, University of Pittsburgh, Pittsburgh, PA

Methane's role in energy production involves challenges in C-H bond activation, traditionally requiring precious metals. Transition Metal Carbides like Titanium Carbide show promise for this activation with lower energy barriers. Using machine learning potentials, we explore Ti/C ratios in Titanium Carbide and their impact on catalytic activity and reaction pathways.

Combined Dry Reforming and Partial Oxidation of Methane over Fe-Modified Ni/γ-Al_2O_3 Catalysts: Insights into the Impact of Iron and the Support Role.

Abbas Khaleel
Chemistry, UAE University, Al Ain, United Arab Emirates; Science, UAE University, Al Ain, United Arab Emirates

Combined catalytic dry reforming and partial oxidation of methane was studied over Fe-modified Ni/alumina catalysts for the production of syngas. Iron ions dispersed in the support of Ni/γ-Al_2O_3 was found to significantly enhance the catalysts' resistance to coking while a negative impact was observed for Fe deposited on the surface

Non-Oxidative Methane Coupling: Towards Electrified C_1 Conversion.

Samay Garg*[1], Joshua O. Crawford[1], Jingguang G. Chen[1,2], and Juliana S.A. Carneiro[1]*
(1)Chemical Engineering, Columbia University, New York, NY, (2)Chemistry Division, Brookhaven National Laboratory, Upton, NY

Ceria-supported single-atom Pt is studied as a model catalyst to uncover structure-property relationships for thermochemical non-oxidative coupling of methane (NOCM), and its catalytic performance is compared to that of Pt-doped barium cerate as a bridge toward developing a novel electrochemical NOCM process which can sustainably convert CH_4 into multicarbon products.

In-Situ and *Operando* Structure-Performance Relationship of Controlled $La_xCe_{x-1}O_{2-x/2}$ Catalysts during Oxidative Coupling of Methane.

Fabiane Trindade[1]*, Andre Ferlauto*[2]*, and Cristiane Barbieri Rodella*[3]
(1)Paineira beamline, Brazilian Synchrotron Light Laboratory, Campinas, Sao Paulo, Brazil, (2)Center for Engineering, Modeling and Applied Social Sciences, Federal University of ABC, Santo Andre, Brazil, (3)Brazilian Synchrotron Light Laboratory, Campinas, Sao Paulo, Brazil

In-situ and operando structure-performance relationship of controlled $La_xCe_{x-1}O_{2-x/2}$ catalysts to establish a fundamental understanding of the relationship between structural changes and C2 selectivity improvements in oxidative coupling of methane.

CO2 - CO2 CAPTURE AND UPGRADING

CO2 - CO_2 CONVERSION TO METHANOL 2

Thursday, June 12, 2025 3:40 PM - 5:40 PM
Centennial Ballroom IV

Chair: Alvaro Amieiro Fonseca, Johnson Matthey

Co-Chair: Elizabeth Bickel Rogers, University of Minnesota

Pressure-Induced Changes in the Characterization of Copper-Based Catalysts for CO_2 Hydrogenation to Methanol.

Sai Teja Nekkanti*, Francielle Candian Firmino Marcos, Franchesca Hauck, and Ana Alba-Rubio*
Department of Chemical and Biomolecular Engineering, Clemson University, Clemson, SC

In this study, we highlighted the limitations of atmospheric pressure characterization and emphasized the need for techniques capable of analyzing the catalysts under reaction pressures. Notably, our results demonstrated a substantial difference in the interpretation of copper surface area and catalyst basicity when the catalysts are characterized at varying pressures.

Understanding the Catalytic Phenomena of CO_2 Hydrogenation to Methanol Based on Catalytic Sites Contiguity: Structural Speciation of ZnO Sites Using XAS Spectral Simulation.

Jingye Chen[1]*, Dongdong Chen*[2]*, Ning Chen*[3]*, Liang Zhao*[2]*, Weifeng Chen*[3]*, Mohsen Shakouri*[1,3]*, and Hui Wang*[1]
(1)Department of Chemical and Biological Engineering, University of Saskatchewan, Saskatoon,

SK, Canada, (2)China University of Petroleum (Beijing), Beijing, Beijing, China, (3)Canadian Light Source, Saskatoon, SK, Canada

This study explores the **Catalytic Sites Contiguity (CSC)** concept in Cu-ZnO catalysts for CO_2 hydrogenation to methanol. Atomic layer deposition (ALD) was used to prepare model catalysts. *In situ* X-ray absorption spectroscopy (XAS) and spectra simulations identified that highly dispersed ZnO species enhanced methanol synthesis.

Effect of Catalyst Structure on the Competitive Reaction Pathways in CO_2 Hydrogenation to Methanol on Copper.

Kaustav Niyogi *and Matteo Maestri*
Laboratory of Catalysis and Catalytic Processes - Dipartimento di Energia, Politecnico di Milano, Milano, Italy

This work uses atomistic calculations and structure-dependent microkinetic modeling to decipher the effect of the catalyst structure on the competitive reaction pathways in copper-based CO_2 hydrogenation. Our analysis resolves the contradictory experimental reports regarding the effect of water in accelerating the reactions and whether the different products share common intermediates.

Boosting ZnO_x-Cu Interfacial Interactions for Methanol Productivity.

Franchesca Hauck[1]*, Francielle Candian Firmino Marcos*[1]*, Sai Teja Nekkanti*[1]*, Jose Rodriguez*[2]*, and Ana Alba-Rubio*[1]
(1)Department of Chemical and Biomolecular Engineering, Clemson University, Clemson, SC, (2)Chemistry, Brookhaven National Laboratory, Upton, NY

This work investigates the impact of controlling the interaction between copper and zinc oxide to promote methanol production from CO_2 hydrogenation, as the proximity of these components helps facilitate favorable reaction pathways. The characterizations under reaction conditions provided a deeper understanding of the catalysts and the promoted pathways to methanol.

Tracking the Evolution of ZnO Dispersion in $ZnZrO_x$ CO_2 Hydrogenation Catalysts and Its Consequence for MeOH Formation.

Alexander Oing[1]*, Paula Abdala*[1]*, Felix Donat*[2]*, and Christoph R. Müller*[1]
(1)Department of Mechanical and Process Engineering, ETH Zurich, Zurich, Switzerland, (2)Laboratory of Energy Science and Engineering, ETH Zürich, Zürich, Switzerland

To attain a detailed structural understanding of the active site of $ZnZrO_x$ CO_2 hydrogenation catalysts, we developed a model system in which the Zn dispersion continuously increases under reaction conditions allowing us to hypothesize sub-nanometer ZnO clusters within ZrO_2 as the most active motif driving methanol formation.

Elucidating the Effect of Proton Source, Capture Agent, and Catalyst on the Electroreduction of Captured CO_2 into CO.

Robert M. Kowalski[1]*, Avishek Banerjee*[1]*, Huiyun Jeong*[2]*, Christopher Hahn*[2]*, Carlos Morales-Guio*[3]*, and Philippe Sautet*[1]
(1)Chemical and Biomolecular Engineering, University of California, Los Angeles, Los Angeles, CA, (2)Lawrence Livermore National Laboratory, Livermore, CA, (3)Department of Chemical and Biomolecular Engineering, University of California, Los Angeles, Los Angeles, CA

We present a Sabatier plot for the electroreduction of captured CO_2 into CO. We find that the proton source defines the theoretical maximum, the catalyst has the largest effect on the descriptor, and the capture agent can tune the activity. We hope this will accelerate material discovery for this reaction.

ELECTRO PHOTO - ELECTROCATALYSIS AND PHOTOCATALYSIS

ELECTRO PHOTO - ELECTROCATALYSIS FOR CO2 CONVERSION 2

Thursday, June 12, 2025 3:40 PM - 5:40 PM
Centennial Ballroom I

Chair: Max Huelsey, Technical University of Munich

Co-Chair: Ezra Clark, Penn State

New Opportunities Beyond Copper Catalysts for Electrochemical CO_2 Reduction.

Samira Siahrostami
Department of Chemistry, Simon Fraser University, Burnaby, BC, Canada

Copper-based catalysts are efficient for CO_2 reduction but prone to degradation, prompting the search for non-copper alternatives. Using high-throughput DFT calculations, we screen unconventional materials like transition metal nitrides, metal-organic frameworks, and perovskites to identify more stable and efficient CO2RR catalysts.

Experimental Trends and Theoretical Descriptors for Electrochemical Reduction of Carbon Dioxide to Formate over Sn-Based Bimetallic Catalysts.

Qiaowan Chang
Gene & Linda Voiland School of Chemical Engineering and Bioengineering, Washington State University, Pullman, WA

This study explores CO_2 to formate electrocatalytic conversion by analyzing real-time catalyst structural evolution and the role of key reaction intermediates in influencing the formate selectivity. *In-situ* XANES revealed Sn valence dynamics influenced by secondary metals. A multidimensional descriptor was developed to evaluate formate selectivity through a 2D volcano plot.

Interplay between Catalysts Restructuring and Activity for Electrocatalytic Reduction on Copper.

Dongfang Cheng[1], Ziyang Wei[2], Zisheng Zhang[3], Peter Broekmann[4], Anastassia Alexandrova[3], and ***Philippe Sautet***[1]
(1)Chemical and Biomolecular Engineering, University of California, Los Angeles, Los Angeles, CA, (2)Department of Chemistry and Biochemistry, University of California, Los Angeles, Los Angeles, CA, (3)Department of Chemistry and Biochemistry, University of California - Los Angeles, Los Angeles, CA, (4)University of Bern, Bern, Switzerland

We show that major restructuring events occur on copper in electroreduction conditions, by formation of adatoms or stabilization of steps. This leads to the creation of new active sites, not present on the initial catalyst, resulting in a strong enhancement of the catalytic activity.

New Insights into the Role of Organic Cation Promoters for Non-Aqueous CO_2 Reduction.

Jon-Marc McGregor*, Louise Canada, Joan F. Brennecke, and Joaquin Resasco*
McKetta Department of Chemical Engineering, The University of Texas at Austin, Austin, TX

Our work examines how organic phosphonium-based cations influence CO_2 electrochemical reduction in non-aqueous media. Kinetic and in-situ spectroscopy reveals that interfacial electric fields over Ag catalysts depend on cation size and packing density. These insights will deepen our understanding of catalysis in electrochemical environments.

Control of Heteroatom Configurations in Carbon Materials for Electrocatalytic Applications.

Dohyung Kim
Chemical and Biomolecular Engineering, University of Pennsylvania, Philadelphia, PA

We investigated the temperature- and time-dependent evolution and stability of nitrogen configurations in N-doped carbon materials, observing that a mixture of configurations is thermodynamically favored. By kinetically trapping specific N-functionalities, we successfully synthesized N-doped carbon materials with distinct N-configurations and evaluated their fundamental activity in CO2 electroconversion.

Insights to so_2 Poisoning Impacts on CO_2rr over Single-Atom Transition Metal Molecular Catalysts.

Yiqing Wu[1], ***Chang Liu***[1]*, Yuanyuan Li[2], and Zili Wu[2]*
(1)Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN, (2)Chemical Sciences Division, Oak Ridge National Laboratory (ORNL), Oak Ridge, TN

We investigated the immobilization of transition metal phthalocyanine (TM-Pc) molecular catalysts on graphene support in electrochemical CO_2RR. Our results demonstrate that the SO_2

adverse impacts are closely related to the electronic properties of the center TM active sites, providing a pathway to design of robust and effective electrocatalysts for CO_2RR.

ENERGY INPUTS - NOVEL ENERGY INPUTS FOR CATALYSIS

ENERGY INPUTS - HYDROCARBON CATALYSIS DRIVEN BY MICROWAVES AND PLASMA

Thursday, June 12, 2025 3:40 PM - 5:40 PM
Hanover Hall CDE

Chair: Manish Shetty, Texas A&M University

Co-Chair: Sijie Guo, University of Tennessee, Knoxville

Toward Mechanistic Understanding of Plasma-Assisted C1 Conversions Via *Operando* Infrared Spectroscopy.

***James Trettin**, Bruce Koel, and Michele Sarazen*
Department of Chemical and Biological Engineering, Princeton University, Princeton, NJ

Mechanistic understanding of plasma-assisted catalysis will advance effective implementation of this electrified fuel and chemical production technology. This work employs a plasma jet interfaced with *operando* DRIFTS-MS to study plasma-assisted CO oxidation and methanol decomposition on supported Pt catalysts as probes to better understand plasma-assisted C1 conversions.

Microwave-Assisted Activation of Mo/HZSM5 in Methane Dehydroaromatization.

***Swarom Kanitkar**[1,2], Xinwei Bai[1], Duy Hien Mai[1,2], Evgeniy M. Myshakin[3,4], and Daniel Haynes[2]*
(1)NETL Support Contractor, Morgantown, WV, (2)National Energy Technology Laboratory, Morgantown, WV, (3)National Energy Technology Laboratory, Pittsburgh, PA, (4)NETL Support Contractor, Pittsburgh, PA

This study provides insight into how microwave cavity configuration and the pre-treatment gas environment play a strong role in catalyst stability and benzene yield in methane DHA.

Microwave-Driven Methane Pyrolysis for Clean Hydrogen and Carbon Nanostructure Production.

***Sijie Guo**[1] and Siris Laursen[2]*
(1)Chemical and Biomolecular Engineering, University of Tennessee, Knoxville, Knoxville, TN, (2)Chemical and Biomolecular Engineering, University of Tennessee, Knoxville, TN

This study utilizes microwave radiation to generate hot phonons in catalytic materials, driving methane pyrolysis for clean hydrogen and carbon nanostructures. Hot phonon-driven catalysis advances thermal catalysis, providing a path to electrify the chemical industry, improve energy efficiency, and reduce CO_2 emissions.

Specific Heating and Thermometry in Tandem Catalysis for the Selective Conversion of Ethylene into Propylene.

Marcos G. Farpón[1,2,3], *Raquel Peláez Fernández*[1], *Verónica Recio*[1], *Burak Atakan*[4], *Carlos Zaldo*[5], *and Gonzalo Prieto*[1,3]
(1)Instituto de Tecnología Química (ITQ UPV-CSIC) 46022, Valencia, Spain, (2)Department of Chemical Engineering, Massachusetts Institute of Technology (MIT) 02139, Cambridge, MA, (3)Max-Planck-Institut für Kohlenforschung, 45470, Mülheim a.d. Ruhr, Germany, (4)Thermodynamik ,EMPI, University of Duisburg-Essen, 47057, Duisburg, Germany, (5)Instituto de Ciencia de Materiales de Madrid, CSIC, 28049, Madrid, Spain

The design of multifunctional materials integrating catalytic, auxiliary magnetic susception and thermal sensing functionalities enables catalyst-specific heating and thermometry for spatially proximate solid catalysts in a single reactor. The new concept alleviates temperature limitations in tandem catalysis, as demonstrated in the direct conversion of ethylene into propylene via dimerization-metathesis.

KEYNOTE: Using Electrochemistry to Understand and Control Thermochemical Catalysis.

Yogesh Surendranath[1], *Deiaa Harraz*[1], *Kunal Lodaya*[1], *Karl Westendorff*[2], *and Yuriy Roman*[2]
(1)Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA, (2)Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, MA

The role of charge transfer reactions and interfacial polarization is poorly understood in the context of thermochemical catalysis. We have developed general methods for tracking and controlling the degree of interfacial polarization during catalytic turnover and have used this approach to understand and tune thermochemical oxidation, hydrogenation, and acid catalysis.

FUNDAMENTALS - FUNDAMENTALS OF CATALYSIS AND SURFACE SCIENCE

FUNDAMENTALS - HYDROCARBON AND OXYGENATE CONVERSIONS

Thursday, June 12, 2025 3:40 PM - 5:40 PM
Centennial Ballroom II

Chair: Manuela Serban, Honeywell UOP

Co-Chair: William Broomhead, Georgia Institute of Technology

Selective Chemical Looping Combustion of Acetylene in Ethylene-Rich Streams.

Matthew Jacob[1], *Huy Nguyen*[1], *Rishi Raj*[1], *Javier Garcia-Barriocanal*[1], *Jiyun Hong*[2], *Jorge Perez-Aguilar*[2], *Adam Hoffman*[2], *K. Andre Mkhoyan*[1], *Simon Bare*[2], *Matthew Neurock*[1], *and Aditya Bhan*[1]
(1)Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN, (2)Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, Menlo Park, CA

We report the selective chemical looping combustion of acetylene in ethylene-rich gas mixtures which occurs with >99% selectivity by lattice oxygen of bismuth oxide as an alternative to acetylene semi-hydrogenation to reduce acetylene concentrations below 2 ppm in ethylene streams.

Ni Promotes Selective Ethylene Epoxidation on Ag.

Anika Jalil[1], *Elizabeth E. Happel*[2], *Laura Cramer*[2], *Adrian Hunt*[3], *Adam Hoffman*[4,5], *Iradwikanari Waluyo*[3], *Matthew Montemore*[6], *E Charles Sykes*[2,7], *and Phillip Christopher*[1]
(1)Department of Chemical Engineering, University of California, Santa Barbara, Santa Barbara, CA, (2)Department of Chemistry, Tufts Univ, Medford, MA, (3)Brookhaven National Laboratory, Upton, NY, (4)SUNCAT Center for Interfacial Science and Catalysis, SLAC National Accelerator Laboratory, Menlo Park, CA, (5)Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, Menlo Park, CA, (6)Chemical and Biomolecular Engineering, Tulane University, New Orleans, LA, (7)Department of Chemical and Biological Engineering, Tufts University, Medford, MA

Ultra-dilute NiAg alloys were identified as promising selective oxidation catalysts from theory and surface science studies. Addition of ppm amounts of Ni enhances the selectivity of supported Ag ethylene epoxidation catalysts by ~25%, comparable to the effect of Cl co-flow.

Uncovering the Role of Pd-Acetate Trimers and Dimers in Heterogeneous Vinyl Acetate Synthesis.

Hunter Jacobs[1,2], *Welman C. Elias*[2], *Kimberly N. Heck*[2], *Shan Jiang*[3], *Justin J. Dodson*[4], *Byeong Jun Cha*[2], *Jacob H. Arredondo*[2], *Laiyuan Chen*[4], *Sean G. Mueller*[4], *Steven R. Alexander*[4], *Jeffrey T. Miller*[3], *and Michael Wong*[2]
(1)Manufacturing Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN, (2)Department of Chemical and Biomolecular Engineering, Rice University, Houston, TX, (3)Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN, (4)Celanese Corporation, Pasadena, TX

Molecular Pd-acetate trimers and dimers are known to form during vinyl acetate monomer (VAM) synthesis. Although they are suspected to participate in the reaction, their mechanistic role in heterogeneous VAM chemistry remains unclear. This work utilizes *in situ/operando* techniques to uncover the dynamics of these species on the catalyst surface.

Chemisorbed:Lattice Oxygen Ratios As a Lens for Interpreting Dynamic Enhancement during the Catalytic Oxidation of Ethane.

Austin Morales, Michael Harold, and ***Praveen Bollini***
William A. Brookshire Department of Chemical and Biomolecular Engineering, University of Houston, Houston, TX

We rationalize dynamic selectivity enhancement during the oxidative dehydrogenation of ethane through the quantitative analysis of transient chemisorbed to lattice oxygen ratios. We present a

framework for predicting dynamic enhancement under both kinetic and diffusion-controlled regimes that can be applied broadly to a variety of catalytic partial oxidation reactions.

Electrocatalytic Oxidation of Ammonia to Nitrate Occurs on NiOOH with OH/O Vacancies.

Vi Thi Thuy Phan[1]*, Quy Nguyen*[2]*, Bin Wang*[2]*, and Ian Burgess*[1]
(1)Department of Chemistry, University of Saskatchewan, Saskatoon, SK, Canada, (2)School of Sustainable Chemical, Biological and Materials Engineering, University of Oklahoma, Norman, OK

This study combines surface enhanced infrared absorption spectroscopy (SEIRAS) and density functional theory (DFT) calculations to determine potential-dependent intermediates, active catalytic sites, and ammonia electrooxidation reaction (AOR) pathways on Ni-based catalysts to gain mechanistic insight into AOR, thus paving the way for future research on catalyst design and AOR optimization.

Anomalous Diffusion of Metal Atoms on Oxide Surfaces: A Machine Learning Molecular Dynamics Study of Pt_1/TiO_2.

Shaama Mallikarjun Sharada and ***Usama Saleem***
Mork Family Department of Chemical Engineering and Materials Science, University of Southern California, Los Angeles, CA

Employing machine learned interatomic potentials to simulate the dynamical evolution of the metal-support interface in atomically dispersed Pt on TiO_2, we show that the metal exhibits anomalous or sub-diffusive behavior, with a propensity to stabilize via coordination with one or more bridging oxygen atoms.

HYDRO ECON - CATALYSIS FOR THE HYDROGEN ECONOMY

HYDRO ECON - THERMOCATALYSIS

Thursday, June 12, 2025 3:40 PM - 5:40 PM
Hanover Hall FG

Chair: Zahra Almisbaa, Saudi Aramco

Co-Chair: Aayush Singh, SandboxAQ

Hydrogen Production in Ammonia Decomposition over Direct Reduced Iron Catalyst Obtained from Ironmaking Process.

Jaemin Park[1] *and Do Heui Kim*[2]
(1)Department of Chemical and Biological Engineering, Seoul National University, Seoul, Korea, Republic of (South), (2)Seoul National University, Seoul, Korea, Republic of (South)

This study explores the use of direct reduced iron (DRI) as a low-cost catalyst for ammonia decomposition to produce hydrogen. It investigates the impact of reaction conditions on DRI's

nitridation and hydrogen production, highlighting the potential for carbon-neutral steel production by using DRI for both hydrogen generation and steel manufacturing.

Development of Advanced Catalysts for the Generation of Clean H_2 from Liquid Organic Hydrogen Carriers: Dehydrogenation of Methylcyclohexane.

Yanjiao Yi[1]*, Donna Chen*[2]*, Jochen Lauterbach*[3]*, Christopher Williams*[1]*, and John Regalbuto*[1]
(1)Chemical Engineering, University of South Carolina, Columbia, SC, (2)Chemistry, University of South Carolina, Coulmbia, SC, (3)Department of Chemical Engineering, University of South Carolina, Columbia, SC

The study explores advanced catalysts for the dehydrogenation of methylcyclohexane to toluene. Pt/γ-Al_2O_3 catalysts synthesized using SEA exhibit enhanced catalytic activity compared to those prepared by DI. The combined SEA and Sn wetting method offers a simple and effective approach for synthesizing $PtSn_x$ alloy nanoparticles with a core-shell structure.

Methanol Steam Reforming: Basicity Effect of Alkali-Pt/m-ZrO_2 Catalysts.

Denzel Megafu[1]*, Braedon McFee*[1]*, Michela Martinelli*[2]*, and* ***Gary Jacobs***[3]
(1)Department of Biomedical Engineering and Chemical Engineering, University of Texas at San Antonio, San Antonio, TX, (2)Center for Applied Energy Research (CAER), University of Kentucky, Lexington, KY, (3)Dept. of Biomedical Engineering and Chemical Engineering, The University of Texas at San Antonio, San Antonio, TX

Type and loading of alkali added to Pt/m-ZrO_2 greatly alters H_2 selectivity of the MSR reaction by modifying surface basicity. The catalyst was tuned with Li, K moving from 68.2% undesired CO selectivity (H_2-unselective pathway) for unpromoted catalyst to >80% CO_2 selectivity (H_2-selective pathway) with adding 0.54% Li or 3.1%K.

Selective Hydrogen Combustion over Silica-Supported Sodium Tungstate Catalysts.

Elijah Kipp *and Aditya Bhan*
Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN

Supported sodium tungstate catalysts preferentially combust hydrogen in mixtures with hydrocarbons at 923 K. Kinetic and isotopic studies to probe the kinetically relevant step, reoxidation pathway, and oxidant identity suggest kinetically relevant H-H dissociation over an O* species which is rapidly replenished by O_2.

Interpretable Machine Learning Guided Plasma Catalysis for Hydrogen Economy.

Saleh Ahmat Ibrahim[1]*, Shengyan Meng*[2]*, Charles Milhans*[1]*, Magda Barecka*[3]*, Yilang Liu*[4]*, Qiang Li*[1]*, Jiaqi Yang*[1]*, Yabing Sha*[1]*, Yanhui Yi*[2]*, and* ***Fanglin Che***[1]
(1)Chemical Engineering, University of Massachusetts Lowell, Lowell, MA, (2)2School of Chemical Engineering, Dalian University of Technology, Dalian, China, (3)Department of

Chemical Engineering, Northeastern University, Boston, MA, (4)Delaware Energy Institute, University of Delaware, Newark, DE

Plasma-assisted NH_3 decomposition enables cost-effective, low-carbon H_2 generation using earth-abundant catalysts, supporting industrial decarbonization. Machine learning accelerates the identification of high-performance, non-critical bimetallic catalysts, validated experimentally for practical applications. Plasma catalysis achieves H_2 production cost under $1/kg with a low carbon footprint, offering a scalable, eco-friendly energy solution.

Coked Ni/CeO_2 Catalyst Regeneration: An *Operando* Etem Insight.

Yuanyuan Zhu
MSE, University of Connecticut, Storrs, CT

Catalyst deactivation by coking and unsatisfactory regeneration pose major challenges for sustainable hydrogen economy. To bridge the crucial gap in understanding of regeneration processes that ultimately determine catalyst longevity and operational costs, this study establish microstructure-informed kinetics for filamentous carbon gasification under technical relevant air-like conditions.

NITRO CHEM - NITROGEN CHEMISTRY

NITRO CHEM - ELECTROCHEMISTRY FROM WASTES TO AMMONIA

Thursday, June 12, 2025 3:40 PM - 5:40 PM
Centennial Ballroom III

Chair: Huiyuan Zhu, University of Virginia

Co-Chair: Andrew Medford, Georgia Institute of Technology

KEYNOTE: High-Temperature Electrocatalytic Nitrogen Activation Using Mixed Anion (Oxide/Nitride)-Type Cathodes.

Umit Ozkan
William G. Lowrie Department of Chemical & Biomolecular Engineering, The Ohio State University, Columbus, OH

This project targets acquiring a fundamental understanding of the high-temperature electrocatalytic nitrogen reduction reaction using a highly versatile class of materials, double perovskite oxynitrides as cathode catalysts and manipulation of their anionic and cationic ordering through synthesis parameters.

Theoretical Study of Electrocatalytic Nitrate Reduction on Dilute Atom Alloys.

Arnold Sison[1] *and Kasun Gunasooriya*[2]
(1)School of Sustainable, Chemical, Biological, and Materials Engineering, University of Oklahoma, Norman, OK, (2)Chemical, Biological & Materials Engineering, University of Oklahoma, Norman, OK

We analyzed the electrocatalytic nitrate reduction with density functional theory and microkinetic modeling to understand the reaction mechanism over dilute atom alloys. We observed that ruthenium single atom alloys have an electronic structure similar to a free-atom and nitrate reduction is more favorable on single atom alloys than pure metals.

Determining Aqueous and Gaseous Product Composition for Electrocatalytic Nitrate Reduction to Ammonia.

Wrayzene Willoughby[1], *Michaela Burke Stevens*[2], *Adam Nielander*[3], *and Thomas Jaramillo*[4]
(1)Department of Chemical Engineering, Stanford University, Stanford, CA, (2)McKetta Department of Chemical Engineering, UT, Austin, TX, (3)SUNCAT Center for Interface Science and Catalysis, SLAC National Accelerator Laboratory, Menlo Park, CA, (4)Chemical Engineering, Stanford University, Stanford, CA

Reactive nitrogen is vital for agriculture but poses challenges, including the energy-intensive Haber-Bosch process and environmental pollution from overfertilization. This research aims to develop electrocatalysts for nitrate-to-ammonia conversion, enabling simultaneous fertilizer production and water purification. Using advanced analytical methods, the team investigates reaction mechanisms to optimize efficiency and sustainability.

Electrochemical Nitrate-to-Ammonia Conversion Using Titanium-Nitrogen Doped Carbon Flowers.

Carlos Fernadnez[1], *Matthew Liu*[2,3], *Diego Uruchurtu Patino*[1,3], *Huaxin Gong*[1,3], *Jesse Matthews*[1,3], *Kindle S. Williams*[1], *Alfred Vargas*[1,3], *Michael J. Zachman*[4], *Adam Hoffman*[5], *Md Delowar Hossain*[1,3], *Michal Bajdich*[3], *Simon Bare*[3,5], *Michaela Burke Stevens*[3], *Thomas Jaramillo*[1,3], *Zhenan Bao*[1,3], *and William A. Tarpeh*[3,6]
(1)Chemical Engineering, Stanford University, Stanford, CA, (2)Chemical Engineering, MIT, Cambridge, MA, (3)SUNCAT Center for Interface Science and Catalysis, SLAC National Accelerator Laboratory, Menlo Park, CA, (4)Oak Ridge National Laboratory, Oak Ridge, TN, (5)Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, Menlo Park, CA, (6)Department of Chemical Engineering, Stanford University, Stanford, CA

We evaluate titanium-nitrogen-doped carbon nanoflowers as catalysts for electrochemical nitrate reduction to ammonia in complex environments. By optimizing catalyst morphology and reaction parameters, we achieved selective ammonia production, demonstrating the potential of this approach for sustainable wastewater treatment and nitrogen recovery.

Electrocatalytic Conversion of NOx Waste to Useful Chemicals Using Metal Single Atom Catalysts (M-SACs).

Xianqin Wang
Chemical and Materials Engineering, New Jersey Institute of Technology, Newark, NJ

M-BN catalysts are promising for electrochemical nitrate reduction reaction (NO_3RR) to ammonia Superior NH_3 productivity of 3,184.9 $\mu g/mg_{cat}/h$ and selectivity of 95% with

outstanding stability are obtained on CuBN. XAS results confirm active Cu single atoms with strong interaction between Cu and BN play an important role for NO_3RR performance.

POLYMER - CATALYSIS FOR POLYMER SYNTHESIS, UPCYCLING, AND RECYCLING

POLYMER - PVC AND PS CONVERSION

Thursday, June 12, 2025 3:40 PM - 5:40 PM
Regency Ballroom VI

Chair: Tracy Lohr, Northwestern University

Co-Chair: Houqian Li, New Mexico State University

Hydrodechlorination of PVC to Value-Added Waxes Via Tandem Dechlorination and Hydrogenation.

*Scott Svadlenak[1], Artur Spiridonov[2], and **Konstantinos Goulas**[2]*
(1)Renewcat Inc., Corvallis, OR, (2)Oregon State University, Corvallis, OR

The dechlorination of waste PVC can be achieved using an organic base followed by heterogeneous hydrogenation. Catalyst activity requires the presence of a chlorine sink, to avoid catalyst poisoning. Conversely, catalyst longevity requires the presence of a heterogeneous chlorine adsorbent, specifically a basic solid.

Chloroaluminate Ionic Liquid Catalyzed Polymer Upcycling for Mixed PVC and Polyolefin Waste.

***Boda Yang**[1], Wei Zhang[1], Benjamin Jackson[1], Junbo Zhao[2], Donald M. Camaioni[1], Sungmin Kim[3], Huamin Wang[3], Janos Szanyi[3], Jingguang G. Chen[4], Mal Soon Lee[1], and Johannes Lercher[1,2]*
(1)Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA, (2)Department of Chemistry and Catalysis Research Center, Technische Universität München, Garching, Germany, (3)Pacific Northwest National Laboratory, Richland, WA, (4)Chemistry Division, Brookhaven National Laboratory, Upton, NY

We present a new low-temperature upcycling process for polyvinyl chloride into fuel-range isoalkanes and HCl. Polyolefins can be effectively integrated into the process with enhanced conversion rate. A detailed dehydrochlorination mechanism is proposed and shown how it couples with cracking and alkylation with the assist of computational simulation.

Low-Temperature Dechlorination of Polyvinyl Chloride (PVC) for Production of H_2 and Carbon Materials Using Liquid Metal Catalysts.

***Felipe Polo-Garzon**[1], Zili Wu[1], Yuanyuan Li[1], Junyan Zhang[1], Xinbin Yu[2], Elena Toups[3], Eddie Lopez-Honorato[4], Joshua Damron[5], Jeffrey Foster[6], Yongqiang Cheng[7], Luke L. Daemen[7], Annabal Ramirez-Cuesta[8], and Harry M. Meyer III[1]*
(1)Chemical Sciences Division, Oak Ridge National Laboratory (ORNL), Oak Ridge, TN,

(2)Pacific Northwest National Laboratory, Richland, WA, (3)University of New Orleans, New Orleans, LA, (4)Nuclear Energy and Fuel Cycle Division, Oak Ridge National Laboratory, Oak Ridge, TN, (5)Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN, (6)Sandia National Laboratories, Albuquerque, NM, (7)Chemical and Engineering Materials Division, Oak Ridge National Lab, Oak Ridge, TN, (8)Oak Ridge National Lab, Oak Ridge, TN

A catalytic route was developed to dechlorinate PVC (~90% reduction of Cl content) at mild temperature (200 °C) to produce gas H_2 (with negligible co-production of corrosive gas HCl) and carbon materials, using Ga as a liquid metal (LM) catalyst.

Kinetics of Self-Cleaning Catalysts to Enable Recycling of Multilayered Plastic Films.

Dai Phat Bui, Samira Abdolbaghi, Thamid Karim, Duc Nam, Laura Alejandra Gomez Gomez, Bin Wang, Lance Lobban, and ***Steven Crossley***
School of Sustainable Chemical, Biological and Materials Engineering, University of Oklahoma, Norman, OK

Multilayered films present unique challenges for polymer recycling. In this contribution, we present a catalytic biphasic system that selectively cleans impurities (EVOH, PVC) from multilayered polyolefin films through selective heteroatom scission over metal catalysts supported on reducible oxides while preserving the carbon backbone.

Upcycling Polystyrene Waste to Adipic Acid through Combined Chemical and Biological Reactions.

Hyunjin Moon[1]*, Jason DesVeaux*[2]*, Hannah Alt*[1]*, Joel Miscall*[1]*, Clarissa Lydia Lincoln*[1]*, Christine A. Singer*[1]*, Nicolette R. Meyer*[1]*, Kelsey J. Ramirez*[1]*, Taylor Uekert*[2]*, Davinia Salvachua*[1]*, Allison Werner*[1]*, Shannon S. Stahl*[3]*, and Gregg T. Beckham*[4]
(1)Renewable Resources and Enabling Sciences Center, National Renewable Energy Laboratory, Golden, CO, (2)Strategic Energy Analysis Center, National Renewable Energy Laboratory, Golden, CO, (3)Department of Chemistry, University of Wisconsin-Madison, Madison, WI, (4)BioEconomy and Sustainable Transportation, National Renewable Energy Laboratory, Golden, CO

PS was converted to benzoic acid at 94 mol% yield through modified Amoco process. The benzoic acid was then bioprocessed to muconic acid (30-40 g/L) and finally to adipic acid at >99% yield. This process reduces greenhouse gas emissions by ~50% compared to traditional methods.

Upcycling of Waste Polystyrene to Polyvinylcyclohexane Via Catalytic Hydrogenation.

Kaiwalya Sabnis*, Reggie Tennyson, Ryan Gilbert-Wilson, Matthew Heberle, Paulette Hazin, and Travis Conant*
SABIC Technology Center, SABIC Americas Inc., Sugar Land, TX

We report a catalytic pathway for upcycling of waste expanded polystyrene (EPS). Polyvinylcyclohexane was synthesized via solution-phase hydrogenation of EPS over Pt/Al_2O_3 catalyst. Standard adsorption techniques were used to remove additives/impurities from EPS that poison the catalyst. Effect of solvent on hydrogenation rates will be discussed during this presentation.

C2+ - CATALYSIS OF C2+ CHEMISTRY

C2+ | C3+ HYDROCARBONS C-C COUPLING, ISOMERIZATION, AND CRACKING REACTIONS

Friday, June 13, 2025 8:00 AM - 9:00 AM
Hanover Hall CDE

Chair: Nicholas Jaegers, University of New Mexico

Co-Chair: Xiang WANG, Dalian University of Technology

Assessing the Influence of Acid Site Location in MFI Zeolites on Propene Oligomerization Rates and Selectivity.

Diamarys Salome Rivera[1], *Lauren Kilburn*[1], *David Hibbitts*[1,2], *and Rajamani Gounder*[1]
(1)Charles D. Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN, (2)Department of Chemical Engineering, University of Florida, Gainesville, FL

Measured propene oligomerization rates, which are influenced by both kinetics and diffusional restrictions imposed by bulky hydrocarbons occluded within micropores, were higher for MFI zeolites with H^+-sites biased in smaller channels and away from larger intersections, due to shifts in product selectivity that lead to higher effective molecular diffusivities.

Progression of Catalyst Activation and Deactivation Fronts in Fixed Bed Reactor Explains Reactivity Profile of Butene Isomerization over Ferrierite in Experiment and Theory.

Pawel Chmielniak[1], *Karoline L. Hebisch*[1], *and Carsten Sievers*[2]
(1)School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA, (2)School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA

Isomerization of butene over ferrierite requires 3-5 wt% carbonaceous deposits for optimal performance. Experiments and stochastic modeling attribute the reactivity profile to propagating activation and deactivation fronts. These fronts maintain a constant number of active sites, explaining the steady-state reactivity and selectivity observed in the fixed bed.

Enhanced Aerobic Epoxidation of Styrene Using Mesoporous Co-Ni Catalysts.

Chathupama Abeyrathne[1], *Steven L. Suib*[2], *Musatafa S. Yavuz*[2], *Inosh P. Perera*[1], *Isaac Olowookere*[1], *Luisa Posada*[1], *and Samantha Rubio*[1]
(1)Department of Chemistry, University of Connecticut, Storrs, CT, (2)Institute of Materials Science, University of Connecticut, Storrs, CT

This work reports the synthesis and characterization of an efficient, environmentally benign mesoporous catalyst, 73CoNi-250, for styrene epoxidation, demonstrating exceptional catalytic activity with high conversion rates and excellent yield.The catalyst demonstrated remarkable reusability, up to 4 catalytic cycles, without altering the mesoporosity of the catalyst.

CO2 - CO2 CAPTURE AND UPGRADING

CO2 - CO_2 CONVERSION BY FUNCTIONAL METAL OXIDES

Friday, June 13, 2025 8:00 AM - 9:00 AM
Centennial Ballroom IV

Chair: Honghong Shi, Pacific Northwest National Laboratory

Co-Chair: Zhuoran Gan, Oak Ridge National Laboratory (ORNL)

Tuning Catalytic Selectivity Via Dynamic Mobility of Catalytically Active Dopants in Perovskite Oxides for CO_2 Hydrogenation.

Samiha Bhat[1]*, Miguel Sepulveda*[2]*, Camilo A. Ortega-Vega*[2]*, Yomaira Pagan Torres*[2]*, and Eranda Nikolla*[1]
(1)Department of Chemical Engineering, University of Michigan, Ann Arbor, MI, (2)Chemical Engineering, University of Puerto Rico at Mayaguez, Mayaguez, PR

Perovskite oxides inherently housing single cationic sites in their structure generate metal clusters at the close interface with the parent oxide under reducing conditions. The metal's uniform dispersion within the perovskite, controlled size (upon exsolution), and anchored interaction with the parent oxide are knobs for tuning CO_2 hydrogenation selectivity.

Oxygen Vacancy Dynamics Determine Activity and Stability of In2O3-Based Catalysts in CO2 Hydrogenation.

Matthias Becker*, Alexey Fedorov, Paula Abdala, and Christoph R. Müller*
Department of Mechanical and Process Engineering, ETH Zurich, Zurich, Switzerland

Sn- or Zr-doped In_2O_3 nanocrystals were synthesized using a colloidal approach to modify the active oxygen vacancy sites in In_2O_3. In-depth operando analyses revealed diverging effects on the CO_2 hydrogenation performance. The contrasting effects were rationalized by the different reactivities of the oxygen vacancies towards CO_2.

Overcoming Equilibrium Limitations in Reverse Water-Gas-Shift Reaction with Mixed Oxides Via Chemical Looping.

William Martin*, Chongyan Ruan, Tochukwu Aniekwensi, Abigail Mathias, and Fanxing Li*
Department of Chemical and Biomolecular Engineering, North Carolina State University, Raleigh, NC

We report "super-equilibrium" yields under a reverse flow chemical looping scheme in the reverse water-gas-shift reaction utilizing doped-Ceria at relatively low temperatures, overcoming conventional thermodynamic limitations with improved catalyst kinetics.

DYNAMICS - DYNAMIC CATALYSIS

DYNAMICS - DYNAMIC CATALYSIS

Friday, June 13, 2025 8:00 AM - 9:00 AM
Regency Ballroom VI

Chair: Steven Chavez, University of California, Los Angeles

Co-Chair: Audrey Dannar, Harvard University

Electron Doping for Adsorbate Binding Surface Chemistry Regulation.

Benjamin Page[1], *Tzia Ming Onn*[2], *Kyungryul Oh*[2], *Paul J. Dauenhauer*[2,3], *and Omar Abdelrahman*[4,5]
(1)Department of Chemical and Biomolecular Engineering, University of Houston, Houston, TX, (2)Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN, (3)Center for Programmable Energy Catalysis, University of Minnesota, Minneapolis, MN, (4)William A. Brookshire Department of Chemical and Biomolecular Engineering, University of Houston, Houston, TX, (5)Center for Programmable Energy Catalysis (CPEC), Minneapolis, MN

This work explored how modulating the electron density of a catalyst active site using a new type of architecture changed the binding energy of a kinetically relevant adsorbate. Practical application of this work can predict reaction conditions necessary to observe a macroscopic rate enhancement for the overall chemical reaction.

X-Ray Diffraction Computed Tomography (XRD-CT) Experiments on a Working Magnetic Induction Reaction during CO_2 Conversion.

Lucy Costley-Wood[1], *Antonis Vamvakeros*[2], *Christian Cerezo Navarrete*[3], *Simon S. D. M. Jacques*[2], *Pascual Oña Burgos*[3], *and* ***Andrew Beale***[2]
(1)UCL, London, United Kingdom, (2)Finden Ltd, Didcot, United Kingdom, (3)ITQ, Valencia, Spain

Advanced operando synchrotron experiments using X-ray diffraction computed tomography on novel reactors were conducted, during a magnetic induction study. The study revealed significant temperature gradients inside the reactor. The results of the study led to a redesign of the reactor to mitigate thermal gradients, improving RWGS conversion by 10%.

Assembly, Disassembly, and Reassembly of Pt Nanocatalysts during Reverse Water Gas Shift Reaction.

Rafat Hossain Aunkon[1], *Ryuichi Shimogawa*[1,2], *Yuanyuan Li*[3], *and Anatoly I. Frenkel*[1,4]
(1)Materials Science & Chemical Engineering, Stony Brook University, Stony Brook, NY,

(2)Mitsubishi Chemical Corporation, Science and Innovation Center, Yokohoma, Japan, (3)Chemical Sciences Division, Oak Ridge National Laboratory (ORNL), Oak Ridge, TN, (4)Brookhaven National Laboratory, Upton, NY

This study investigates the aggregation and subsequent fragmentation of Pt catalysts on ceria-titania support under reaction conditions using in situ DRIFTS, XAFS, and theoretical simulation. Key descriptors identified were CO binding, Pt-support interactions, and hydrogen coverage, providing insights into catalyst design for enhanced stability and performance.

ENERGY INPUTS - NOVEL ENERGY INPUTS FOR CATALYSIS

ENERGY INPUTS - CATALYSIS DRIVEN BY MECHANICAL, DYNAMIC HEATING, AND NONTHERMAL PLASMA

Friday, June 13, 2025 8:00 AM - 9:00 AM
Hanover Hall FG

Chair: Qiaowan Chang, Washington State University

Co-Chair: Sijie Guo, University of Tennessee, Knoxville

Dynamic Electrification of Nonoxidative Propane Dehydrogenation.

Yeonsu Kwak[1]*, Arnav Mittal*[2]*, Kewei Yu*[1]*, Weiqing Zheng*[3]*, and Dionisios Vlachos*[4]
(1)Chemical and Biomolecular Engineering, University of Delaware, Newark, DE, (2)University of Delaware, Newark, DE, (3)Delaware Energy Institute, University of Delaware, Newark, DE, University of Delaware, Newark, DE, (4)Delaware Energy Institute, University of Delaware, Newark, DE

This work reveals how dynamic heating modes influence reaction control, catalyst activity, and stability in nonoxidative propane dehydrogenation. By comparing rapid pulse and continuous Joule heating conditions, we uncover reaction pathways and mechanistic insights, advancing our understanding of renewable electricity-driven propylene production.

Mechanocatalytic Dehydrogenation of Propane in Ball Mills.

Aubrey Hepstall[1]*, Jouke van Westrenen*[1]*, Rongge Zou*[2]*, Felipe Polo-Garzon*[2]*, Zili Wu*[2]*, Yuanyuan Li*[2]*, David Sholl*[3]*, and Carsten Sievers*[4]
(1)School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA, (2)Chemical Sciences Division, Oak Ridge National Laboratory (ORNL), Oak Ridge, TN, (3)University of Tennessee-Oak Ridge Innovation Institute, Oak Ridge National Laboratory (ORNL), Oak Ridge, TN, (4)School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA

Propane dehydrogenation (PDH) is an important process for meeting the growing demand for propylene, but traditional thermal reaction processes face shortcomings like catalyst deactivation and high heating requirements. This work details the first known PDH reaction carried out using ball mill mechanochemistry in the absence of bulk heating.

Performance Predictions and Design Strategies for Nonthermal-Plasma-Promoted Ethane Reforming.

***Denver Haycock**, Russell J. Clarke, Jason Hicks, and William Schneider*
Chemical and Biomolecular Engineering, University of Notre Dame, Notre Dame, IN

We identified ideal dehydrogenation conditions for ethane in a nonthermal plasma using kinetic modeling techniques. We also expanded capabilities to design and explore plasma-chemical ethane reforming by applying kinetic models within advanced reactor models. This will push the field towards realization of decarbonized ethane reforming.

HYDRO ECON - CATALYSIS FOR THE HYDROGEN ECONOMY

HYDRO ECON - NOVEL ROUTES TO HYDROGEN PRODUCTION

Friday, June 13, 2025 8:00 AM - 9:00 AM
Centennial Ballroom III

Chair: Mingwu Tan, Institute of Sustainability for Chemicals, Energy and Environment (ISCE2)/Agency for Science, Technology and Research (A∗STAR)

Co-Chair: Hongliang Xin, Virginia Tech

The Role of Water on Methane Conversion for Hydrogen and Carbon Nanotube Production over Ni-Mo/MgO As a Catalyst.

***Phuong Nguyen Thi**, Laura Alejandra Gomez Gomez, Caleb Bavlnka, Le Thy Thy Ho, Bin Wang, Daniel Resasco, and Steven P. Crossley*
School of Sustainable Chemical, Biological and Materials Engineering, University of Oklahoma, Norman, OK

Incorporating water with methane at the initial stage of catalytic methane pyrolysis disrupts the catalyst evolution, resulting in lower production yield, while at steady state, it enhances catalyst regeneration and hydrogen yield by cleaning active sites. Lower temperatures amplify these benefits, and water can reduce the activation energy of reaction.

A New Catalytic Process for H2S Splitting to H2 and Elemental S.

*Anna Nova[1], **Emanuele Moioli**[2], and Flavio Manenti[3]*
(1)Politecnico di Milano, Milano, Italy, (2)Politecnico di Milano, Milano, None, Italy, (3)Dipartimento di Chimica, Materiali e Ingegneria Chimica, Politecnico di Milano, Milano, Italy

This paper presents the catalyst synthesis, characterisation and performance testing of a metal sulfide catalyst for H_2S splitting. The results are used to design a dedicated unit to produce H_2 from H_2S in oil refineries

Low-Carbon Hydrogen Production with in-Situ CO_2 Adsorption.

Diana Iruretagoyena Ferrer
Department of Chemical Engineering, Faculty of Chemistry, National Autonomous University of Mexico, Mexico City, Mexico

Sorption-enhanced H_2 production (SE-H_2) is a promising strategy to low-carbon H_2 at large scale. To aid its deployment, this work investigates a range of attractive mixed oxides to be used as CO_2 adsorbents and/or catalysts in SE-H_2. Comprehensive thermodynamic and kinetic studies to improve process design are also carried out.

LIQUID - CATALYSIS IN LIQUID, SUPERCRITICAL, AND MULTIPHASE SYSTEMS

LIQUID - INTERFACIAL CATALYSIS

Friday, June 13, 2025 8:00 AM - 9:00 AM
Regency Ballroom VII

Chair: Ali Hussain Motagamwala, Shell

Co-Chair: Benjamin Jackson, Pacific Northwest National Laboratory

Stimulus-Responsive Control of Electric Fields Near Water-Metal Interfaces Dictates Activity of Thermo-Catalysts.

Pengcheng Huang[1], Yu Yan[2], Ricardo P. Martinho[3], Leon Lefferts[4], Bin Wang[5], and ***Jimmy A. Faria***[6]
(1)School of Petrochemical Engineering, Changzhou University, Changchou, Netherlands, (2)School of Chemical, Biological and Materials Engineering, University of Oklahoma, Norman, OK, (3)Department of Molecules and Materials, University of Twente, Enschede, Netherlands, (4)Catalytic Processes and Materials (CPM) - TNW Faculty, University of Twente, Enschede, Netherlands, (5)School of Sustainable Chemical, Biological and Materials Engineering, University of Oklahoma, Norman, OK, (6)Faculty of Science and Technology, University of Twente, Enschede, Overijssel, Netherlands

This work lays down the foundation for developing homeostatic catalysts that can operate autonomously in dynamic reaction environments. These results underscore the ability of these polymers to alter the electric fields near metal-aqueous interfaces, which can have great potential in modulating activity in thermo- and electro- catalysts.

Reduced and Oxidized Ga Species Impact the Catalytic Hydrogenation of Olefins By Pd over Liquid Metal Catalysts.

Kathryn MacIntosh[1], *Felix Messick[2], Iklim Gokce[2], and Robert Rioux[3,4]*
(1)Chemical and Biomedical Engineering, The Pennsylvania State University, University Park, PA, (2)Chemical Engineering, The Pennsylvania State University, University Park, PA, (3)Department of Chemistry, The Pennsylvania State University, University Park, PA, (4)Department of Chemical Engineering, The Pennsylvania State University, University Park, PA

Supported liquid Pd/Ga catalysts consist of highly dynamic single metal atom active sites. The oxide layer on the surface of liquid metal droplets plays a significant role in their catalytic performance during ethylene hydrogenation, which may be associated with the stabilization of Pd ensembles on the liquid metal surface.

From Methane to Methanol: Pd-Ic-CeO_2 Catalysts Engineered for High Selectivity Via Mechanochemical Synthesis.

Juan Jimenez[1], *Pablo G. Lustemberg*[2], *Maila Danielis*[3], *Estefania Fernandez-Villanueva*[2], *Alessandro Trovarelli*[4], *Jose A. Rodriguez*[1,5], *Sara Colussi*[3], *M. Veronica Ganduglia-Pirovano*[2], *and Sanjaya D. Senanayake*[1]
(1)Chemistry Division, Brookhaven National Laboratory, Upton, NY, (2)CSIC, Instituto de Catálisis y Petroleoquímica, Madrid, Madrid, Spain, (3)Polytechnic Department, University of Udine, Udine, Italy, (4)Polytechnic Department, Università di Udine, Udine, Italy, (5)Chemistry Department, Stony Brook University, Stony Brook, NY

Milled Pd-CeO_2, with a unique interface composed of Pd-iC-CeO_2, enables the conversion of CH_4 into CH_3OH at a rate of 117 $\mu mol/g_{cat}$ in peroxide and water at 75 °C. Experiment and theory reveal that the role of interfacial carbon is to enables the 100% selective transformation of methane into methanol.

NEW COMP - NEW METHODS IN COMPUTATIONAL CATALYSIS

NEW COMP - COMPLEX SYSTEMS

Friday, June 13, 2025 8:00 AM - 9:00 AM
Centennial Ballroom II

Chair: Bjarne Kreitz, Georgia Institute of Technology

Co-Chair: Richard West, Northeastern University

Automated Uncertainty Estimation of Catalytic Mechanisms in Reaction Mechanism Generator (RMG).

Sevy Harris *and Richard West*
Department of Chemical Engineering, Northeastern University, Boston, MA

This work implements automated uncertainty estimation for catalysis mechanisms built by the Reaction Mechanism Generator (RMG). It allows investigators to easily compute correlated uncertainties for all the model input parameters and propagate them through a reactor simulation to determine the overall accuracy of model outputs like species concentrations.

A Similarity-Determining Algorithm to Theoretically Understand Catalysis with Multiple Reactants at Defected Metallic Sites.

Jin Zeng *and Siddharth Deshpande*
Chemical Engineering, University of Rochester, Rochester, NY

We introduce a novel configurational similarity algorithm and showcase it can significantly reduce the vast configurational space in the important case of multiple types and numbers of adsorbate on defected metal/metal alloy surfaces.

Elucidating the Mechanistic Pathways for Electrochemical CO and CO_2 Reduction to Different Multi-Carbon Products on Cu(100) Using DFT within a Hybrid Model.

Nkechi Kingsley[1] *and Craig Plaisance*[2]
(1)Chemical Engineering, Louisiana State University, Baton Rouge, LA, (2)Cain Department of Chemical Engineering, Louisiana State University, Baton Rouge, LA

This study introduces a hybrid solvation model that combines implicit and explicit water treatments in density functional theory (DFT) simulations. By accurately capturing hydrogen-bonding interactions during electrochemical CO and CO_2 reduction on copper surfaces, the framework improves kinetic barrier calculations and enhances understanding of product selectivity for multi-carbon formation.

NITRO CHEM - NITROGEN CHEMISTRY

NITRO CHEM - COUPLING AND DECOMPOSITION REACTIONS

Friday, June 13, 2025 8:00 AM - 9:00 AM
Centennial Ballroom I

Chair: Xianqin Wang, New Jersey Institute of Technology

Co-Chair: Raul Montesano, Topsoe

Electrocatalytic Activity and Selectivity for Urea Synthesis through the Co-Reduction of CO_2 and Nitrite..

Mohammadreza Karamad
Chemistry and School of Sustainable Energy Engineering, Simon Fraser University, Burnaby, BC, Canada

We employed density functional theory calculations to get insight into factor governing the selectivity in the co-reduction of CO_2 and nitrite for urea synthesis, on different electrocatalysts reported in experimental studies. This research establishes critical design principles for developing efficient electrocatalysts for urea synthesis.

Oxidative Coupling of NH_3 and CO on Pt for Urea Synthesis.

Haocheng Xiong[1]*, Qi Lu*[2]*, and Bingjun Xu*[3]
(1)Department of Chemical Engineering, Tsinghua University, Beijing, China, (2)Chemical Engineering, Tsinghua University, Beijing, China, (3)Catalysis Center for Energy Innovation, Department of Chemical and Biomolecular Engineering, University of Delaware, Newark, DE

I will demonstrate a novel approach for urea production by proposing the oxidative coupling of NH_3 with CO on Pt catalysts under ambient conditions.

If time permits, I will also discuss the intersection between thermocatalytic and electrocatalytic methods for urea production.

Iron Catalysts for Methane Pyrolysis: Understanding the Effects of Carbon Build-up on Structure and Activity.

Veronica Piazza*, Lidia Castoldi, Chiara Negri, Marco Orsenigo, Davide Cafaro, Matteo Maestri, Gianpiero Groppi, and Alessanda Beretta*
Laboratory of Catalysis and Catalytic Processes - Dipartimento di Energia, Politecnico di Milano, Milano, Italy

This work examines Fe-Al_2O_3 catalysts at high Fe load for methane pyrolysis. The compositional effects, the role of reduction, the transformations that follow the incipient and extensive growth of carbon are investigated to better elucidate C build-up chemism and obtain rational guidelines to scale-up and industrialization.

BIOMASS - BIOMASS AND WASTE VALORIZATION CATALYSIS

BIOMASS - BIOMASS TO FUELS 3

Friday, June 13, 2025 9:20 AM - 10:40 AM
Regency Ballroom VI

Chair: Zhexi Lin, Columbia University

Co-Chair: Elizabeth Biddinger, The City College of New York

En Route to Identifying a Benchmark Catalyst for the Deoxydehydration (DODH) of Biomass Derived Polyols.

Han Wang[1], Bhushan Murjani[2], Mark Gandelman[3], ***Friederike Jentoft****[2], and Oz Gazit[1]*
(1)Chemical Engineering, Israel institute of Technology Technion, Haifa, Israel, (2)Department of Chemical Engineering, University of Massachusetts Amherst, Amherst, MA, (3)Chemistry, Israel institute of Technology Technion, Haifa, Israel

In the current work we show, for the first time, that the Cp*ReO_3 catalyst is active and ~100% selective for the deoxydehydration of 1,2-propanediol to propylene. We rigorously investigate the condition and factors affecting the stability of the Cp*ReO_3 and evaluate its potential as a benchmark homogeneous DODH catalyst.

Few Layer MoS_2 As a Catalyst for the Fatty Acid Hydrodeoxygenation to Alkanes.

Fuli Deng*[1], Yuyang Fan[1], Ruixue Zhao[1], and Johannes Lercher[1,2]*
(1)Technical University of Munich, Garching b. München, Germany, (2)Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA

The few-layered type MoS_2 catalysts demonstrate exceptional activity, selectivity, and stability for the conversion of fatty acids into long-chain alkanes. This performance highlights its

potential for industrial applications in biomass conversion, paving the way for adopting this novel catalyst in sustainable fuel production.

Enhanced Electrochemical Hydrodeoxygenation of Bio-Oil Model Compounds Using Bimetallic Platinum Catalysts.

Jeffrey Page[1], *Büşra Çetiner*[2], *Alp Yürüm*[2], *Juan A. Lopez-Ruiz*[3], *and Julia A. Valla*[1]
(1)Chemical and Biomolecular Engineering, University of Connecticut, Storrs, CT, (2)Nanotechnology Research and Application Center, Sabanci University, Istanbul, Turkey, (3)Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA

This study aims to shed light on the effects and synergy of metals on the electrochemical hydrodeoxygenation of phenol to cyclohexane through the development of structure reactivity relationships in mono- and bi-metallic catalysts.

Pt Supported on $ZnAl_2O_4$ Spinel for Selective C=O over C=C Hydrogenation.

Clara Ehinger[1], *Wenda Hu*[2], *Hao Xu*[1], *Mingwu Tan*[3], *and Yong Wang*[2]
(1)Chemical and Bio Engineering, Washington State University, Pullman, WA, (2)The Gene and Linda Voiland School of Chemical Engineering and Bioengineering, Washington State University, Pullman, WA, (3)4Agency for Science, Technology and Research (A∗STAR), Singapore, Singapore

A Pt-enriched PtZn alloy on $ZnAl_2O_4$ achieves 90% selectivity for cinnamyl alcohol (C=O hydrogenation) in cinnamaldehyde hydrogenation, outperforming ZnO and Al_2O_3 supports. This demonstrates that tailored supports can modulate selective hydrogenation, advancing biofuel production and contributing to decarbonization efforts.

C2+ - CATALYSIS OF C2+ CHEMISTRY

C2+ | C2 HYDROCARBONS/OXYGENATES OXIDATION AND C-C COUPLING REACTIONS

Friday, June 13, 2025 9:20 AM - 10:40 AM
Hanover Hall CDE

Chair: D Jan, Honeywell - UOP

Co-Chair: Juan Jimenez, Brookhaven National Laboratory

Direct Conversion of Ethanol to Olefins over Cu-Rare Earth/Beta Catalysts: The Critical Role of Lewis Acid Sites on Catalyst Behavior.

Meijun Li[1,2], *Stephen Purdy*[2], *Shivangi Nandkumar Borate*[3], *Junyan Zhang*[4], *Kinga A. Unocic*[5], *Zili Wu*[4], *Huamin Wang*[6], *James W. Harris*[3], *Brian H. Davison*[7], *Andrew D. Sutton*[2], *and Hunter Jacobs*[2]
(1)Manufacturing Science Division, ORNL, Oak Ridge, TN, (2)Manufacturing Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN, (3)Department of Chemical and Biological Engineering, The University of Alabama, Tuscaloosa, AL, (4)Chemical Sciences Division, Oak

Ridge National Laboratory (ORNL), Oak Ridge, TN, (5)Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, TN, (6)Pacific Northwest National Laboratory, Richland, WA, (7)Biosciences Division, Center for Bioenergy Innovation, Oak Ridge National Laboratory, Oak Ridge, TN

We have developed Cu-RE/Beta catalysts that yield high C_{3+} alkene selectivity from direct ethanol upgrading. The intermediates and reaction steps are probed as a function of RE LAS. The catalyst deactivation mechanism was identified. The work highlights the critical role of LAS in influencing reaction pathways, product distribution and stability.

Anaerobic Wacker-Type Reaction Enabled By Isolated Pd(II) Stabilized on MnO_2.

***Jacklyn Hall**, Yu Lim Kim, Cong Liu, A. Jeremy Kropf, Massimiliano Delferro, and David Kaphan*
Chemical Sciences and Engineering Division, Argonne National Laboratory, Lemont, IL

This work applies isolated Pd catalysts for the heterogeneous Wacker-type oxidation of ethylene to acetaldehyde under both aerobic and anaerobic reaction conditions. A combination of kinetic and spectroscopic tools aid in establishing a clear relationship between catalytic properties and interactions of supported Pd with the oxide surfaces.

Controlling Single-Atom Rhodium Sites for Hydroformylation Using Phosphonic Acids.

***Zachary W. Meduna**, Daniel K. Schwartz, and J. Will Medlin*
Department of Chemical and Biological Engineering, University of Colorado Boulder, Boulder, CO

Atomically disperse catalysts have gained traction due to their potential to perform reactions unfeasible on metal nanoparticles; here, we investigate the effects of phosphonic acid modifiers on the hydroformylation of ethylene over isolated rhodium on titania catalysts and correlate to descriptors found by CO DRIFTS.

Interactions Amongst Inorganic and Gaseous Promoters in Ag/α-Al_2O_3 Ethylene Epoxidation Catalysts.

***Michael Gresh-Sill** and Aditya Bhan*
Chemical Engineering and Materials Science, University of Minnesota Twin Cities, Minneapolis, MN

Cs-promoted Ag/α-Al_2O_3 ethylene epoxidation catalysts feature abundant coverages of bidentate carbonates rationalizing the inverse half-order dependence of rate with CO_2 pressure. Organochloride promotional effects on rate and selectivity remain unchanged suggesting that the surfaces of Cs-promoted catalysts are abundantly covered in both carbonates and Cl-adatoms on distinct sites.

CO2 - CO2 CAPTURE AND UPGRADING

CO2 - CO_2 CAPTURE AND CONVERSION

Friday, June 13, 2025 9:20 AM - 10:40 AM
Centennial Ballroom IV

Chair: Chae Jeong-Potter, National Renewable Energy Laboratory

Co-Chair: Mathew Rasmussen, National Renewable Energy Laboratory

Ocean Carbon Capture- Electrochemical Ocean Deacidification, Carbonate Mineralization, and General Techno-Economic Analysis.

Hussein Badr[1]*, Isabela Rios Amador*[1]*, Ryan Hannagan*[2]*, Dong Un Lee*[1]*, and Thomas Jaramillo*[1]
(1)Chemical Engineering, Stanford University, Stanford, CA, (2)Chemical Engineering, Stanford University, Palo Alto, CA

Design and fabricate realistic and scalable hybrid oceanwater electrolysis/chlorine-hydrogen fuel cell system for direct carbon capture from oceanwater. Techno-economic analysis showed that electrolysis byproducts, themselves, can jump start an enormous mineral extraction industry from the ocean to pay itself for carbon capture.

Energy-Efficient Removal of O_2 from CO_2 Stream Using Catalysts.

Yeonshil Park*, Todd Toops, Sreshtha Sinha Majumdar, Hai-Ying Chen, and David Sholl*
Oak Ridge National Laboratory, Oak Ridge, TN

Purification of captured CO_2 streams is essential for its pipeline transportation to avoid corrosion and two-phase flow issues. Through our systematic study, insights into the technical feasibility of the various catalytic oxygen reduction technologies can be gained for oxygen removal to meet the CO_2 pipeline specifications.

Active Phase Evolution in Fe-Zn Based Catalysts for CO_2 Hydrogenation to C_{2+} Oxygenates.

Zhuoran Gan[1]*, Zili Wu*[2]*, and Yuanyuan Li*[2]
(1)Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN, (2)Chemical Sciences Division, Oak Ridge National Laboratory (ORNL), Oak Ridge, TN

Selectivity towards C2+ oxygenates were tuned by employing different pretreatment conditions using H2 and CO in CO2 hydrogenation. The evolution of active phases Fe_5C_2 and $ZnFeO_x$ was investigated over Fe-Zn based catalysts.

Catalytic Activity of Ensemble Sites for CO_2 Hydrogenation to Methanol on a ZrO_2 on Cu Inverse Catalyst.

Zihan Yang[1] *and Philippe Sautet*[2]
(1)UCLA, Los Angeles, CA, (2)Chemical and Biomolecular Engineering, University of California, Los Angeles, Los Angeles, CA

We developed an electronic feature-based descriptor to predict active sites on ZrO_2/Cu catalysts for CO_2 hydrogenation to methanol, enabling efficient screening for large catalyst ensembles, followed by reaction pathway simulation and catalytic activity evaluation. This represents an efficient workflow for studying diverse catalysts under operating conditions, guiding rational catalyst design.

ENVIRO AUTO - ENVIRONMENTAL AND AUTOMOTIVE CATALYSIS

ENVIRO AUTO - NEW DEVELOPMENTS IN NO_X EMISSION CONTROL

Friday, June 13, 2025 9:20 AM - 10:40 AM
Hanover Hall FG

Chair: Fudong Liu, University of California, Riverside

Co-Chair: Maria Pia Ruggeri, Johnson Matthey Technology Centre

From Atoms to Nanoparticles and Back – Site Transformations in Pd/AEI Zeolite for NO_x Adsorption.

Petr Koci[1], *Tetyana Zheleznyak*[1], *Richard Knopp*[1], *Maria Pia Ruggeri*[2], *Djamela Bounechada*[2], *and Andrew P.E. York*[2]
(1)University of Chemistry and Technology, Prague, Czech Republic, (2)Johnson Matthey Technology Centre, Sonning Common, United Kingdom

Pd ions exchanged into zeolite transform reversibly into clusters and nanoparticles during catalyst operation. The combination of lab experiments and kinetic modeling allows us to build a physically relevant, predictive model of PNA activity and adsorption capacity depending on the trajectory of operating conditions, including possible catalyst reactivation strategies.

An NMR Identification of the Ag Anchoring Sites of Al_2O_3 to Explain the Enhancement of (H_2-)C_3H_6-SCR Performance of Ag/Al_2O_3 Catalysts Prepared from Warm-Water-Treated Al_2O_3.

Yannick Millot[1], *Guylène Costentin*[1], *Sandra Casale*[1], *Clémence Rodigue*[1], *Thomas Onfroy*[1], *and* ***Cyril Thomas***[2]
(1)Sorbonne Université, Paris, France, (2)Sorbonne Université, Laboratoire de Réactivité de Surface, Paris, France

This work not only paves the way for further improvement of the HC-SCR and H_2-HC-SCR performance of the Ag/Al_2O_3 system, but also identifies the Ag anchoring sites of Al_2O_3 through unprecedented in-depth NMR investigations (μ^1-OH groups at the crystallite edges).

High Throughput Design of Catalytic Converters for NO_x Reduction from Aircrafts Emissions.

Anshuman Goswami[1,2,3], *Joakim Halldin Stenlid*[3], *John W. Lawson*[4], *and Frank Abild-Pedersen*[1,2]
(1)Department of Chemical Engineering, Stanford University, Stanford, CA, (2)SUNCAT Center

for Interface Science and Catalysis, SLAC National Accelerator Laboratory, Menlo Park, CA, (3)KBR Intelligent System Division, NASA Ames Research Center, Mountain View, CA, (4)Intelligent System Division, NASA Ames Research Center, Moffett Field, CA

We employ machine learned potentials from the Open Catalyst Project (OCP) to explore materials spaces optimum for NO_x reduction. We construct a database of adsorption energies on different transition metal surfaces. We benchmark ML potentials against this database, identify alloy candidates and analyse site compositions optimal for catalysing NO_x conversion.

Transition-Metal Aluminate Spinels for PGM-Free, Direct NO Decomposition.

***Griffin Canning**, Kimber L. Stamm Masias, and Charles A. Roberts*
Toyota Research Institute of North America, Ann Arbor, MI

Advanced combustion engines expected to dominate the automotive market in the coming decades require catalysts that can operate at lower temperatures than before. Design principles of PGM-free aluminate spinel catalysts for the decomposition of NO at these low temperatures are discussed.

FUNDAMENTALS - FUNDAMENTALS OF CATALYSIS AND SURFACE SCIENCE

FUNDAMENTALS - FUNDAMENTALS IN THERMOCATALYSIS AND ELECTROCATALYSIS

Friday, June 13, 2025 9:20 AM - 10:40 AM
Centennial Ballroom II

Chair: Audrey Dannar, Harvard University

Co-Chair: Kausthubh Savant, University of California, Los Angeles

Descriptor Analysis of Heterogeneous Mo-Based Olefin Metathesis Catalysts Reveals an Olefin Structure-Dependent H-Donation Mechanism Facilitated By Silanols.

***Dimitri Gatzios**[1], Stephen Stockton[1], Hannah Frankovic[1], Avery Hill[2], Matthew Montemore[2], and Lucas Ellis[1]*
(1)School of Chemical, Biological, and Environmental Engineering, Oregon State University, Corvallis, OR, (2)Chemical and Biomolecular Engineering, Tulane University, New Orleans, LA

We pretreated SiO_2-supported MoO_x catalysts for propene metathesis with olefins of varying methyl branching. Highly branched olefins promote better surface adsorption and hydrogen donation via dehydrogenation. Temperature-programmed studies and FTIR reveal that branched olefins enhance active site creation through a silanol-facilitated, H-assisted mechanism.

Tuning the Catalytic Fate of Interfacial Hydrogen in Thermo- and Electrocatalytic Phenol Hydrogenation and Substitution.

***William Broomhead**[1,2], Julia de Barros Dias Moreira[2], Kamal Nayan[1], Udishnu Sanyal[2],*

Sungmin Kim[2], Thuy Le[2], Huamin Wang[2], Johannes Lercher[2,3], and Ya-Huei (Cathy) Chin[1]
(1)Department of Chemical Engineering and Applied Chemistry, University of Toronto, Toronto, ON, Canada, (2)Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA, (3)Technical University of Munich, Garching b. München, Germany

Using phenol electrophilic substitution and hydrogenation as kinetic probes for interfacial protons and hydrogen atoms at the metal-water interface, we derive a unified dependence of their rates on the electrostatic potential for open circuit, cathodic, and anodic potentials, for a range of transition metals (Pt, Rh, Ru, and Rd)

Diagnosing Enhancement Mechanisms for CO Electro-Oxidation across Bimetallic Alloy Compositions Using Kinetic Measurements and Modeling.

Todd Whittaker *and Adam Holewinski*
Chemical and Biological Engineering, University of Colorado Boulder, Boulder, CO

Alloy enhancement mechanisms are not fully understood for CO electro-oxidation. This talk discusses efforts to characterize these enhancement mechanisms, namely the bifunctional and electronic enhancement, for Pd-based alloy electrocatalysts using kinetic measurements and microkinetic modeling. A unique, non-integer electrosorption valency for hydroxide on silver sites was revealed for AgPd catalysts.

Facet Preferencing By Doping Controls Semi-Hydrogenation Selectivity in Ternary Pyrite-Type Intermetallics.

Mustafa Eid[1]*, Nilanjan ROY[2], Kathryn MacIntosh[3], Michael Janik[2], and Robert Rioux[4,5]*
(1)Chemistry, The Pennsylvania State University, University Park, PA, (2)Chemical Engineering, The Pennsylvania State University, University Park, PA, (3)Chemical and Biomedical Engineering, The Pennsylvania State University, University Park, PA, (4)Department of Chemistry, The Pennsylvania State University, University Park, PA, (5)Department of Chemical Engineering, The Pennsylvania State University, University Park, PA

The partial substitution of Pd with Au in $PdSb_2$ intermetallics introduced geometric effects by preferentially exposing (100) surfaces and diminishing (111) surfaces. The (100) surface possess weaker binding to ethylene and demonstrated higher net ethylene selectivity compared to (111) surfaces during the semi-hydrogenation of acetylene-propylene mixtures in excess alkene.

HYDRO ECON - CATALYSIS FOR THE HYDROGEN ECONOMY

HYDRO ECON - THERMOCATALYSIS 2

Friday, June 13, 2025 9:20 AM - 10:40 AM
Centennial Ballroom III

Chair: Yizhen Chen, University of Virginia

Co-Chair: Ugochukwu Nwosu, Simon Fraser University

Innovative Methanol Production Technology Integrating Hydrogen Storage and Waste CO_2 Valorization.

Andrzej Rogala[1] *and Izabela Frackiewicz*[2]
(1)SUNCAT, Stanford University, Stanford/Menlo Park, CA, (2)Department of Process Engineering and Chemical Technology, Gdansk University of Technology, Gdansk, Poland

The transformation of the global energy system is no longer a plan but a reality. This work introduces an innovative intermediate technology to enhance the sustainability of gas recovery and replace outdated methods as hydrocarbon extraction declines. It combines process and catalytic advancements to address practical industrial challenges.

Novel Close-Contact Cu-Ni Bimetallic Catalysts for Enhanced Methylcyclohexane Dehydrogenation.

Md Fakhruddin Patwary[1]*, Haiying Zhou*[2]*, John Meynard Tengco*[2]*, and John Monnier*[2]
(1)Chemical Engineering, UNIVERSITY OF SOUTH CAROLINA, Columbia, SC, (2)Chemical Engineering, University of South Carolina, Columbia, SC

Highly dispersed Close-contact Cu-Ni catalysts synthesized by galvanic displacement and electroless deposition method. These catalysts show superior performance for Methylcyclohexane dehydrogenation as compared to dry impregnated catalysts. Increasing Cu content from 0.1wt% to 1.7wt% in a 5 wt% Ni base catalyst significantly improved the TOF.

Zr-Promoted Ni Nanoparticles in Mesoporous Silica Spheres (NiZr/*m*SiO_2) for Catalytic Decomposition of Methane.

Mohammadreza Kosari[1]*, Samuel Portillo*[1]*, Abhijit Talpade*[2]*, and Fanxing Li*[3]
(1)Chemical & Biomolecular Engineering, North Carolina State University, Raleigh, NC, (2)Eastman Chemical Company, Kingsport, NC, (3)Department of Chemical and Biomolecular Engineering, North Carolina State University, Raleigh, NC

A highly active catalyst for catalytic decomposition of methane is presented comprising of inert mesoporous silica sphere (*m*SiO_2) as a support loaded with Ni NPs and Zr promoter, resulting in an excellent H_2 production rate (4.52 $mol_{H2} \cdot g_{Ni}^{-1} \cdot h^{-1}$). Satisfactory long-term stability, cyclability performance, and CNTs growth mode switching are demonstrated.

Hydrogen Spillover Assisted By Oxygenate Molecules over Nonreducible Oxides.

Mingwu Tan[1] *and Yong Wang*[2]
(1)Institute of Sustainability for Chemicals, Energy and Environment (ISCE2)/Agency for Science, Technology and Research (A∗STAR), Singapore, Singapore, (2)The Gene and Linda Voiland School of Chemical Engineering and Bioengineering, Washington State University, Pullman, WA

This study demonstrates a strategy to enable hydrogen spillover on non-reducible SiO_2 using organic molecules with a carbonyl group, facilitating active hydrogen transfer from Pt to Fe sites in Pt-Fe catalysts, significantly enhancing hydrodeoxygenation rates. This approach provides a new method for optimizing multifunctional heterogeneous catalysts.

NITRO CHEM - NITROGEN CHEMISTRY

NITRO CHEM - EMERGING PATHWAYS TOWARD SUSTAINABLE NITROGEN CYCLE

Friday, June 13, 2025 9:20 AM - 10:40 AM
Centennial Ballroom I

Chair: Raul Montesano, Topsoe

Co-Chair: Nirala Singh, University of Michigan

In Situ Formation of Nickel Nitride Structures and Their Catalytic Activities for Plasma-Assisted Ammonia Synthesis.

Yiteng Zheng[1], *Christopher Kondratowicz*[2], *James Trettin*[1], *and Bruce E. Koel*[1]
(1)Department of Chemical and Biological Engineering, Princeton University, Princeton, NJ, (2)Mechanical and Aerospace Engineering, Princeton University, Princeton, NJ

Plasma-assisted ammonia synthesis is an alternative process to produce ammonia. The dynamics of surface structures under plasma conditions have not been studied due to the limited capabilities for in situ characterization. The in-situ formation of Ni nitride structures was identified by in situ spectroscopic techniques.

Accelerated Computational Materials Discovery for Electrochemical Nutrient Recovery.

Nianhan Tian[1], *Samuel Olusegun*[2], *Haldrian Iriawan*[3], *Ehsan Abbasi*[2], *Kevin O'Halloran*[4], *Joseph Gauthier*[2], *Gerardine Botte*[2], *Yang Shao-Horn*[3], *Paul Kohl*[1], *and Andrew Medford*[1]
(1)School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA, (2)Chemical Engineering, Texas Tech University, Lubbock, TX, (3)Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, MA, (4)Georgia Gwinnett College, Lawrenceville, GA

This work leverages computational material screening and Pourbaix diagram studies to design stable catalysts for electrochemical nutrient recovery. By integrating machine learned potentials, we identify thermodynamically stable and active materials, accelerating discovery while reducing computational costs. This approach provides insight for optimal catalyst material design for sustainable nutrient recovery.

Understanding Activity Trends in Electrochemical Dinitrogen Oxidation over Transition Metal Oxides .

Samuel Olusegun[1], *Yancun Qi*[2], *Nishithan Balaji Chidambara Kani*[3], *Meenesh R Singh*[4], *and Joseph Gauthier*[1]

(1)Chemical Engineering, Texas Tech University, Lubbock, TX, (2)University of Illinois Chicago, Chicago, IL, (3)Chemical Engineering, University of Illinois at Chicago, Chicago, IL, (4)Department of Chemical Engineering, University of Illinois Chicago, Chicago, IL

Our mechanistic study identified the Mars-van-Krevelen(MvK) mechanism as a key pathway for N_2OR, discovered the likely rate-limiting step, illustrated that circumventing competitive water adsorption will be critical for N_2OR on anodic metal oxides, and proposed, tested, and validated dynamic potential control as a possible method to improve N_2OR.

Proton Donor Effects on Lithium Nitride (Li_3N) Formation in Lithium-Mediated Ammonia Synthesis (LiMEAS).

Victor Azumah[1]*, Lance Kavalsky*[2]*, and Venkatasubramanian Viswanathan*[2,3]
(1)Chemical Engineering, University of Michigan, Ann Arbor, Ann Arbor, MI, (2)Mechanical Engineering, University of Michigan, Ann Arbor, Ann Arbor, MI, (3)Aerospace Engineering, University of Michigan, Ann Arbor, Ann Arbor, MI

We investigate how proton donors impact lithium nitride formation in lithium-mediated ammonia synthesis. Using density functional theory and statistical analysis, our work reveals significant correlations between proton donor chemistry and nitride stability. These findings can guide the selection of proton donors to enhance ammonia synthesis efficiency.

POLYMER - CATALYSIS FOR POLYMER SYNTHESIS, UPCYCLING, AND RECYCLING

POLYMER - MECHANOCHEMICAL

Friday, June 13, 2025 9:20 AM - 10:40 AM
Regency Ballroom VII

Chair: Linxiao Chen, The University of Akron

Co-Chair: Kinga Golabek, Georgia Institute of Technology

Theory of Kinetics for Mechanocatalytic Reactions Conducted inside Vibratory Ball Mills.

Yuchen Chang[1] *and Carsten Sievers*[2]
(1)School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA, (2)School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA

A reactor theory is formulated to describe mechanocatalytic kinetics in a vibratory ball mill. Time-dependent or steady-state kinetics involving a solid catalyst and gaseous reactants or products can be modeled using the theory.

Surface-Activated Mechano-Catalysis for Ambient Conversion of Plastic Waste.

Adrian H. Hergesell[1]*, Renate J. Baarslag*[1]*, Claire L. Seitzinger*[1]*, Raghavendra Meena*[2]*, Patrick Schara*[3]*, Željko Tomović*[3]*, Guanna Li*[2]*, Bert M. Weckhuysen*[1]*, and Ina Vollmer*[1]

(1)Utrecht University, Utrecht, Netherlands, (2)Wageningen University and Research, Wageningen, Netherlands, (3)Eindhoven University of Technology, Eindhoven, Netherlands

While chemical recycling of polyolefins is typically performed at high temperatures, we show that plastic waste can be depolymerized at ambient conditions using mechano-catalysis. We purposefully incorporated catalytically active sites on the surface of grinding spheres, enabling good contact with the plastic material and stabilization of mechano-chemically generated radical intermediates.

Mechanocatalytic Methanolysis of Polyethylene Terephthalate.

Christopher Kevin Wijaya[1,2]*, Pei Ying Moo*[2]*, Tej Choksi*[1]*, and Amol Amrute*[2]
*(1)School of Chemistry, Chemical Engineering and Biotechnology, Nanyang Technological University, Singapore, Singapore, (2)Institute Of Sustainability for Chemicals, Energy And Environment (ISCE2), Agency for Science, Technology and Research (A*STAR), Singapore, Singapore*

A novel mechanocatalytic methanolysis of PET using benign K_2CO_3 catalyst for 15 minutes was established. Additional experiments and calculations were carried out to understand on the mechanism, revealing the role of ball milling to increase the surface area of PET susceptible for reaction and K_2CO_3 to activate methanol.

Spatially-Resolved Single Impact Tests Revealing Reaction Environments in Mechanochemical Upcycling of Polymers.

Kinga Golabek[1]*, Yuchen Chang*[1]*, Lauren Mellinger*[1]*, Mariana Veiga Rodrigues*[2]*, Cauê de Souza Coutinho Nogueira*[3]*, Fabio B. Passos*[4]*, Yutao Xing*[3]*, Aline Ribeiro Passos*[2]*, Mohammed Saffarini*[5]*, Austin Isner*[5]*, David Sholl*[5]*, and Carsten Sievers*[6]
(1)School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA, (2)Brazilian Synchrotron Light Laboratory, Brazilian Center for Research in Energy and Materials, Campinas, Brazil, (3)Center for Petroleum Industry, Fluminense Federal University, Niteroi, Brazil, (4)Department of Chemical and Petroleum Engineering, Universidade Federal Fluminense, Niteroi, Brazil, (5)Computing and Computational Sciences Directorate, Oak Ridge National Laboratory (ORNL), Oak Ridge, TN, (6)School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA

Carefully controlled single impact measurements that combine multiple spatially resolved analytical methods and simulations were utilized to gain unprecedented information about mechanochemical depolymerization of PET. These measurements highlighted the contributions of plastic deformation, amorphization, and depolymerization during the transfer of kinetic energy in collisions relevant to ball mills.

BIOMASS - BIOMASS AND WASTE VALORIZATION CATALYSIS

BIOMASS - DFT & MECHANISTIC STUDIES

Friday, June 13, 2025 10:50 AM - 12:10 PM
Regency Ballroom VI

Chair: Reda Bababrik, Phillips 66 Research Center

Co-Chair: Stephen Schuyten, Johnson Matthey Inc.

Elucidating the Essential Role of Hydrogen Bonding and Direct H-Transfer in Transfer Hydrogenation of Carbonyl Group on Transition Metal Catalysts.

Aojie Li[1] *and Srinivas Rangarajan*[2]
(1)Department of Chemical and Biomolecular Engineering, Lehigh University, Bethlehem, PA, (2)Chemical and Biomolecular Engineering, Lehigh University, Bethlehem, PA

Presenting a detailed mechanistic analysis of our coverage-cognizant microkinetic model for HCHO hydrogenation by formic acid, and further discuss the kinetic relevance of direct H-transfer in transfer hydrogenation and hydrogenolysis of sugar-derived aldehydes and alcohols. This insight enables sustainable hydrogenation design, leveraging H-donor selection as a tunable parameter.

Redox-Activated Catalytic CO_2 Sorbents for Green Hydrogen Production.

Mahe Rukh[1]*, Runxia Cai*[1]*, Fanxing Li*[1]*, Kunran Yang*[1]*, Xijun Wang*[2]*, and Leo Brody*[1]
(1)Department of Chemical and Biomolecular Engineering, North Carolina State University, Raleigh, NC, (2)Department of Chemical & Biological Engineering, Northwestern University, Evanston, IL

Sorption-enhanced reforming and gasification simplifies H_2 production but struggles with energy-intensive decarbonation and sorbent stability. We introduce redox-activated perovskites for isothermal SERG, leveraging oxygen and CO_2 partial pressure shifts for efficient carbonation-decarbonation. Moreover, these sorbents catalyze reforming, ensuring cyclic stability. A thermodynamic framework, DFT screening, and experimental validation are presented.

Catalyst Testing for Renewable Diesel / SAF Production from Renewable Feedstocks.

Ioan-Teodor Trotus*, Giada Innocenti, Jochen Berg, and Kai Dannenbauer*
R&D solutions, hte GmbH, Heidelberg, Germany

The Net-Zero CO_2 emission goals for the next decades require a rethink of how fuels and chemicals are manufactured. Sustainable fuels can be produced from different feedstocks, like vegetable oils, animal fat, syngas, alcohols and pyrolysis oils. This contribution focuses on the conversion of vegetable oils to produce sustainable fuels.

Selective Isobutanol Dehydration Catalyzed By Hfer: Mechanism Investigation By Operando IR, Chemometrics and Microkinetics.

Eleonora Vottero[1]*, Reda Aboulayt*[1]*, Alexandre Vimont*[1]*, Philippe Bazin*[1]*, Karine Thomas*[1]*, Sylvie Maury*[2]*, Céline Chizallet*[3]*, and Arnaud Travert*[1]

(1)Université de Caen Normandie, Caen, France, (2)IFP Energies nouvelles, Solaize, France, (3)IFP Energies Nouvelles, Solaize, France

HFER is a promising catalyst for the direct dehydration and isomerization of bio-sourced isobutanol to linear butenes. By combining *operando* IR, chemometrics and microkinetic modelling, we managed to shed new light to the unusual reaction mechanism.

C1 - CATALYSIS OF C1 CHEMISTRY

C1 - C1 OXIDATION

Friday, June 13, 2025 10:50 AM - 12:10 PM
Regency Ballroom VII

Chair: Zhenzhen Yang, Oak Ridge National Laboratory (ORNL)

Co-Chair: Hyewon Lee, National Renewable Energy Laboratory

Influence of Titania Structure and Particle Size on the Catalytic Activity of IrO_2-Based Catalysts in Methane Oxidation Reactions.

Helena Weaver[1] *and Li-Yin Hsiao*[2]
(1)Chemical Engineering, University of Florida, Gainesville, FL, (2)Department of Chemical Engineering, University of Florida, Gainesville, FL

The complete oxidation of methane was investigated over IrO_2 supported on TiO_2 nanoparticles with different structure (anatase, rutile and brookite) and particle sizes (5, 10 and 15 nm). The activity in this reaction is very sensitive to anatase particle size. The best performing catalyst was IrO_2 on 10-nm anatase TiO_2.

Efficient Pd Catalysts for Methane Combustion.

Yuanyuan Li[1]*, Weiwei Yang*[2]*, Haohong Song*[3]*, Felipe Polo-Garzon*[2]*, De-en Jiang*[3]*, and Zili Wu*[1]
(1)Chemical Sciences Division, Oak Ridge National Laboratory (ORNL), Oak Ridge, TN, (2)Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN, (3)Interdisciplinary Materials Science, Vanderbilt University, Nashville, TN

Efficiently removing/converting methane via methane combustion imposes challenges on catalyst design. By manipulating the local structure and atomic distance of isolated Pd atoms, herein we show that the intrinsic activity of Pd catalysts can be significantly improved for methane combustion.

Operando-FTIR Study of Methanol Partial Oxidation over MoO_3/TiO_2 catalysts.

Gabriel Galdames[1]*, Bastián Fuentes*[1]*, Daviel Gómez*[2]*, Patricia Concepción*[2]*, Romel Jiménez*[1]*, and Alejandro Karelovic*[1]
(1)Chemical Engineering, Universidad de Concepción, Concepción, Región del Biobío, Chile, (2)Instituto de Tecnología Química, Valencia, Spain

Operando-FTIR studies of methanol oxidation over MoO_3/TiO_2 catalysts reveal distinct pathways for methyl formate and dimethoxymethane formation. Formate species form methyl formate on low loading catalysts while on higher loadings it is formed by two parallel pathways. A redox, acid, and interfacial three-site mechanism explains the observed activity and selectivity.

Manganese Cobalt Oxide Catalysts for the Preferential Oxidation of Carbon Monoxide Studied *in Situ*.

Thulani Nyathi[1], *Mohamed Fadlalla*[1], *Felix Herold*[2], *Samuel Regli*[2], *Magnus Rønning*[2], *and Michael Claeys*[1]
(1)Department of Chemical Engineering, Catalysis Institute, University of Cape Town, Cape Town, Western Cape, South Africa, (2)Chemical Engineering, Norwegian University of Science and Technology, Trondheim, Trøndelag, Norway

Our work demonstrates the improved chemical phase stability and CO oxidation activity of Co-based oxides achieved through Mn doping for the CO-PrOx reaction. We also show the positive impact of *in situ*/*operando* characterization in gaining deeper insights into the functions of working CO-PrOx catalysts, which aids in their further development.

C2+ - CATALYSIS OF C2+ CHEMISTRY

C2+ | C2+ HYDROCARBONS/OXYGENATES DEHYDROGENATION, OXIDATION, AND C-C COUPLING

Friday, June 13, 2025 10:50 AM - 12:10 PM
Hanover Hall CDE

Chair: Meijun Li, ORNL

Co-Chair: Michael Cordon, Oak Ridge National Laboratory

Revealing the Unique Reactive Properties of Chemically-Treated Oxide Surfaces for Heterolytic C-H Activation Routes in Catalysis.

Nicholas Jaegers[1], *Mikalai Artsiusheuski*[1], *Vardan Danghyan*[1], *Junnan Shangguan*[1], *Prashant Deshlahra*[2], *Carlos Lizandara-Pueyo*[3], *and Enrique Iglesia*[1,4]
(1)University of California at Berkeley, Berkeley, CA, (2)Department of Chemical and Biological Engineering, Tufts University, Medford, MA, (3)BASF SE, Ludwigshafen, Germany, (4)Chemical Engineering, Purdue University, West Lafayette, IN

Lewis acid-base (LAB) pairs at ZrO_2 surfaces activate C–H bonds via heterolytic mechanisms during alkane dehydrogenation. Chemical treatments expose these sites through dehydroxylation without catalyst sintering, enabling high hydrocarbon dehydrogenation and hydrogenation rates (thermodynamically linked). DFT and kinetic studies confirm reaction pathways and active site identity on earth-abundant oxides .

Mechanistic Details of Multifunctional Propane Conversion to Acrylic Acid on M1 Phase Oxides.

Prashant Deshlahra[1]*, Adam Twombly*[1]*, and Yilang Liu*[2]
(1)Department of Chemical and Biological Engineering, Tufts University, Medford, MA, (2)Chemical Engineering, University of Massachusetts Lowell, Lowell, MA

Redox-active metal oxides often contain acid-base properties but their mechanistic role beyond the methanol probe reaction is often unclear. This work analyzes reactivity for multiple reactions and combines experiment and DFT to understand the importance of acid-redox bifunctionality and provides guidance for improving selectivity in propane to acrylic acid conversion.

Essential Role of Isolated Ce Species and OH Groups in Dealuminated BEA Zeolite for C-C Coupling and Deoxygenation Reactions.

Karen Vannessa Caballero[1]*, Wenda Hu*[2]*, Hao Xu*[3]*, Konstantin Khivantsev*[4]*, and Yong Wang*[5]
(1)Voiland School of Chemical Engineering and Bioengineering, Washington State University, Pullman, WA, (2)Pacific Northwest National Laboratory, Richland, WA, (3)Chemical and Bio Engineering, Washington State University, Pullman, WA, (4)Physical and Computational Sciences Directorate and Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA, (5)Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA

The catalytic performance of isolated Ce species in dealuminated-BEA zeolite catalyzes the selective C-C coupling and deoxygenation reactions in the acetone-to-isobutene formation, reaching 100% theoretical selectivity. This work established the cooperative role of Ce species and OH group in the activation of acetone molecules and stabilization of the C-C coupling.

First Principles Study of Low Temperature Electrocatalytic Propane Activation on Platinum.

Durvesh Eknath Parab[1]*, Ashutosh Bhadouria*[1]*, Joseph Heil*[1]*, Viswanath Pasumarthi*[1]*, Brian M. Tackett*[1]*, and Jeffrey Greeley*[2]
(1)Charles D. Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN, (2)Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN

We investigate electrocatalytic propane activation on a Pt surface through computational methods. Our findings show that hydrogen competes with propane adsorption and weakens its binding. Additionally, we predict that deeply dehydrogenated products are likely to form on the Pt catalyst, highlighting the potential of our study for selective propane dehydrogenation.

CO2 - CO2 CAPTURE AND UPGRADING

CO2 - CO_2 CONVERSION OVER CARBIDE CATALYSTS

Friday, June 13, 2025 10:50 AM - 12:10 PM
Centennial Ballroom IV

Chair: Ashraf Abedin, NETL Support Contractor

Co-Chair: Brian M. Tackett, Purdue University

Is There a Maximum Achievable Conversion in Direct CO_2-Hydrogenation?.

*Nicholas Featherstone[1], Alisa Govender[2], and **Eric van Steen**[3]*
(1)Catalysis Institute, Department of Chemical Engineering, University of Cape Town (South Africa), Rondebosch (Cape Town), South Africa, (2)Energy Operations, R&T, SASOL, Sasolburg, Free State, South Africa, (3)Catalysis Institute, Dpt. Chemical Engineering, University of Cape Town, Cape Town, South Africa

The CO2-conversion in the CO2-hydrogenation to long chain hydrocarbons over an Fe-based catalyst was found to be independent of the space velocity, which was attributed to the oxidation of the catalytically active iron carbide to magnetite

Deciphering the Multiphase Challenge of Tungsten Carbide in the Catalytic Hydrogenation of CO_2.

***Sinhara Perera** and Marc Porosoff*
Department of Chemical Engineering, University of Rochester, Rochester, NY

This study addresses the polymorphic complexity of tungsten carbides (W_xC) by controlling carburization kinetics to selectively synthesize pure phases, enabling accurate evaluation of their CO_2 hydrogenation activity. Phase-pure W_2C and WC are synthesized, identifying W_2C as the catalytically active phase, offering sustainable alternatives to precious metal catalysts.

Evaluation of Mo_2C-Co Catalysts for Low-Temperature CO_2 Conversion Via Rwgs: Effect of K-Promotion and Co/Mo Ratio.

*Giovanni Ulloa[1], Alejandro Karelovic[2], Néstor Escalona[3], Ana B Dongil[4], and **Elodie Blanco**[3]*
(1)Pontificia universidad Católica de chile, santiago, Chile, (2)Chemical Engineering, Universidad de Concepción, (3)Pontificia Universidad Católica de Chile, Santiago, Chile, (4)ICP, Madrid, Spain

This study reports the catalytic performance of $CoMo_2C/H$ for CO_2 conversion into syngas (CO) at 250-350°C, highlighting the role of K and Co in the formation of active species (Mo_2C, Mo_3Co_3C). K promotes RWGS suppressing SR. A synergistic effect between Mo and Co could be observed.

Unsupported Mo_2c Catalysts for Low Temperature CO_2 Hydrogenation to Methanol.

***Elizabeth Bickel Rogers**[1], Frederick Baddour[2], Anh To[2], Daniel Ruddy[2], and Aditya Bhan[1]*
(1)Chemical Engineering and Materials Science, University of Minnesota Twin Cities, Minneapolis, MN, (2)Catalytic Carbon Transformation and Scale-Up Center, National Renewable Energy Laboratory, Golden, CO

Unsupported Mo_2C selectively catalyzes CO_2 hydrogenation to methanol at low temperatures (348–408 K), while also forming methane and CO. Kinetic studies and kinetic modeling indicate

that the Mo_2C surface is highly covered with CO- and CO_2-derived intermediates during catalysis, which favor the formation of methane and methanol, respectively.

ELECTRO PHOTO - ELECTROCATALYSIS AND PHOTOCATALYSIS

ELECTRO PHOTO - PHOTOCATALYTIC CO2 CONVERSION

Friday, June 13, 2025 10:50 AM - 12:10 PM

Centennial Ballroom I

Chair: Jason Adams, University of Illinois Urbana-Champaign

Co-Chair: Chang Liu, University at Buffalo, State University of New York

Investigations of the Surface Impact of MOF-Coatings on Mesoporous and Graphitic Carbon Nitrides in Liquid and Gas-Flow Photocatalytic Reduction of CO_2.

Patrick Nimax[1], *Sonia Zoltowska*[2], *Saloa Vaquero*[1], *Davide Ravelli*[3], *and Iker Aguirrezabal Telleria*[1]

(1)Department of Chemical and Environmental Engineering, Universidad del Pais Vasco, Bilbao, Spain, (2)Department of Colloid Chemistry, Max Planck Institute of Colloids and Interfaces, Potsdam, Germany, (3)Department of Chemistry, University of Pavia, Pavia, Italy

Mesoporous carbon nitride (CN) in heterojunctions with metal-organic frameworks (MOF) act as versatile photocatalysts, however suffer low crystallinity and reduced activity when CN, not MOF is used as template. Depositing MOF structures on CN in layers improves MOF crystallinity and application of MAS-NMR approaches allows highly sensitive identification of CN-MOF-interactions.

Solar-Driven Selective Conversion of Millimolar Dissolved Carbon to CO Under CO2(aq) Molecular Flux.

Xiang Shi[1] *and Shu Hu*[2]

(1)Chemical & Environmental Engineering, Yale University, New Haven, CT, (2)Department of Chemical and Environmental Engineering, Yale University, New Haven, CT

We demonstrate a transformative concept of molecular flux catalysis in which CO_2(aq) reactants in situ generated via HCO_3^- acidification continuously flow to the CO2R catalysts to enable the single-step solar conversion of the dissolved carbon in seawater to gaseous carbon products such as CO.

Tuning the Active Phase of a CO_2 Hydrogenation Co/TiO_2 Catalyst with Light.

D. Nicolette Maaskant[1], *P. Tim Prins*[2], *Bert M. Weckhuysen*[3], *and Matteo Monai*[4]

(1)Inorganic Chemistry and Catalysis group, Utrecht University, Utrecht, Utrecht, Netherlands, (2)Inorganic Chemistry and Catalysis group, Utrecht University, Utrecht, Netherlands, (3)Utrecht University, Utrecht, Netherlands, (4)Inorganic Chemistry and Catalysis, Institute for Sustainable and Circular Chemistry, Utrecht University, Utrecht, Netherlands

By elucidating what effects light has on reactions and catalyst materials, light can be used for (in situ) active phase tuning and optimizing performance, introducing a different approach to control the structure of catalysts under reaction conditions. We investigated the effect of light on CO_2 hydrogenation over a Co/TiO_2 catalyst.

Solar Driven CO_2 Reduction for Selective Methanol Production.

*Anthony Sanderse[1], Koen Vermeulen[1], Jelle Rohlfs[1], Nicole Meulendijks[1], Pascal Buskens Sr.[2], and **Francesc Sastre Sr.**[1]*
(1)Materials Solutions, TNO, Eindhoven, Brabant, Netherlands, (2)Materials, Institute for Materials Research, Design and Synthesis of Inorganic Materia, Hasselt, Brabant, Belgium

This study demonstrates CO_2 hydrogenation to methanol under solar light irradiation using $Cu/ZnO/Al_2O_3$ (CZA) catalysts. Leveraging plasmonic effects, it achieved stable methanol production over 95 hours at 40 bar and 13.8 suns, highlighting catalyst efficiency and stability.

ENVIRO AUTO - ENVIRONMENTAL AND AUTOMOTIVE CATALYSIS

ENVIRO AUTO - CATALYTIC OXIDATION OF TOLUENE AND CO

Friday, June 13, 2025 10:50 AM - 12:10 PM
Hanover Hall FG

Chair: Robin Hu, DCL Inc

Co-Chair: Silvia Marino, University of California, Santa Barbara

Modulation of Co Spin State at Co_3O_4 Crystalline-Amorphous Interfaces for CO Oxidation and N_2o Decomposition.

***Yunpeng Long**[1], Junhua Li[2], and Yue Peng[2]*
(1)Tsinghua University, Beijing, China, (2)State Key Joint Laboratory of Environment Simulation and Pollution Control, Tsinghua University, Beijing, China

Manipulation of spin polarization tune the interaction between d-orbital electrons and adsorbates through quantum spin exchange interactions. Herein, we reported a simple strategy to yield Co3O4 crystalline–amorphous interfaces. Not only new interfacial sites are introduced, but also the spin states are changed, significantly promoting CO and N2O purification.

Role of Hollow @SiO_2 and @TiO_2 Supports in Catalytic Activity of CuO and Co_3O_4 Phases in Total Oxidation of Toluene.

***Anna Rokicinska**, Magdalena Zurowska, Radosław Sadowski, Marek Debosz, and Piotr Kustrowski*
Faculty of Chemistry, Jagiellonian University, Krakow, Poland

The catalytic behavior of Co_3O_4 and CuO phases deposited on two different oxide supports, i.e. SiO_2 and TiO_2, in toluene combustion was studied. In order to determine the actual role of active

phase-support interactions in the VOCs conversion, specially designed hollow @SiO_2 and @TiO_2 supports with similar porosity were used.

Transforming Ceria into 2-Dimensional Clusters Enhances Catalytic Activity.

Konstantin Khivantsev[1]*, Hien N. Pham*[2]*, Mark Engelhard*[3]*, Iskra Z. Koleva*[4]*, Hristiyan A. Aleksandrov*[4]*, Yipeng Sun*[5]*, Jeffrey T. Miller*[6]*, Janos Szanyi*[3]*, Abhaya K. Datye*[7]*, and Yong Wang*[8]
(1)Physical and Computational Sciences Directorate and Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA, (2)Department of Chemical and Biological Engineering and Center for Micro-Engineered Materials, University of New Mexico, Albuquerque, NM, (3)Pacific Northwest National Laboratory, Richland, WA, (4)Faculty of Chemistry, University of Sofia, 1126 Sofia, Bulgaria, (5)BASF, Iselin, NJ, (6)Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN, (7)Department of Chemical & Biological Engineering and Center for Micro-Engineered Materials, University of New Mexico, Albuquerque, NM, (8)Washington State University, Pullman, WA

We describe a new catalytic architecture composed of ~1 monolayer-thin 2-dimensional ceria domains, that form upon treatment of supported ceria nanoparticles under harsh reactive (reducing) conditions, with superior catalytic properties.

Influence of the Impregnation Techniques on Assisted 3D-Printing CeO_x-MnO_x Monoliths Towards Toluene Oxidation.

Isidro Daniel de León Abarte *and Santiago Iván Suárez-Vázquez*
Facultad de Ingeniería Civil, Universidad Autónoma de Nuevo León, San Nicolás de los Garza, NL, Mexico

Catalytic oxidation mitigates VOCs like toluene, a severe health hazard. MnOX, especially Mn_3O_4, is a cost-effective catalyst. This study developed 3D-printed CeOX-MnOX monoliths, achieving superior toluene oxidation through innovative impregnation techniques, enhanced phase homogenization, oxygen vacancies, and efficient active sites, demonstrating improved catalytic performance for atmospheric emission reduction.

FUNDAMENTALS - FUNDAMENTALS OF CATALYSIS AND SURFACE SCIENCE

FUNDAMENTALS - METAL-SUPPORT INTERACTIONS & COMPUTATIONAL APPROACHES

Friday, June 13, 2025 10:50 AM - 12:10 PM
Centennial Ballroom II

Chair: William Broomhead, Georgia Institute of Technology

Co-Chair: Steven Chavez, University of California, Los Angeles

Effect of Metal Nuclearity on Bidirectional Metal-Support Interaction of Pt/CeO_2 and Catalytic Properties.

Md Raian Yousuf[1]*, Hung-Ling Yu*[1]*, Stephen Porter*[2]*, Matthew Bonney*[3]*, Sagar Sourav*[4]*, Eli Stavitski*[5]*, Adam Hoffman*[6]*, Simon Bare*[7]*, Dionisios Vlachos*[8]*, Michael White*[9]*, Abhaya K. Datye*[10]*, and Ayman M. Karim*[1]
(1)Department of Chemical Engineering, Virginia Polytechnic Institute and State University, Blacksburg, VA, (2)Department of Chemical and Biological Engineering and Center for Micro-Engineered Materials, University of New Mexico, Albuquerque, NM, (3)Stony Brook University, Stony Brook, NY, (4)Chemical and Biomolecular Engineering, University of Delaware, Newark, DE, (5)National Synchrotron Light Source II, Brookhaven National Laboratory, Upton, NY, (6)Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, Menlo Park, CA, (7)SUNCAT Center for Interface Science and Catalysis, SLAC National Accelerator Laboratory, Menlo Park, CA, (8)Delaware Energy Institute, University of Delaware, Newark, DE, (9)Brookhaven National Laboratory, Upton, NY, (10)Department of Chemical & Biological Engineering and Center for Micro-Engineered Materials, University of New Mexico, Albuquerque, NM

This study investigates the Pt size-dependent bidirectional electronic interaction between Pt and CeO_2 in Pt/CeO_2 catalysts. Utilizing *in situ* spectroscopy, we reveal how Pt size modulates CeO_2 reducibility and oxygen vacancy dynamics while the O_{vac} and OH^- concentration on CeO_2 impacts Pt electron density and H_2 activation.

Understanding and Harnessing Nanoscale Immiscibility in Ru-in Alloys for Selective CO2 Hydrogenation.

Chengshuang Zhou[1] *and Matteo Cargnello*[2]
(1)Molecular Foundry, Lawrence Berkeley National Lab, Berkeley, CA, (2)Chemical Engineering, Stanford University, Stanford, CA

Bimetallic alloys of immiscible elements behave differently at the nanoscale. In the Ru-In system, albeit immisciblity, In atoms decorate Ru nanoparticles' surfaces, forming superficial immiscible alloys. This enhances catalytic performance, enabling superior methanol production from CO_2 hydrogenation compared to individual elements and ordered intermetallic alloys, offering insights for catalyst design

Non-Mean Field Approaches for Surface Catalysis: Analytical Description of Kinetics from Adsorbate-Adsorbate Interactions.

Purva Paranjape *and Jeffrey Greeley*
Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN

This study develops an analytical microkinetic framework to incorporate adsorbate-adsorbate interactions on fcc(100) surfaces, extending traditional mean field models. By utilizing the Bethe-Peierls approximation, we derive activity coefficient correction factors for adsorption and reaction kinetics, providing insights into how spatial correlations impact reaction rates and activation barriers.

Unraveling Temperature-Dependent Free-Energy Landscapes and Surface Dynamics in Methane Activation on Ni(511) Via Machine Learning and Enhanced Sampling.

Yezhi Jin[1], *Yinan Xu*[1], *Jireh García Sánchez*[1], *Gustavo Perez Lemus*[1], *Pablo Zubieta*[1], *Massimiliano Delferro*[2], *and Juan J. de Pablo*[1]
(1)Pritzker School of Molecular Engineering, University of Chicago, Chicago, IL, (2)Chemical Sciences and Engineering Division, Argonne National Laboratory, Lemont, IL

We combine a ML-based potential and enhanced sampling to reveal temperature-driven enthalpic and entropic contributions in methane activation on stepped Ni(511) surface. We show evolving active sites—initially step-edge atoms, later terrace sites—and the disappearance of key intermediates on free energy surfaces at higher temperatures due to entropic penalties.

HYDRO ECON - CATALYSIS FOR THE HYDROGEN ECONOMY

HYDRO ECON - ELECTROCATALYSIS 2

Friday, June 13, 2025 10:50 AM - 12:10 PM
Centennial Ballroom III

Chair: Ugochukwu Nwosu, Simon Fraser University

Co-Chair: Yizhen Chen, University of Virginia

The Leaching of Cobalt in Platinum-Cobalt Fuel Cell Catalysts Studied Using *in Situ* Magnetometry.

Omishka Ranganthan[1], *Michael Claeys*[1], *Andrew P.E. York*[2], *and Dominic de Oliveira*[1]
(1)Department of Chemical Engineering, Catalysis Institute, University of Cape Town, Cape Town, Western Cape, South Africa, (2)Technology Centre, Johnson Matthey, Sonning Common, United Kingdom

In this study, an *in situ* magnetometer is used to investigate Pt-Co alloy temperatures and the leaching of Co in Pt-Co fuel cell catalysts during catalyst ink preparation. Pt-Co alloys are only formed at higher synthesis temperatures. $PtCo_2$/C experiences the greatest extent of Co leaching and Pt_3Co/C is most stable.

Towards the Complete Mineralization of PFOA with a Pilot-Scale UV-Light, Boron-Nitride—Based Recirculating Reactor Unit.

Juan Donoso[1], *Kimberly N. Heck*[1], *Mohamed Ateia*[2], *and Michael Wong*[1]
(1)Department of Chemical and Biomolecular Engineering, Rice University, Houston, TX, (2)Chemical and Biomolecular Engineering, Rice University, Houston, TX

Heterogeneous photocatalysis shows promise for PFAS destruction but faces challenges like low material activity and byproduct formation. This study demonstrates >99% PFOA defluorination using boron nitride (BN) in a UV flow reactor, outperforming TiO_2. BN's resilience to tap water anions highlights its potential for practical PFAS remediation.

TiO_2 Nanorods Supported $NiFeO_x$ Nanoclusters for the Oxygen Evolution Reaction in Anion Exchange Membrane Electrolysis.

Yizhen Chen *and Sen Zhang*
Chemistry, University of Virginia, Charlottesville, VA

We report the synthesis and characterization of TiO_2 nanorods supported $NiFeO_x$ sub-nanometer clusters. Ni_3Fe_1/TiO_2 catalyst showed outstanding activity and durability in AEMEL testing demonstrating that our catalysts hold significant potential for real clean H_2 produced industrial applications.

Evaluating Molybdenum As a Co-Catalyst for TiO_2 in the Photocatalytic Hydrogen Generation.

Naomi Harrisankar d'Oliveira[1]*, Wijnand Marquart*[1]*, Nico Fischer*[1,2]*, and Eric van Steen*[1,3]
(1)Department of Chemical Engineering, Catalysis Institute, University of Cape Town, Cape Town, Western Cape, South Africa, (2)University of Cape Town, Cape Town, South Africa, (3)Catalysis Institute, Dpt. Chemical Engineering, University of Cape Town, Cape Town, South Africa

The photocatalytic production of hydrogen from water using triethanolamine as a sacrificial reagent was performed over molybdenum supported on the various titania structures and P25. Carburization of molybdenum results in a substantial increase in the activity, but carburization of molybdenum P25 led to rutilization, which reduces the photocatalytic hydrogen production.