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 Kim¹, Wenda Hu², Nicholas Jaegers³, 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 CH₃. 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 °C).

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

*Adli Peck*¹, Michael Claeys¹, Giovanni Hearne², Gustavo Pasquevich³, Deogratias Tumwijukye², and Christopher Mullins¹ (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* ⁵⁷Fe 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-Suarez² (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 Ramos¹, 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 Bare¹, Sarah Hesse¹, Adam Hoffman¹, Christopher J. Tassone¹, Kirsten Winther², Anastassia Alexandrova³, Matteo Cargnello⁴, Phillip Christopher⁵, Ashley Head⁶, Matthew Kanan⁷, Shyam Kattel⁸, Ambarish Kulkarni⁹, Robert Rallo¹⁰, Robert Rioux¹¹, and Judith Yang⁶ (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 Yang¹, Alfred Worrad¹, Salman A. Khan², and Dionisios Vlachos² (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/Al₂O₃-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 Moon¹, Jiwon Kim², Jinwoo Lee², and Jeong Woo Han¹ (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 Ru₁-ZrO₂ 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 ZrO₂. The liquid (C₅-C₂₀) comprises \sim 70% jet-fuel-ranged branched hydrocarbons (C₈-C₁₆), while the gas product is liquefied-petroleum-gas (C₃-C₆) without methane and ethane.

Valorization of Ethanol to Sustainable Aviation Fuels Via n-Butene-Rich Intermediate over Cu-MO_x/SiO₂ Catalysts.

*Martin Affandy*¹, Robert A. Dagle¹, Libor Kovarik², Yong Wang³, and Vanessa Lebarbier Dagle²

(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.

Catalytic Conversion of Captured Monoterpenes to Sustainable Aviation Fuel.

Ajibola Lawal¹, Andrew D. Sutton², and Kim Tutin³ (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.

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

*Chigozie Ezeorah*¹, Aaron Vannucci¹, and John Regalbuto² (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/SiO₂ catalyst of different sizes revealed visible size effects.

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

*Mike Griffin*¹, Steven Rowland¹, Kristiina Iisa¹, Abhijit Dutta¹, Xiaolin Chen¹, Cody Wrasman¹, Calvin Mukarakate¹, Matthew Yung¹, Mark Nimlos¹, Luke Tuxworth², Xavier Baucherel², and Susan Habas¹ (1)National Renewable Energy Laboratory, Golden, CO, (2)Johnson Matthey, Newcastle, United

(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 Sanyal¹, Laura C. Meyer¹, Yang He², Mond F. Guo¹, and Karthikeyan Ramasamy³

(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 Gu², Morgan Hahnert¹, James Lin², Daniel Slanac¹, and Shunzu Wang² (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 2^{nd} 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 ZrO₂ Sequential Addition on Red Mud-Based Catalysts for CO₂ Hydrogenation.

Mahbuba Aktary¹, 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 (KNO₃) and ZrO₂ in a different order on the conversion of CO₂ and the product's selectivity.

Hydrotreatment of Waste Vegetable Oil for Advanced Biofuels Production.

Paula Marmol¹, Patricia Reñones¹, Silvia Morales de la Rosa², 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 Haidar¹, Md Raian Yousuf¹, Hung-Ling Yu¹, Stephen Porter², Sagar Sourav³, Eli Stavitski⁴, Dionisios Vlachos⁵, Abhaya Datye², and Ayman M. Karim¹

(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 CeO₂, 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 Hwang¹, Andrey Karpov², Carlos Lizandara-Pueyo², 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 Winther¹, **Ruchika Mahajan**², and Michal Bajdich³ (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 Lee³, Juan A. Lopez-Ruiz^{3,4}, and Elizabeth Biddinger¹

(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. Adams¹, Minju Chung², Justin Bui³, Yuriy Roman², and Karthish Manthiram⁴ (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 cm²) 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 Medlin², 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, H₂ 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 H₂ formation rates than Cu at only slightly higher overpotential.

Enhancement of Steam-Methane Reforming By Joule Heating of Ni/ZrO₂-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/ZrO₂ wire coil exhibits enhanced performance over conventional heating and over Joule heating of a similarly-shaped wire coated with Ni/Al₂O₃. This enhancement stems from electrical conductivity differences of the supports, with ZrO₂ being more conductive than Al₂O₃.

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 Harraz¹, Kunal Lodaya¹, Cole Cadaram¹, Bryan Tang², and Yogesh Surendranath¹ (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 Razdan¹, 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 Cardwell¹, Sten Lambeets², Isaac Onyango¹, Mark G. Wirth², Eric Vo², Yong Wang², Pierre Gaspard³, Cornelius F. Ivory¹, Daniel Perea², Thierry Visart De Bocarmé³, 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. Albrecht², Joshua M. Terrian², and David W. Flaherty³ (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 Ti₂c 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 Tengco¹, Haiying Zhou¹, Wen Xiong¹, Benjamin Egelske¹, Akkarat Wongkaew², John Regalbuto¹, and John Monnier¹ (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 SO₃ decomposition.

Learnings about Supported Metal Catalysts.

*Stuart Soled*¹, *Chris Kliewer*², and Michael Lanci³ (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 multiwall 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 V

Chair: Eswar Iyyamperumal, Ketjen Corporation

Co-Chair: Jennifer Lee, Harvard University

Hydrothermally Stable Single Atom Cu on CeO2 for Ethanol Upgrading.

Jesse Larence¹, Abhaya Datye², Hien N. Pham², Andrew T. DeLaRiva², Ryan Alcala³, Vanessa Lebarbier Dagle⁴, Huamin Wang⁵, Benjamin Moskowitz⁴, Martin Affandy⁵, Robert A. Dagle⁴, Ted Kim⁶, and Jeffrey T. Miller⁶

(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 H₂ 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 Saha¹, **Ruby Deeter**², Hani M El-kaderi², and Ayman M. Karim¹ (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 Shen¹, Ayman M. Karim², Dionisios Vlachos³, Raymond Gorte¹, 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 nm² 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 Novotny¹, Georgios Giannakakis¹, Yogita Soni¹, E Charles Sykes², and Prashant Deshlahra¹ (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/Al₂O₃.

Jason Malizia¹, Shengguang Wang¹, Stephen Kristy¹, Rong Xing², Mingyong Sun³, and Rebecca Fushimi¹ (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 Hemberger², and Andras Bodi²

(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 (CH₃) and short-lived oxygenates, in the oxidative dehydrogenation of propane, CH₃Cl 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 Ferri¹, and Jeroen A. van Bokhoven² (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 CH₃OH/CD₃OD 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 Ferwerda¹, Valerie Briois², Sebastian Weber³, Michael Kraemer³, Nils Bottke³, Matteo Monai¹, and Bert M. Weckhuysen¹

(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 Suekuni¹ and Alan Allgeier²

(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 CO₂ 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 Lin¹, Nathaniel Blake¹, Xueqi Pang¹, Zhirui He¹, Reza Mirshekari², Oyinkansola Romiluyi², Yoon Jun Son², Suryansh Kabra¹, and Daniel Esposito¹ (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 CO₂ Reduction on a Copper-Gold Catalyst.

Seyed Parsa Amouzesh¹, Taha Baghban-Ronaghi¹, SeyedSepehr Mostafayi¹, Karen A. Castaneda², 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 CO₂RR 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 CO₂ Concentration.

Exploring Design Principles for Tandem Electrochemical CO2 Reduction.

Lun An¹, Wenyu Huang², and Long Qi³

(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 CO₂-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 CO₂ Electrocatalytic Reduction to C₂ Oxygenates.

Isaac Kojo Seim¹, Gbolade Kayode², Charles Dees³, Matthew Montemore², and Ming Yang¹ (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 CO₂ activation, C–C coupling, and ethanol formation.

High-Temperature CO₂ Electroreduction in Molten Salt Electrolyte for Pure Carbon-Negative Carbon Nanotubes.

Andrew Wong¹ and Yukun Hu²

(1)Materials Science and Engineering, National University of Singapore, Singapore, Singapore, (2)Chemical & Biomolecular Engineering, National University of Singapore, Singapore, ---None ---, Singapore

The electrochemical CO₂ 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 CO₂-derived carbon nanotubes, addressing bottlenecks to profitability and commercialization of carbon-negative electrochemical CO₂ 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 CO₂ capture and Conversion.

Eslam Hamed¹ and Sam Li²

(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% CO₂ conversion to bicarbonate via a biomimetic process. The high metal loading (18 wt%) enhances catalytic activity, enabling CO₂ sequestration and amino acid detection in supplements with remarkable sensitivity, showcasing Zn-SAN's potential in environmental and analytical applications.

Scale-up CO₂ Conversion Technology.

Hanif Choudhury¹, Mohamed Sufiyan Challiwala¹, and Nimir Elbashir² (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 Geci¹, Niall Gushue¹, Leah Batoosingh¹, Riley Day¹, Robert Meulenberg², Pascal Raybaud³, Andreas Kafizas⁴, Thomas Schwartz⁵, 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 Marino¹, Anika Jalil¹, Michael Gordon¹, and Phillip Christopher¹ (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 Kumar¹ and Ravi Teja Addanki Tirumala²

(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 Cu₂O-based catalysts for the reverse water-gas shift reaction (RWGSR), converting CO₂ into valuable CO with ~99% selectivity. Dynamic phase changes between Cu₂O and metallic Cu, confirmed via spectroscopy and XRD, influence reaction rates. Visible light enhances performance, with Cu₂O outperforming Cu at lower temperatures.

Unravelling the Role of Visible Light in the Rwgs Reaction over Cu/Al₂O₃: Not All That Shines Is Good.

Kristijan Lorber¹, Iztok Arčon², Matej Huš³, Nataša Novak Tušar¹, 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/Al₂O₃ 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 H₂ Using Ni/Zn₃In₂S₆ Photocatalyst.

Denny Gunawan¹, Cui Ying Toe^{1,2}, Jason Scott¹, and Rose Amal¹ (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/Zn₃In₂S₆ photocatalyst and upscaled photoreactor achieving 1.08% solar-to-H₂ efficiency. Technoeconomic analysis highlights solar-to-H₂ efficiency and solar availability as key feasibility factors. Overall, the findings demonstrate the potential of solar-driven reforming to produce costeffective renewable H₂, 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 Policano¹, Jimmy A. Faria², and Leon Lefferts³ (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/CeO₂-r excels due to abundant oxygen vacancies enhancing redox activity, while Pd/CeO₂-c relies on exceptional stability. Elevated Pd²⁺ 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 Shi¹, Rana Muhammad Haris², Kenneth Rappe³, Michael Harold², and Yong Wang¹ (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/Al₂O₃ Catalyst.

Min Wang¹, **Haiying Chen**¹, Yuliana Lugo-Jose¹, Joseph M. Fedeyko², Todd Toops¹, and Jacqueline Fidler³ (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/Al₂O₃ 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 Al₂O₃ and ZrO₂.

Do Heui Kim¹ 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 H₂O 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-DeBusk¹, **Sreshtha Sinha Majumdar**², and Yensil Park¹ (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/Al₂O₃ and PtPd/Al₂O₃ 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 Palermo¹, Hai-Ying Chen², Phil Evans³, Joseph M. Fedeyko⁴, Jacqueline Fidler⁵, Patrick Flynn⁵, Kerr Gray³, Melissa A Hess⁴, Yuliana Lugo-Jose⁴, and Min Wang² (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 Ibrahim¹, Edgard Lebrón Rodríguez², Jerome Evans¹, Levi Callahan¹, Fabiola Y. Rodríguez-Rodríguez³, Christine Kortendick¹, Nelson Cardona-Martinez³, 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, 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 Khare¹, Yunxiang Sheng¹, 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 Akinsanya¹, Deep M. Patel², Christopher O'Connor³, Marta Perxés Perich⁴, Jessi E.S. van der Hoeven⁴, Christian Reece⁵, Luke T. Roling², and **Nathaniel Eagan¹** (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 LI¹, Mustafa Eid², Nilanjan Roy¹, Robert Rioux^{3,4}, and Michael Janik¹ (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 V

Chair: Tracy Lohr, Shell

Co-Chair: Paul Kim, Shell

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

Dean Miller¹, Matthew Liu¹, Uran Iwata², Neha Sharma¹, Wylie Kau³, Jinyu Guo¹, Samantha Bunke¹, 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 Liu¹, Rajat Daga¹, Yu Kawamata², Phil Baran², 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(sp³)-C(sp³)-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 Ihara¹, Tianwei Yan¹, Matthew Edgar¹, Siddarth Krishna², James A. Dumesic¹, and George W. Huber¹ (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 Quach¹, Mayank Tanwar², Zach A. Nguyen³, Dylan G. Boucher⁴, Kevin M. McFadden³, Shelley D. Minteer³, and Matthew Neurock²
(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. Chen¹ and Stacey I. Zones²

(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 Li¹, Abraham Martinez¹, Oleksandr Trybrat¹, Jinyi Han², Yi-sheng Chen³, C.Y. Chen³, Bi-Zeng Zhan³, Howard S. Lacheen³, Alexander Kuperman⁴, and Alexander Katz⁵ (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 cm³/g), and is an active acid catalyst for HD exchange and CI-test reactions.

Metal Organic Framework Derived Carbon Materials for CO2 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. Zones³, and Mark E. Davis¹ (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 Cui², Daniel Shantz², and Jean-Sabin McEwen³ (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 Bhowmick¹, Lu Liu², Chen Zhang², and **Dongxia Liu¹** (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 Koybasi¹, Dongxia Liu², and Dionisios Vlachos³ (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 Park¹, Marta Hatzell², Carsten Sievers³, and Andreas Bommarius³

(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 Wang¹ and Marc Pera-Titus²

(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 Khan¹, Zhihengyu Chen¹, Adam Hoffman¹, Sarah Hesse¹, Emily K. Schroeder², Phillip Christopher³, Christopher J. Tassone¹, and Simon Bare¹ (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 Chalmers¹, Adam Hoffman², Fernando Vila³, Simon Bare², and Susannah Scott¹ (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 Das¹, Vasyl Marchuk^{1,2}, Dmitry Doronkin^{1,3}, Dario Sanchez⁴, Jan-Dierk Grunwaldt^{1,3}, and Thomas Sheppard¹ (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-Al₂O₃ Supported Pd Nanoparticles Via in-Situ Pair Distribution Function Analyses..

Siddhant Singh¹, Graham King², and Robert W.J. Scott¹

(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 -Al₂O₃ 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 Yu¹, Md Raian Yousuf¹, Eli Stavitski², and Ayman M. Karim¹ (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 Hoffman¹, Florian Meirer², Nina Genz³, and Simon Bare¹

(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/SiO₂ 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 Zhang¹, **Stephen Purdy**², Meijun Li³, Nohor Samad⁴, James W. Harris⁴, Kinga A. Unocic⁵, Evan C. Wegener⁶, Shan Jiang⁷, Jeffrey T. Miller⁷, Felipe Polo-Garzon¹, Dongxia Liu⁸, Theodore Krause⁹, Zili Wu¹, Andrew D. Sutton², 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 Nejadmoghadam¹, Olov Öhrman², Derek Creaser³, and Louise Olsson³ (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 Dorazio¹, James C. Fu², Reinhard Seiser³, and Jessica Olstad⁴
(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 coprocessing 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 biobased 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 Borate¹, Young Gul Hur¹, Meijun Li², Stephen Purdy³, Andrew D. Sutton³, and James W. Harris¹ (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 - CO2 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 CO₂ 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 CO₂ 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 CO₂ to C_{2+} Compounds.

Sankar Meenakshisundaram¹, Alberto Gonzalez-Fernandez¹, Matthew Lindley¹, Sarah Haigh², Chris Hardacre³, Shashikant Kadam⁴, James Paterson⁵, Stephen Poulston⁶, and Christopher Hawkins⁶

(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 CO₂ into C₂₊ 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 CO₂ into C₂₊ 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 Zhou¹, Wei Zhang², Thuy Le², Sungmin Kim¹, Huamin Wang¹, and Johannes Lercher¹ (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 CO₂ is discussed allowing to minimize methane formation.

Metal Oxide Mobility in Zeolite: Impact on Hydrocarbon Pools and Its Inhibition Via Silicalite-1 Coating during CO₂ Hydrogenation.

*Fatima Mahnaz*¹, C D Balaji², Jasan Robey Mangalindan¹, Jenna Vito¹, Jithin John Varghese³, and Manish Shetty¹

(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 CO₂-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/CO₂ 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 CO₂ Hydrogenation to Olefins over Znzrox-Aei Tandems.

*Ahmed Sajid*¹, Julien Devos², Ibrahim Khalil¹, and Michiel Dusselier¹ (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 CO₂ 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 Bender¹, Rohan Sanspeur², Nicolas Bueno Ponce³, Angel Valles¹, Alyssa Uvodich¹, Delia Milliron⁴, John Kitchin², and Joaquin Resasco¹ (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 Matalkeh¹, Jin LI¹, Andrew Wong¹, Bryan Vogt², Michael Janik², and **Ezra L. Clark¹** (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 O₂ 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 Chen¹, Xiao Zhao², Yizhi Zhang³, Peifen Lyu⁴, Bo Yang³, Hao Chen⁵, Marina Leite⁴, Haiyan Wang³, Miquel Salmeron², 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/TiO₂ Catalysts Under Reverse Water Gas Shift Conditions That Dictate Stability.

Seunghwa Hong¹, Emily K. Schroeder¹, Selin Bac², Xiaobo Chen³, Adam Hoffman⁴, Jake A. Heinlein⁵, Ashley Head³, Simon Bare⁴, Matteo Cargnello⁶, and Phillip Christopher² (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, (6)Chemical Engineering, Stanford University, Stanford, CA, (7)Chemical Engineering, Stanford

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 Ahsan¹, Matthew Edgar¹, Jingrui Wei², Sirinada Chantachaiwat¹, Paul Voyles², and Siddarth Krishna¹ (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 Berry¹, Michael Gordon¹, and Phillip Christopher¹ (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 Nwosu¹ and Samira Siahrostami²

(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-Al₂O₃ Catalysts for Propane Dehydrogenation.

*Melis Yarar*¹, Zixuan Chen¹, Paula Abdala¹, Christophe Copéret², Alexey Fedorov¹, and Christoph R. Müller¹ (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-Al₂O₃ 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 Ga³⁺ sites and increasing relative fraction of ^[5,6]Ga³⁺ 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 Misicko¹ 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 Mo₂TiC₂ 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 Qi¹, Wenda Hu^{1,2}, Chia-Yu Chang³, Jinshu Tian², Mingwu Tan⁴, Hao Xu¹, Zihao Zhang², Jian Zhi Hu^{1,2}, Bing Joe Hwang³, 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/CeO₂ 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 Zeng¹ and Yogesh Surendranath²

(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 H₂ 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 Shekhar¹ and K. K. Pant²

(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 Deo¹, Wenyu Sun¹, Tanusree Chatterjee¹, Victoria Ehlinger², Thomas Moore³, Mengyao Yuan², Giovanna Bucci², Matthew Mcnenly², and Sneha Akhade¹ (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 protectedbut-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 \sim 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 Tengco², John Monnier², John Regalbuto², Madan Bhasin³, and Hamid Reza Godini⁴ (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 V

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 Kelly¹, Asmaul Hoque², Shannon S. Stahl³, and Marcel Schreier⁴ (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 Waters¹, Elnaz Jamalzade², Hussein T. Abdulrazzaq³, Nathaniel Kuch⁴, Sampath Gunukula¹, James A. Dumesic⁵, Philip Kersten⁴, and **Thomas Schwartz³** (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

Microkinetic Modelling of Ethylene Oligomerization on H-BEA Zeolites.

Sai Praneet Batchu¹, Boen Cao², Rajamani Gounder², and Linda Broadbelt¹ (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.

The Role of Zinc in Fe-Co-Zn Trimetallic Catalysts for CO₂ 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.

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

*Xin Deng*¹ and Weijie Li² (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.

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.

Synthesis and Application of Re or Ru-Doped Mg_xAlO_y–SiO₂ Catalysts for Ethanol Conversion to 1,3-Butadiene.

*Maynara Santos*¹, Fabio Toniolo², Michael Lanci³, Trong Pham⁴, Naveen Agrawal⁴, 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.

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.

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

Sophie Brauer¹, Paul J. Dauenhauer¹, and Christopher Nicholas²

(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.

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

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 Hauber¹ and Matthias Stehle² (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.

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

Ali Mohammed¹ and Omar Abdelrahman²

(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.

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

Hans-Joerg Woelk¹, Franziska Heck¹, and Ingo Graef²

(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.

Understanding CO₂ 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.

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

Nidhi Kushwaha¹, Arindam Modak², Ejaz Ahmad³, and K. K. Pant⁴ (1)Department of Chemical Engineering, Indian Institute of Technology Delhi, New Delhi, Delhi, India, (2)Institute of Applied Sciences, Amity University, Uttar Pradesh, India, (3)Department of Chemical Engineering, Indian Institute of Technology (ISM) Dhanbad, Dhanbad, India, (4)Chemical Engineering Department, Indian Institute of Technology Delhi, New Delhi, India

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.

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

Damilola Akinneye¹ and J. Will Medlin²

(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 SiO₂ led to improved activity.

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

Heloisa Bortolini¹, Rita M. B. Alves², Elisabete Assaf⁸, and Justin Notestein⁴
(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 LE¹, Manh Tung Nguyen¹, Emma Olsson Månsson¹, Hoang Phuoc Ho¹, Quoc Khanh Tran¹, Olov Öhrman², Derek Creaser¹, and Louise Olsson¹ (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 Mahajan¹, Kirsten Winther², and Michal Bajdich³

(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 Sackey¹, Michael Timko², Xinhua Liang³, and Jesse Bond¹ (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/SiO₂ 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 Al₂O₃-Nb₂O₅ for Simultaneous Hdo/HDS Co-Processing.

Luis Jorge Rodriguez Castillo^{1,2}, Franklin J. Méndez³, Jorge García-Macedo³, Lina A. Calzada⁴, Elim Albiter⁴, Jose Eduardo Hernandez¹, Felix Cancino¹, Juan A. Alcantara¹, Carlos Eduardo Santolalla-Vargas¹, and Victor Florencio Santes Hernandez¹ (1)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, (2)Energia, Unidad Profesional Interdisciplinaria en Ingeniería y Tecnologías Avanzadas UPIITA-IPN Avenida Instituto Politécnico Nacional No. 2580, Col. Barrio la Laguna Ticomán, Gustavo A. Madero, Ciudad de México, C.P. 07340., Mexico City, DF, Mexico, (3)Departamento de Estado Sólido, Instituto de Física, Departamento de Estado Sólido, Instituto de Física, Universidad Nacional Autónoma de México, Ciudad Universitaria 04510, Ciudad de México, México., Mexico City, DF, Mexico, (4)Catalisis y Materiales, Laboratorio de Catálisis y Materiales. Instituto Politécnico Nacional-ESIQIE. Zacatenco, C. P. 07738, Ciudad de México, México., Mexico, DF, Mexico NiW catalysts supported γ -Al₂O₃ mixed with Nb₂O₅ were investigated to examine the influence of Nb content in the simultaneous HDO/HDS co-processing. Supports and catalysts were studied through SEM-EDX, N₂ physisorption, powder XRD, UV-vis DRS, Raman spectroscopy, and H₂-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 Schwartz²

(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. Beas³, and Joshua Gorimbo⁴ (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 Cordon¹, Abishek Kasturi¹, Gyoung Gug Jang¹, Diana Stamberga², Jong K. Keum³, Dhruba Jyoti Deka⁴, Aye Meyer¹, Radu Custelcean², and Costas Tsouris¹

(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 aminebased 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 To¹, Daniel A. Ruddy¹, Eric Tan¹, Jonathan Martin², Wilson McNeary¹, Martha A. Arellano-Treviño¹, Chae Jeong-Potter¹, and Alexander J. Hill¹ (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 Flippo¹, 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 Boricha¹, Nitharshni R. G.¹, Marcello B. Solomon², Aravind Chandiran¹, Deanna D'Alessandro², 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 CO₂ 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 CO₂ 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 watergas shift reaction (RWGS-CL). Impregnation of Ni on doped CeO₂ improved H₂ 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 CO₂ 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 Davide¹, Jayalatha Robinson¹, Sanjaya D. Senanayake², and Cheng Zhang¹ (1)Long Island University Post, Brookville, NY, (2)Chemistry Division, Brookhaven National Laboratory, Upton, NY

This study tackles climate change by leveraging CO₂ as a resource. Using CeO₂-supported Fe-Co bimetallic catalysts with varying Fe/Co ratios, researchers achieved efficient CO₂ 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 CO₂ Hydrogenation and Reactive CO₂ 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 (CO₂ 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 CO₂ Hydrogenation By Combining Na-Promoted Fe₃O₄ and Pt/WO₃-ZrO₂ Catalysts.

Changhun Hur¹ and Kwangjin An²

(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 Fe₃O₄ and acidic Pt/WO₃-ZrO₂ (PtWZ) catalysts with dual-bed system in a single reactor enhanced the synthesis of isoparaffin-rich hydrocarbons in CO₂ 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°C to 600°C 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/CeO₂ Catalysts in CO₂ Hydrogenation.

*Maria Isabella Soares*¹, Ananda V. Paladino Lino², Jose Assaf³, Elisabete Assaf⁴, and Luiz Vieira⁵

(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/CeO₂ catalysts influences CO₂ 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 H₂ spillover and undesired CH₄ 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 CO₂ 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 CO₂ Conversion to Light Olefins.

*Jawad Mahmud*¹, Cheng Zhang², Jared Lugo², and Jayalatha Robinson² (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 CO₂ 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 Robinson¹, Tyler Davide¹, Sanjaya D. Senanayake², and Cheng Zhang¹ (1)Long Island University Post, Brookville, NY, (2)Chemistry Division, Brookhaven National Laboratory, Upton, NY

We aim to catalytically transform CO₂ 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 CO₂ conversion efficiency with excellent selectivity for light olefins.

Zeolite-Metal Nanoparticle Catalysts for Methane Partial Oxidation.

Hannah Even¹, Cole Hullfish², and Michele Sarazen²

(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 Mai¹, **Swarom Kanitkar¹**, **Evgeniy M. Myshakin²**, Xinwei Bai¹, Wissam A. Saidi³, Biswanath Dutta¹, and Daniel Haynes⁴

(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 Goyal¹, Horia Metiu², and Vishal Agarwal¹

(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 (BiCl₃) and metal (Bi) systems to investigate the catalytic activity of methane activation as it is envisaged that doping molten BiCl₃ 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 Wierzbicki¹, Davide Ferri², Anna Wach³, and Maarten Nachtegaal² (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 Wan¹ and Arun Majumdar²

(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 Jackson¹, Wei Zhang¹, Boda Yang¹, Mal Soon Lee¹, Sungmin Kim¹, Huamin Wang¹, Janos Szanyi¹, 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 AlCl₃-based chloroaluminate ionic liquids to catalyze the room-temperature upcycling of PVC waste into liquid iso-alkanes.

Improvement of Polyethylene Hydrogenolysis Performance on Ru/Al₂O₃ 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 Al₂O₃ (NA-Al₂O₃), Ru formed Ru–Al bonds, resulting in high dispersion and small size. The 1Ru/NA-Al₂O₃ catalyst achieved optimal Ru structure, showing the highest PE conversion rate and liquid/wax production.

Bimetallic Moru/TiO₂ 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 Fabris¹, Elio Sarotto², Tomás Cordero-Lanzac³, Izar Capel Berdiell¹, Sebastian Prodinger⁴, Andrea Jouve², Valentina Brunella², Silvia Bordiga², and Stian Svelle¹ (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 Bozkurt¹, Anna Brenner², Griffin Drake², Jorge Perez-Aguilar¹, Adam Hoffman¹, Yuriy

Roman², and Simon Bare¹

(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 Sun¹, Dionisios Vlachos², and Esun Selvam³

(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 Campos¹, **Luis F. Bordini**¹, Giullia Bertrand Marçano¹, Pedro Romano², and João Monnerat³

(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 Sousa², Nilson de Paula³, Pedro Romano⁴, Donato Aranda⁵, 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 de Janeiro, Rio de Janeiro, Brazil, (4)Campus D. de Caxias, Federal University of Rio de Janeiro, Rio de Janeiro, Brazil, (5)School of Chemistry, Federal University of Rio de Janeiro, Rio de Janeiro, Brazil, (6)Chemistry Institute, Federal University of Rio de Janeiro, Rio de Janeiro, Brazil

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.

*Van Son Nguyen*¹, Yuchen Chang¹, Erin V. Phillips², Jacob A. Dewitt¹, and Carsten Sievers³ (1)School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA, (2)Chemistry & Biochemistry, Georgia Institute of Technology, Atlanta, GA, (3)School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA

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).

Yuchen Chang¹, Aubrey Hepstall¹, Adrian H. Hergesell², Claire L. Seitzinger², Pawel Chmielniak¹, Ina Vollmer², and Carsten Sievers³ (1)School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA, (2)Utrecht University, Utrecht, Netherlands, (3)School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA

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.

Haoxiang Zhang¹, Jong In Choi¹, Saira Kanwal^{1,2}, and **Do-Young Hong**^{1,2} (1)Research Center for Nanocatalysts, Korea Research Institute of Chemical Technology (KRICT), Daejeon, Korea, Republic of (South), (2)Advanced Materials and Chemical Engineering, Korea National University of Science and Technology (UST), Daejeon, Korea, Republic of (South) PtSn/Al₂O₃ 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.

Napat Lertthanaphol¹, Jie Dong², Shashi Lalvani³, Scott Renneckar⁴, and Noppadon Sathitsuksanoh¹

(1)Conn Center for Renewable Energy Research, University of Louisville, Louisville, KY, (2)Southern Illinois University Edwardsville, Edwardsville, IL, (3)Maimi university, Oxford, OH, (4)University of British Columbia, Vancouver, Canada

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.

Kathryn Fasold and Gina Noh

Chemical Engineering, Pennsylvania State University, University Park, PA

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 Wu¹, Rahul Prasad Bangalore Ashok², Matthew Webber¹, **Xiao Wang**¹, Anna Brenner¹, Griffin Drake¹, Joel Miscall³, Clarissa L. Lincoln³, Shannon S. Stahl⁴, Jason DesVeaux², Taylor Uekert⁵, Elisabeth Van Roijen⁵, Yang Shao-Horn⁶, Gregg T. Beckham³, and Yuriy Roman¹ (1)Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, MA, (2)Catalytic Carbon Transformation and Scale-Up Center, National Renewable Energy Laboratory, Golden, CO, (3)Renewable Resources and Enabling Sciences Center, National Renewable Energy Laboratory, Golden, CO, (4)Department of Chemistry, University of Wisconsin-Madison, Madison, WI, (5)Strategic Energy Analysis Center, National Renewable Energy Laboratory, Golden, CO, (6)Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, MA

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 Zhu¹, Justin T. Douglas², and Bala Subramaniam³ (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 Bathena¹, Byun Mi Yeon², Alia Cooper², Uriah Kilgore², S Thomas Autrey², and Mark Bowden³ (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 Ukuku¹ and Craig Plaisance² (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 Kim¹, Eun-Su Yoon¹, Jae-Hak Lim¹, Chae-Min Yoon¹, Kyung-Won Jeon², Won-Jun Jang³, Jung Sang Cho⁴, and Jae-Oh Shim¹ (1)Wonkwang University, Iksan-si, Korea, Republic of (South), (2)Kunsan National University, Gunsan-si, Korea, Republic of (South), (3)Ajou University, Suwon-si, Korea, Republic of (South), (4)Chungbuk National University, Cheongju, Korea, Republic of (South)

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 CeO₂ supports, while acidity is key for Al₂O₃ 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/Al₂O₃ yolk-shell catalysts, prepared via spray pyrolysis, showed excellent stability and activity in SRM under alkali poisoning. Ni/pys-Al₂O₃ outperformed others with high CH₄ 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 Vennala¹, Snehal Patil¹, James N. Gyamfi¹, Seval Gunduz¹, Anne Co², and Umit Ozkan¹

(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 NaBH₄ 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 Kumar¹, Bar Mosevitzky Lis², Musa Najimu³, Yoon Jin Cho⁴, Kandis Leslie Gilliard-Abdulaziz³, Eranda Nikolla⁵, and Israel Wachs⁶

(1)Chemical and Biomolecular Engineering, Lehigh University, Bethlehem, PA, (2)Department of chemical and biomolecular engineering, Lehigh University, Bethlehem, PA, (3)Sonny Astani Civil and Environmental Engineering Department, University of Southern California, Los Angeles, CA, (4)Chemical Engineering, University of Michigan, Ann Arbor, MI, (5)Department of Chemical Engineering, University of Michigan, Ann Arbor, MI, (6)Department of Chemical and Biomolecular Engineering, Lehigh University, Bethlehem, PA

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 Kim¹, James Spragg², Isaac Daniel², Graham J. Hutchings², Samuel Pattisson², and Steven McIntosh¹ (1)Department of Chemical and Biomolecular Engineering, Lehigh University, Bethlehem, PA, (2)School of Chemistry, Cardiff University, Cardiff, United Kingdom 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.

Hoseong Yang¹, Song Gyun Kim¹, Yong Won Kim¹, and **Chanho Pak²** (1)Graduate School of Energy Convergence, Gwangju Institute of Science and Technology, Gwangju, Korea, Republic of (South), (2)Graduate School of Energy Convergence, Institute of Integrated Technology, Gwangju Institute of Science and Technology, Gwangju, Korea, Republic of (South)

Ir/WO₃ catalysts were developed to enhance HOR and OER activities for URFCs. WO₃ 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.

Umar Jafar¹, Mustapha Umar², Yahaya Gambo³, Khalid Alhooshani⁴, and Yousef A. Alsunni¹ (1)Chemical Engineering, King Fahd University of Petroleum and Minerals, Dhahran, Dammam, Saudi Arabia, (2)Chemical Sciences, North Eastern University, Gombe, Gombe, Nigeria, (3)Interdisciplinary Research Center for Refining and Advanced Chemicals, King Fahd University of Petroleum and Minerals, Dhahran, Dammam, Saudi Arabia, (4)Chemistry, King Fahd University of Petroleum and Minerals, Dhahran, Dammam, Saudi Arabia

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 TiO₂ 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. TiO₂ 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 Fe³⁺ and Ti⁴⁺ 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 -TiO₂ catalysts were synthesized through a solid-state reaction of ilmenite combined with TiO₂ 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. TiO₂-coated CdS particulate panels, decorated with Ni nanoparticle cocatalysts, were used for the photocatalytic conversion of benzyl alcohol to benzaldehyde and H₂.

Understanding Strong Metal Support Interactions for Electrocatalysis.

Akshat Singh¹, Delia Milliron², and Joaquin Resasco¹

(1)McKetta Department of Chemical Engineering, The University of Texas at Austin, Austin, TX, (2)Chemical Engineering, The University of Texas at Austin, Austin, TX

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 Hurst⁶

(1)Catalytic Carbon Transformation and Scale-Up Center, National Renewable Energy Laboratory, Golden, CO, (2)Chemical Engineering, Columbia University, New York, NY,
(3)University of California Irvine, Irvine, CA, (4)Department of Physics and Astronomy, University of California-Irvine, Irvine, CA, (5)Department of Chemical Engineering, Columbia Electrochemical Energy Center, Lenfest Center for Sustainable Energy, Columbia University, New York, NY, (6)National Renewable Energy Laboratory, Golden, CO

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 CO₂ Reduction.

Jiwon Kim¹ and Joaquin Resasco²

(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 CO₂ activation and suppresses the hydrogen evolution reaction (HER), resulting in enhanced electrocatalytic activity and selectivity for CO₂-to-CO conversion.

Fe-Beta Zeolite for Simultaneous SCR of NOx and N₂0 with NH₃: 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 Febeta considering the Si/Al ratio, Fe sources, and loading method.

Impact of NO₂ on Sulfur Poisoning and Impact of Sulfur on NO₂ Reactions on Cu-SSZ-13 Catalysts.

Afrina Zaman Shoronika¹, Poonam Rani¹, Rohil Daya², and William Epling¹
(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 NO₂ affects sulfation, and that sulfation affects the formation of ammonium nitrate and copper nitrate. Controlling NO₂ exposure time helps manage sulfur species on the catalyst surface, with long NO₂ exposure time being detrimental to desulfation.

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

*Kanika Meena*¹, Rohil Daya², Christopher Paolucci¹, and William Epling¹ (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 Foulon¹, Erin Thomson², Ujjal Das¹, and Leo DeRita¹ (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 splitcycle 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 NH₃ Storage in SSZ-13.

Arig-Undram Zolboot¹, William Epling¹, Rohil Daya², Christopher Paolucci¹, and Asanka Wijerathne¹ (1)Chemical Engineering, University of Virginia, Charlottesville, VA, (2)Cummins Inc., Columbus, IN

The fundamental understanding of sulfation effects on Cu speciation and NH₃ 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 NH₃ desorption behaviors of sulfated and non-sulfated Cu dimers.

NO_x-Assisted Mercury Oxidation in the Selective Catalytic Reduction of NO By NH₃ over a V₂O₅-WO₃/TiO₂ 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 Rukh¹, **Karoline Menze**², Xunhua Mo², Austin Gallagher², and Mehdi Allahverdi² (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.

N₂o Formation during Selective Catalytic NO_x Reduction on Cu-Exchanged Zeolite Catalysts.

Dhruba Jyoti Deka¹, Garam Lee¹, Kenneth Rappe¹, Janos Szanyi¹, 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-programmeddesorption 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 CeO₂(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 Tang¹, Robson Schuarca², and Jesse Bond² (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/SiO₂ and Pt-Sn/SiO₂ Catalysts.

Mohammed Tahseen Islam¹, Yaqin Tang², Robson Schuarca³, and Jesse Bond³ (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 $Pt-Sn/SiO_2$ 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 CO₂ Hydrogenation Catalysts.

Cherie Hsu¹, Luca J. Weigel¹, Robin Gutounig¹, Shabaaz Abdullah², Rabia Ilica^{1,3}, Erisa Saraçi^{1,3}, Anna Zimina^{1,3}, Mohamed Fadlalla², Jan-Dierk Grunwaldt^{1,3}, Michael Claeys², 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 CO₂ hydrogenation condition to provide further insights

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

Huston Locht¹, David S. Potts², Zahra Rangoonwala¹, and David Flaherty^{1,2} (1)School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA, (2)Chemical and Biomolecular Engineering, University of Illinois Urbana-Champaign, Urbana, IL

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.

Shoutian Sun¹, Thomas Salas¹, Gengnan Li^{1,2}, Daniel Resasco¹, and Bin Wang¹ (1)School of Sustainable Chemical, Biological and Materials Engineering, University of Oklahoma, Norman, OK, (2)Center for Nanoscale Materials, Argonne National Laboratory, Lemont, IL

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 Verma¹, Silvia Marino², Asanka Wijerathne¹, Colby Whitcomb¹, William Epling¹, Robert Davis¹, and Christopher Paolucci¹ (1)Chemical Engineering, University of Virginia, Charlottesville, VA, (2)Department of Chemical Engineering, University of California, Santa Barbara, Santa Barbara, CA

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 CO₂ As a Promoter in H₂O₂ 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 CO₂ and adsorbate induced restructuring.

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

Richa Ghosh¹, Dingqi Nai², Andrew Medford¹, and David Flaherty¹ (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

We correlate transient OCP and *operando* Raman spectroscopy measurements after Au surface polarization to examine the creation of reactive oxygen species (O^*) by H₂O electrooxidation and their consumption at open circuit by reaction with CH₃OH. We hypothesize that OCP decay rates will reflect thermochemical reaction rates of CH₃OH with O*.

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

Alexander von Rueden¹, Julia de Barros Dias Moreira¹, Benjamin Jackson², Thuy Le¹, Udishnu Sanyal², Simuck Yuk³, Mal Soon Lee¹, and Johannes Lercher⁴ (1)Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA, (2)Pacific Northwest National Laboratory, Richland, WA, (3)Department of Chemistry & Life Science, United States Military Academy, West Point, NY, (4)Technical University of Munich, Garching b. München, Germany

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 NH₃ synthesis on Pd(111), kinetic analysis has revealed that 4% tensile strain can increase the turnover frequency by $\sim 10^{\times}$.

Mechanistic Studies of H₂ Reduction of Mononuclear Cu²⁺ Sites to Cu⁺ in Cu-Exchanged Chabazite Zeolites.

Angel Santiago-Colón¹, Jose Rebolledo-Oyarce², William Schneider³, and Rajamani Gounder⁴ (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/CeO₂ Single Atom Catalysts Alters the Reaction Mechanism of CO Oxidation.

Saba Rahman¹, Alireza Javanmard¹, Kayla Eudy¹, Michael Janik¹, 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/CeO₂ strengthens CO binding to Pd by inhibiting the formation of PdO₂. 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 Javanmard¹, Kayla Eudy¹, Michael Janik¹, 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/CeO₂ 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 Sarbacker², David W. Flaherty³, and Christopher Paolucci¹

(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 TiO₂ 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 TiO₂ 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-Gilbert¹ and Steven Tait²

(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 CeO₂ Aerogels for Degradation of Organophosphorus Chemical Warfare Simulants.

Travis Novak¹, Janna Domenico², Alex Balboa³, Wesley O. Gordon³, Austin Herzog⁴, Evan Glaser⁵, Paul A. DeSario⁶, and Debra Rolison¹

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CeO₂ and Gd-doped CeO₂ 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 C₆–C₁₂ Methylbenzenes in H-MFI Zeolite.

*Ayotunde Alabi*¹, *Reilly Afflerback*², *David Hibbitts*¹, and Hansel Montalvo-Castro² (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 NH₃-SCR.

Daniel Gilleland¹, Logan Spell¹, and Alessandro Turrina² (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 Spell¹, Alessandro Turrina², Ugursan Aydogan², Agnes Raj², and Alexander Green² (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 Gonzalez¹, Julia Aguilar Pliego², Misael Garcia Ruiz², Enrique Sastre de Andrés³, Marisol Grande Casas³, and Carlos Márquez Alvarez³ (1)Applied Chemistry, Universidad Autónoma Metropolitana, Mexico City, DF, Mexico, (2)C.B, UAM-Azcapotzalco, (3)Tamices Moleculares, Consejo Superior de Investigaciones Científicas, Instituto de Catálisis y Petroleoquímica, Madrid, Madrid, Spain

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 Shankar¹, Deepak Sonawat², Siddarth Krishna², and Christopher Paolucci¹ (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 CO₂ Hydrogenation.

*Fatima Mahnaz*¹, C D Balaji², Jasan Robey Mangalindan¹, Jenna Vito¹, Jithin John Varghese³, and Manish Shetty¹

(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 (In₂O₃, ZnZrOx, Cr₂O₃) 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 CO₂ hydrogenation.

Ni and Ru Metallic Nanoparticles Supported on Crystalline and Embryonic HZSM-5 for CO₂ Methanation.

Ana Simões¹, Robson De Souza Filho¹, Amanda Guimarães², Leandro V. Pontual³, Joyce R. Oliveira⁴, Larissa G. Souza⁴, Ludmila P. C. Silva⁵, Fabio B. Passos⁶, Maria H. Araujo¹, Sara S. Vieira⁴, and **Lisiane Veiga Mattos**³

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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 CH₄ 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 Sison¹, Keishana Navodye S. a.¹, Michael Quaynor¹, and Kasun Gunasooriya² (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 highthroughput 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 Marques⁶, Joris Thybaut⁷, and Pedro Mendes^{5,6}

(1)Machine Learning, Technische Universität Berlin, Berlin, Berlin, Germany, (2)Berlin Institute for the Foundations of Learning and Data (BIFOLD), Berlin, Germany, (3)BASLEARN – TU Berlin/BASF Joint Lab for Machine Learning, Berlin, Germany, (4)Chemical Engineering, KULeuven, Leuven, Belgium, (5)Laboratory for Chemical Technology, Ghent University, Ghent, Belgium, (6)Department of Chemical Engineering, Instituto Superior Técnico, Lisbon, Portugal, (7)Laboratory for Chemical Technology (LCT), Department of Materials, Textiles, and Chemical Engineering, Technologiepark 125, B-9052, Ghent University, Ghent, Belgium

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 Hong¹, Giovanni Pireddu², Wei Fan¹, Rocio Semino², and Scott M. Auerbach³ (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 Timmerman¹, Andrew Medford², and Phanish Suryanarayana³ (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 CO₂ and Water for Direct Air Capture Using ML Modelling.

Romalya Ranasinghe¹, Navya Tyagi², Sonika Tyagi², Paul Webley¹, and Akshat Tanksale¹ (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 CO₂ 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-CO₂ 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 Han¹ and **Seokhyun Choung**²

(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)

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/CeO₂ 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. Benites¹, Andressa Andrade Alves da Silva¹, **Héctor Napoleão Cozendey da Silva**^{2,3}, João Felipe Mitre¹, 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, R²: 0.80).

Catbench: Benchmark of Graph Neural Networks for Adsorption Energy Predictions in Heterogeneous Catalysis.

Jinuk Moon¹, Uchan Jeon², and Jeong Woo Han¹

(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 Kim¹, Dongjae Shin¹, and Jeong Woo Han²

(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 Cozzarolo¹, Federica Romanelli¹, Claudio Ferroni¹, Matteo Ambrosetti¹, Bruna Mello Gabbrielleschi², Mauro Bracconi¹, Alessandra Beretta¹, Gianpiero Groppi¹, Bryce Williams², and Enrico Tronconi¹

(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 Ferri², Alessandra Beretta¹, Gianpiero Groppi¹, and Enrico Tronconi¹ (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 Ko¹, Kian Kwa¹, Han Wang¹, Carlos L. Pueyo², Jianping Chen³, Roel Sanchez-Carrera⁴, and Erdem Sasmaz¹

(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 Lambert¹, Ankush Rout¹, Debalina Sengupta², Micah Green¹, Benjamin Wilhite³, and Mark Barteau¹ (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 Hatwar¹, Akshat Tanksale¹, and Hamza Asmat² (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 CO₂ 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 Tanksale²

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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 Yu¹, Letícia Rasteiro¹, Van Son Nguyen¹, Kinga Golabek¹, Carsten Sievers², and Andrew Medford¹

(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 MoO₃ 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 Zarth¹, **Li Li**², Antonio Marchi Netto², and Diogo Lima Marques da Silva¹ (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 CO₂ Hydrogenation Using the *in-Situ* mass Analyzer..

*Mei Ju Goemans*¹, Pio Gramazio¹, Björn Frederik Baumgarten¹, Rune Myrstad², Jia Yang³, and Edd Blekkan¹ (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 CO₂ 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 Abuothman¹, Atharva Burte², and Omar Abdelrahman² (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 Paykar¹, Simon Friedrich², John Regalbuto³, and Christopher Williams³ (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@GaOx Catalysts for Propane Dehydrogenation.

Yiyi Xu¹ and Andrew Beale² (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 Patil¹, Alejandra Torres Velasco², and Juan Bravo-Suarez³ (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 CO₂ Hydrogenation.

Jorge Moncada¹, Evan Jahrman², Eli Stavitski³, and Jose Rodriguez⁴ (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 Nguyen¹, Bar Mosevitzky Lis^{1,2}, Agustin De Arriba³, Jose Manuel Lopez-Nieto Sr.³, and Israel Wachs⁴

(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/Al₂O₃ Dehydrogenation Catalyst..

*Vladimir Fridman*¹, Renqin Zhang², and Rong Xing³ (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 Clarkson¹, Andrew Coe², James Paterson³, and Virginie Viseur² (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 (CANStm), 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 H₂ Pumping Enhances the Activity of Selective Semi-Hydrogenation Catalysts.

Michael Lemelin¹ and Ezra L. Clark²

(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 H₂ pumping since the overall rate of reaction is limited by H₂ activation in conventional thermal reactors.

Hierarchical Zeolite-Based Catalysts for Tandem One-Step Renewable Diesel Production Via Fischer-Tropsch Synthesis.

Binchao Zhao¹, Chunxiang Zhu^{1,2}, Fangyuan Liu³, 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 multilayer 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 Barber¹, Christopher Lieb¹, 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/Al₂O₃ As a Catalyst for Propane Dehydrogenation through Multiscale Characterization and Model Development.

Nicholas Thornburg¹, **Adam Yonge**², Meagan Crowley², Hariswaran Sitaraman², Dingqi Nai³, Jason Malizia⁴, Stephen Kristy⁴, Rong Xing⁵, Mingyong Sun⁶, Lars Grabow⁷, Rebecca Fushimi⁴, Andrew Medford³, and Peter Ciesielski²

(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 informaticsbased 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. Senftle¹, Ezra L. Clark², and Marc Porosoff³

(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 Gyamfi¹, Snehal Patil¹, Luke Gillespie¹, Chidimma Maryjane Nwankwaor¹, Anant Sohale¹, Seval Gunduz¹, Paul Edmiston², and Umit Ozkan¹ (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 solventdependent 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 Zheng¹, Bailey Holmes², Asuka Firdaus³, and Jingyue Liu¹ (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 Albrechtsen¹ and Alexander Bagger²

(1)DTU Physics, Technical University of Denmark, Kongens Lyngby, Denmark, (2)Chemistry, University of Copenhagen

Electrochemical CO₂ 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). CeO₂ 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 Kim¹, Seongmin Yuk¹, Jinseong Choi¹, Jaejun Ko¹, and Chang Hyuck Choi² (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 Yuk¹, Kyounghee Kim¹, Jinseong Choi¹, Jaejun Ko¹, and Chang Hyuck Choi² (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 realtime 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.