PLENARY LECTURES

2025 MICHEL BOUDART AWARD PLENARY LECTURE BY BERT WECKHUYSEN

Wednesday, June 11, 2025 8:00 AM - 9:00 AM
Centennial Ballroom

Chair: Carsten Sievers, Georgia Institute of Technology

Operando Spectroscopy of Heterogeneous Catalysts: Foundation, Developments & Applications.

Bert M. Weckhuysen
Utrecht University, Utrecht, Netherlands

Operando spectroscopy has turned into an important field of research. This methodology approaches industrial-like reaction environments and catalyst materials complexity. Further closing this "*operando* gap" results in more insights in reaction and deactivation mechanisms, providing practical leads to develop new catalyst formulations and monitor the "catalyst health" during real-life operation.

BIOMASS - BIOMASS AND WASTE VALORIZATION CATALYSIS

BIOMASS - LIGNIN

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

Chair: Ana Alba-Rubio, Clemson University **Co-Chair:** Huamin Wang, Pacific Northwest National Laboratory

KEYNOTE: Advancing the RCF Lignocellulose Biorefinery: From Molecular Insights to Practical Safer Applications.

Bert Sels
Center for Surface Science and Catalysis, KU Leuven, Leuven, Belgium

This presentation will offer a comprehensive exploration of the complexities of catalysis in biomass recycling, providing innovative solutions to current challenges and promoting the transition to a more sustainable, circular economy.

Selective Oxidation of Humins to Maleic Acid Using Transition-Metal-Substituted Keggin-Type Polyoxometalate Catalysts.

*Tobias Esser, André Wassenberg, Jan-Christian Raabe, **Dorothea Voß**, and Jakob Albert*
Hamburg University, Hamburg, Germany

In this study we could for the first time show the selective oxidation of humins to maleic acid using tailor-made POM catalysts to gain a deeper understanding of the structure-activity-selectivity relationships in the selective catalytic oxidation of furanic compounds.

Acid Pretreatment Effects on the Structure and Catalytic Depolymerization of Corn Cob Lignin.

Nakisha Mark[1], *Sandip Kumar Singh*[1], *Anoop Uchagawkar*[1], *Erik Hagberg*[2], *Thomas Binder*[3], *and Bala Subramaniam*[3,4]
(1)Center for Environmentally Beneficial Catalysis, University of Kansas, Lawrence, KS, (2)Archer Daniels Midland Company, Decatur, IL, (3)Center for Environmentally Beneficial Catalysis, The University of Kansas, Lawrence, KS, (4)Chemical & Petroleum Engineering, The University of Kansas, Lawrence, KS

Sulfuric acid as a catalyst in the acetosolv process eliminates β-O-4 linkages and introduces sulfur into the extracted lignin causing sulfur poisoning of Pd/C catalyst used in lignin catalytic fractionation. In contrast hydrochloric acid avoids these challenges and improve monomer yields. The findings provide guidance for effective lignin valorization strategies.

Tuning Performance of Ni–Mo Catalysts for the Hydrodeoxygenation of Lignin Oils to Fuels.

Tove Kristensen[1,2], *Sara Blomberg*[1], *Marcus Jawerth*[3], *Christian Dahlstrand*[3], *and Christian P. Hulteberg*[2,4]
(1)Department of Process and Life Science Engineering, Lund University, Lund, 221 00, Sweden, (2)Hulteberg Chemistry Engineering AB, Malmö, 212 25, Sweden, (3)Ren Fuel K2B AB, Uppsala, 754 50, Sweden, (4)Division of Chemical Engineering, Department of Process and Life Science Engineering, Lund University, Lund, Scania, Sweden

In this work, a beneficial tailoring approach of a La- and Ce-promoted NiMo/Al_2O_3 catalyst with enhanced potential for long-term activity in the industrial HDO of lignin oils to fuels is demonstrated. A high deoxygenation degree of a lignin oil feedstock is achieved and diffusion limitation and carbon polymerization are suppressed.

Synergistic Cu-ReO_x Catalysis for Hydrogen-Free Transfer Hydrogenation of Furfural: Pathway to Value-Added Chemicals and Fuels.

Debarun Banerjee[1,2,3], *Jack Clegg*[2], *and Sreedevi Upadhyayula*[3]
(1)UQ-IITD Research Academy (UQIDRA), Indian Institute of Technology Delhi, New Delhi, Delhi, India, (2)School of Chemistry and Molecular Biosciences, University of Queensland, Brisbane, QLD, Australia, (3)Chemical Engineering, Indian Institute of Technology Delhi, New Delhi, India

This study explores a hydrogen-free catalytic process for the selective transfer hydrogenation of furfural to value-added chemicals and fuels. The approach offers a tunable pathway for high-conversion, sustainable production of furfuryl alcohol and 2-methylfuran, providing insights into catalyst design and reaction mechanism for similar transformations.

C1 - CATALYSIS OF C1 CHEMISTRY

C1 - METHANOL CONVERSION

Wednesday, June 11, 2025 9:30 AM - 11:30 AM

Centennial Ballroom IV

Chair: Benjamin Moskowitz, Pacific Northwest National Laboratory

Co-Chair: Marc Porosoff, University of Rochester

True Activation Energies Relevant to Methanol-to-Olefins Chemistry.

Dipti Bhave[1]*, Oleksiy V. Shvets*[2]*, Mykhailo M. Kurmach*[2]*, Nataliya Shcherban*[3]*, and Friederike Jentoft*[1]
(1)Department of Chemical Engineering, University of Massachusetts Amherst, Amherst, MA, (2)L.V. Pisarzhevsky Institute of Physical Chemistry, National Academy of Sciences of Ukraine, Kyiv, Ukraine, (3)Department of porous substances and materials, L.V. Pisarzhevsky Institute of Physical Chemistry, National Academy of Sciences of Ukraine, Kyiv, Ukraine

The kinetics of surface reactions relevant to methanol-to-olefins conversion were monitored spectroscopically, and the activation energies for ring contraction of cycloalkenyl cations and for cyclization of alkadienyl cations were determined. The influence of zeolite framework topology, acid site density and isomorphous substitution by boron, gallium, and iron will be discussed.

On the Redox Mechanism of Methanol Carbonylation on the Dispersed ReO_x/SiO_2 Catalyst.

Neil Tran *and Alexander V. Mironenko*
Chemical and Biomolecular Engineering, University of Illinois Urbana-Champaign, Urbana, IL

This study investigates methanol carbonylation on ReO_x/SiO_2 catalyst using DFT, NBO analysis, and the energetic span model. We find that Re reduction is crucial for catalyst activation. C–C coupling is favorable in Re(III), but challenges arise with C–O scission, suggesting multinuclear sites enable the high catalytic activity.

Impact of Mesoporosity and Alkaline-Earth Metal Species in the Deactivation of Zeolite Y in the Methanol-to-Hydrocarbons Reaction.

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

This systematic study highlighted how the modification of the catalyst materials influences the MTH reaction, with a rationalization for different Si/Al: mesoporosity affected the kinetics of deactivation while alkaline-earth metal species suppressed the aromatic selectivity, thus extending the catalyst lifetime.

Brønsted Acid-Site Density Controls the Mechanistic Cycle and Product Selectivity in the Methanol-to-Hydrocarbons Reaction in BEA Zeolite.

Juan Carlos Navarro de Miguel Sr.
King Abdullah University of Science and Technology, Thuwal, Saudi Arabia

The methanol-to-hydrocarbons reaction on beta zeolite is controlled by Brønsted acid-site density. Low density favors the olefinic cycle, boosting propylene selectivity, while high density promotes the aromatic cycle, increasing ethylene and aromatics production. Operando UV-vis spectroscopy links monoenylic carbocations to the olefinic cycle and polyalkylated aromatics to the aromatic cycle.

Ceria Facet Effect on Microwave-Assisted Dry Reforming of Methane.

***Sinmyung Yoon**[1], Alfred Worrad[2], and Dionisios Vlachos[1]*
(1)Delaware Energy Institute, University of Delaware, Newark, DE, (2)University of Delaware, Newark, DE

This work presents a novel investigation of facet-engineered CeO_2 catalysts for MW-assisted DRM, establishing structure-performance relationships that provide new design principles for electrified catalysis.

Dynamic Active Sites on the Mo/HZSM-5 Catalyst for Methane Dehydro-Aromatization (MDA).

***Han Chau**[1], Md Sifat Hossain[2], Shengguang Wang[1], Debasish Sarkar[1], Debtanu Maiti[1], Sheima Khatib[2], and Rebecca Fushimi[1]*
(1)Catalysis and Transient Kinetics Group, Idaho National Laboratory, Idaho Falls, ID, (2)Chemical Engineering, Virginia Tech, Blacksburg, VA

The dynamic nature of active sites in Mo/HZSM-5 catalysts was elucidated by transient kinetic investigations in the Temporal Analysis of Products (TAP) reactor. This work sheds light on the genesis of molybdenum (oxy-) carbide active sites and catalyst deactivation upon exposure to methane under non-oxidative and oxidative methane dehydro-aromatization pathways.

C2+ - CATALYSIS OF C2+ CHEMISTRY

C2+ | C3+ OLEFINS C-C COUPLING, ISOMERIZATION, AND OXIDATION REACTIONS

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

Chair: Alan Allgeier, University of Kansas

Co-Chair: Weixin Huang, University of North Dakota

Bilayered Supported $MoO_x/AlO_x/SiO_2$ Catalyst for Olefin Metathesis.

Eli Ream[1], Joseph Thompson[1], Adhika Setiawan[1], Srinivas Rangarajan[2], and ***Israel Wachs**[1]*
(1)Department of Chemical and Biomolecular Engineering, Lehigh University, Bethlehem, PA,
(2)Chemical and Biomolecular Engineering, Lehigh University, Bethlehem, PA

Surface modification of SiO_2 with AlO_x was used to tune the molecular structure and activity of surface MoO_x for olefin metathesis. The isolated surface $(O=)_2Mo^{6+}$(-O-Al)(-O-Si) sites on bilayered supported $MoO_x/AlO_x/SiO_2$ allow a more energetically favorable mechanism, resulting in enhanced performance over MoO_x/SiO_2. This work provides new insights regarding support effects.

Deciphering the Active Sites of Tandem $\mathrm{M_1}@M_2O_x$ Catalysts for Selective Alkane Chemistry.

Snehitha Srirangam *and Siddharth Deshpande*
Department of Chemical Engineering, University of Rochester, Rochester, NY

We investigate Oxidative Propane Dehydrogenation (ODHP) on $\mathrm{M_1}@M_2O_x$ catalyst, In_2O_3-Pt/Al_2O_3, a highly stable catalyst[1], at an atomic level using a novel data-driven framework. We find Indium oxide to stabilize selective ODHP by blocking Pt(322) defect sites and preventing deep dehydrogenation.

[1] Yan., H. et al., *Science* 371, 1257–1260 (2021)

Carbonaceous Deposits As the Active Sites for Butene Isomerization.

Karoline L. Hebisch[1], Pawel Chmielniak[1], and **Carsten Sievers**[2]
(1)School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA, (2)School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA

This work elucidates the synergistic effects of carbonaceous deposits and solid acidity in confined spaces on the example of ferrierite-catalyzed skeletal butene isomerization. A combination of kinetic studies and spectroscopic analyses provides insights into the reaction location and active species, laying the foundation for prolonging catalyst lifetime.

The Role of Carbonates in the Selective Epoxidation of Propylene on Promoted Ag Catalysts.

***Joseph Esposito**[1]* *and Aditya Bhan[2]*
(1)Chemical Engineering and Material Science, University of Minnesota, Minneapolis, MN,
(2)Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN

Kinetic experiments in tandem with post-reaction surface characterization reveal three required promoters—solid K^+ and gaseous, co-fed CO_2 and trace NO—feature co-dependent promotional interactions. Alkali promotion is shown to stabilize surface carbonates, generated by co-fed CO_2, which deactivate the catalyst in the absence of NO and improve selectivity.

Spectroscopic Insights into the Effects of Pretreatment and K Promotion on Direct Propylene Epoxidation over Cu/SiO_2.

Hashim Alzahrani[1,2,3] *and* ***Juan Bravo-Suarez***[2]
(1)Center for Environmentally Beneficial Catalysis, The University of Kansas, Lawrence, KS, (2)Chemical & Petroleum Engineering, The University of Kansas, Lawrence, KS, (3)Chemical and Materials Engineering Department, King Abdulaziz University, Jeddah, Saudi Arabia

A systematic study investigated K promotion and gas pretreatment effects on propylene epoxidation over Cu/SiO_2. The results revealed a synergy between Cu oxidation states and K, suggesting K-modified Cu^{1+} as the selective site for propylene oxide formation, likely formed through K-Cu interactions when the catalyst starts in a reduced state.

Selective Propene Oxidation: A Transient Kinetic Investigation.

Debasish Sarkar[1], ***Debtanu Maiti***[1], *M. Ross Kunz*[1], *Kenneth Kusima*[2], *Lars Grabow*[3], *and Rebecca Fushimi*[1]
(1)Catalysis and Transient Kinetics Group, Idaho National Laboratory, Idaho Falls, ID, (2)William A. Brookshire Department of Chemical and Biomolecular Engineering, University of Houston, Houston, TX, (3)William A. Brookshire Department of Chemical and Biomolecular Engineering & Texas Center for Superconductivity (TcSUH), University of Houston, Houston, TX

This work delves into the intrinsic kinetics of selective oxidation of propene to acrolein on industrial bismuth molybdate catalysts. Effect of dynamic availability of oxygen sites on different redox states of the catalyst and at various reaction temperatures has been explored towards tuning the product selectivity.

ELECTRO PHOTO - ELECTROCATALYSIS AND PHOTOCATALYSIS

ELECTRO PHOTO - ELECTROCATALYSIS FOR CO2 CONVERSION 1

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

Chair: Astrid Müller, University of Rochester

Co-Chair: Nitish Govindarajan, Nanyang Technological University

Hydronium Ions Inhibit CO_2 Reduction on Coinage Metals.

Max Huelsey[1], *Bryan Tang*[2], *and Yogesh Surendranath*[3]
(1)Department of Chemistry, Technical University of Munich, Garching, Germany, (2)Chemistry and Chemical Biology, Harvard University, Cambridge, MA, (3)Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA

We uncover by transient electrochemical methods paired with electrochemical mass spectrometry the mechanistic basis of the lack of CO_2 reduction in acidic medium. Supporting electrolyte cations are required to increase the interfacial pH under electrolysis conditions allowing CO_2 reduction to occur.

Controlling Temperature to Engineer the Local pH of CO_2 Electrolyzers for Selective Multi-Carbon Products Synthesis.

Victor Brandão *and Carsten Sievers*
School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA

Surface enhanced Raman spectroscopy was coupled with product analysis to investigate how potential and temperature control local pH and the local concentrations of bicarbonate and carbonate for selective multi-carbon products formation under CO_2 reduction conditions.

Activation and Regeneration of an Indium-Bismuth Electrocatalyst for CO_2 Reduction Via Quasi Simultaneous *in Situ* XAS and XRD in a Gas Diffusion Electrode System.

Mariangela Biggiero[1]*, Hugo P. Iglesias van Montfort*[2]*, Vaishnavi Ganesh*[1]*, Jan den Hollander*[1]*, Joris Janssens*[1]*, Roos Grote*[1]*, Kirill A. Lomachenko*[3]*, Tom Burdyny*[2]*, Brian Rawls*[4]*, Florian Meirer*[1]*, Ward van der Stam*[1]*, Annelie Jongerius*[4]*, Bettina Baumgartner*[5]*, and Bert M. Weckhuysen*[1]
(1)Inorganic Chemistry and Catalysis, Institute for Sustainable and Circular Chemistry, Utrecht University, Utrecht, Netherlands, (2)Chemical Engineering, TU Delft, Delft, Netherlands, (3)European Synchrotron Radiation Facility, Grenoble, France, (4)Avantium, Amsterdam, Netherlands, (5)Van 't Hoff Institute for Molecular Sciences, University of Amsterdam, Amsterdam, Netherlands

Industrial implementation of an indium-bismuth catalyst for CO_2 electroreduction towards formate requires understanding of catalyst composition, activation and regeneration. To this end, we investigate catalyst oxidation state and crystalline structure in a Gas Diffusion Electrode cell during industrial-like conditions, combining quasi in simultaneous *in situ* X-ray Absorption Spectroscopy and Diffraction.

Analysis of the Role and Reactivity of Bicarbonate on Silver Gas Diffusion Electrodes for Electrochemical CO_2rr.

Claire Yin[1]*, Nirala Singh*[2]*, and Suljo Linic*[1]
(1)Chemical Engineering, University of Michigan, Ann Arbor, MI, (2)Department of Chemical Engineering, University of Michigan, Ann Arbor, MI

We present a combined experimental and modeling approach to explore the role of bicarbonate in CO2RR by quantifying its and water's contributions to the hydrogen evolution reaction (HER) on a silver electrocatalyst in a gas diffusion electrode flow cell.

How Interfacial Fields Influence Electrocatalytic Rates.

Joaquin Resasco
McKetta Department of Chemical Engineering, The University of Texas at Austin, Austin, TX

Electrocatalytic rates are strongly affected by the electrolyte in which the reaction is run. Here, we propose that the electric field present at the catalyst surface is sensitive to the identity of the cation in the electrolyte. This interfacial field alters the energetics of the reaction and consequently catalytic performance.

Carbon-Neutral Syngas Production Via Electrolysis: In-Situ/Operando Investigation of Cathode Behavior Under Reaction Conditions.

Seval Gunduz, *Dhruba Jyoti Deka, Jaesung Kim, Serra Yesilata, and Umit Ozkan*
William G. Lowrie Department of Chemical & Biomolecular Engineering, The Ohio State University, Columbus, OH

Our research targets acquiring a fundamental understanding of the structure-performance relationship within perovskite-type electrode materials for high-temperature co-electrolysis of CO_2 and H_2O. In-situ and operando characterization techniques showed migration of B-site atoms to the surface, leading to significant changes in the electrode activity, stability, and product composition.

FUNDAMENTALS - FUNDAMENTALS OF CATALYSIS AND SURFACE SCIENCE

FUNDAMENTALS - ZEOLITES AND ACID-BASE CATALYSIS 1

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

Chair: James W. Harris, The University of Alabama

Co-Chair: Siddarth Krishna, University of Wisconsin-Madison

Correlating Atomic-Scale Compositions, Structures, and Reaction Properties of Bifunctional Pt/H$^+$usy Zeolite Catalysts.

Anna Pischer[1], *Bradley F. Chmelka*[2], *Stacey Zones*[3], *and Michael Girgis*[4]
(1)Chemical Engineering, University of California, Santa Barbara, Santa Barbara, CA, (2)Department of Chemical Engineering, University of California Santa Barbara, Santa Barbara, CA, (3)Chevron Energy Technology Company, Richmond, CA, (4)Chevron Research, Richmond, CA

This study uses advanced solid-state 2D, ^{195}Pt, and *in situ* NMR methods to provide detailed new atomic-level insights on the impact of dealumination treatments on the locations and distributions of Al^{IV} sites within zeolite frameworks. These insights are correlated with their catalytic activities, offering insights to improve catalyst performance.

Impact of Polar and Non-Polar Interaction on Alcohol Adsorption in MFI Frameworks.

***Benjamin Jackson**[1], Mal Soon Lee[1], Ruixue Zhao[2], Sungmin Kim[1], Fuli Deng[2], Xiaomai Chen[2], Yue Liu[2,3], Roger Rousseau[1], and Johannes Lercher[1,2]*
(1)Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA, (2)Technical University of Munich, Garching b. München, Germany, (3)Shanghai Key Laboratory of Green Chemistry and Chemical Processes, School of Chemistry and Molecular Engineering, East China Normal University, Shanghai, China

Combined computational and experimental methods elucidate the role of hydrophobic zeolite pore wells and hydrophilic acid-base sites in the adsorption of C1–C4 alcohols on Si-MFI (without BAS) and H-MFI (with BAS) zeolites at the atomic scale which is crucial for design of catalysts with enhanced activity and selectivity.

Investigating Heterogeneity of Partial Confinement in External-Surface Pockets of SSZ-70 Zeolite Catalysts.

***Shankar Ramaswamy**[1], Stacey I. Zones[2], and Alexander Katz[2]*
(1)Department of Chemical and Biomolecular Engineering, University of California - Berkeley, Berkeley, CA, (2)Chemical and Biomolecular Engineering, University of California, Berkeley, Berkeley, CA

We investigate the effect of varying degrees of partial confinement within external-surface pockets of zeolite SSZ-70 on epoxidation catalysis. Our data demonstrate a lack of heterogeneity when only one silanol environment is possible, and a high degree of heterogeneity when silanols are localized at different depths within the pockets.

Quantifying the Kinetics of Framework Dealumination during Hydrothermal Aging of Proton-Form CHA Zeolites.

***Tania Class-Martinez**[1], Craig Waitt[2], Steven Yeo[2], Subramanian Prasad[3], Ahmad Moini[4], William Schneider[2], and Rajamani Gounder[1]*
(1)Charles D. Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN, (2)Chemical and Biomolecular Engineering, University of Notre Dame, Notre Dame, IN, (3)BASF Corporation, Iselin, NJ, (4)BASF Environmental Catalyst and Metal Solutions, Iselin, NJ

Dealumination kinetics measured during hydrothermal aging of proton-form chabazite (CHA) zeolites, with varying amounts of framework Al (Al_f) and 6-MR paired Al site arrangements, reveal that Al_f-O hydrolysis and extra-framework Al agglomeration are both kinetically relevant steps to extents that depend on hydrothermal aging conditions (e.g., temperature, H_2O pressure).

Deactivation, Site Requirements, and Product Inhibition over Au/TS-1 Bifunctional Propene Epoxidation Cascades.

***Ryoh-Suke Sekiya**[1], Enrique Iglesia[1,2], and Rajamani Gounder[1]*

(1)Charles D. Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN, (2)University of California, Berkeley, Berkeley, CA

Dioxygen activation rates and O-based propylene oxide (PO) selectivities are reported for bifunctional propene epoxidation cascades on Au/TS-1 to demonstrate the structural stability of encapsulated Au domains during catalysis, catalytic functions provided by TS-1 for parasitic side reactions, and promotional and inhibitory roles of water on Au.

Surface Tuning of Promoted MoO_x Catalysts for Selective Hydrodeoxygenation of Carboxylic Acids As Hydrogen Carriers.

***Thomas Salas**, Laura Alejandra Gomez Gomez, Daniel E. Resasco, and Steven P. Crossley*
School of Sustainable Chemical, Biological and Materials Engineering, University of Oklahoma, Norman, OK

Acetic acid/ethanol systems are candidate liquid organic hydrogen carriers but require kinetically controlled catalysis to achieve sufficient selectivity to the hydrogen carrier form. Promoted MoO_3 catalysts show enhanced activity with high selectivity for the selective hydrodeoxygenation of acetic acid. The catalyst can be optimized with pretreatment and kinetic analysis.

HYDRO ECON - CATALYSIS FOR THE HYDROGEN ECONOMY

HYDRO ECON - ELECTROCATALYSIS 1

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

Chair: Sen Zhang, University of Virginia

Co-Chair: Samira Siahrostami, Simon Fraser University - Burnaby Campus

Atomically Thin Layer of Iridium Oxide over Cobalt Oxide Nanocrystals for Water Electrolysis.

Gengnan Li
Center for Nanoscale Materials, Argonne National Laboratory, Lemont, IL

An atomically thin layer of iridium oxide has been uniformly dispersed onto cobalt oxide nanocrystals to improve the efficient use of iridium. The resulting iridium cobalt oxide outperforms the commercial iridium oxide for acidic oxygen evolution reaction.

Intrinsic Metal-Support Interactions Break the Activity-Stability Dilemma in Electrocatalysis.

***Lingxi Zhou** and Ruitao Lv*
Tsinghua University, Asian (Including Pacific Islander), Beijing, China

We report a steam-assisted synthesis armed with machine learning screening of an integrated ruthenium-titanium-manganese electrode, featuring intrinsic metal-support interactions. These atomic-scale interactions with self-healing capabilities radically address the activity-stability dilemma across all pH levels. This breakthrough highlights the potential of intrinsic metal-support interactions for enhancing electrocalysis in diverse applications.

Ionic Liquid-Based Electrocatalytic Systems for Sustainable Synthesis at Intermediate Temperatures.

Clare Yijia Xie[1], *Devan Solanki*[2], *and Zachary Schiffer*[1]
(1)School Of Engineering And Applied Sciences, Harvard University, Cambridge, MA,
(2)Harvard John A. Paulson School of Engineering and Applied Sciences, Harvard University, Cambridge, MA

This work advances intermediate-temperature electrochemistry by designing ionic liquid-based systems for sustainable synthesis at 100–250°C. Combining voltage with intermediate temperatures enables efficient electrocatalytic reactions that are challenging or impossible under ambient conditions. We use an ionic liquid electrolyte to explore fundamental thermodynamics and kinetics of benzaldehyde reduction, a prototypical hydrogenation.

Theory Guided Design of $MoO_3/NiMoO_4$ Heterostructures Hybridized Active Pt Co-Catalyst for Efficient Water Splitting.

Nikhil Komalla *and Nelson Dzade*
Energy and Mineral Engineering, The Pennsylvania State University, State College, PA

By combining novel synthesis with catalytic activity measurements, and advanced theoretical modelling, we present a cost-effective bifunctional Pt-$MoO_3/NiMoO_4$ electrocatalyst that shows excellent water-splitting efficiency comparable to current industrial-grade (noble metals) catalysts, with low overpotentials and robust durability, resulting from synergistically improved charge transfers.

KEYNOTE: Catalyst and Electrode Design for Durable Alkaline-Membrane Electrolysis.

Shannon Boettcher
and Energy Storage and Distributed Resources Division, Lawrence Berkeley National Laboratory, Berkeley, CA

Alkaline-exchange-membrane electrolyzers promise high performance for H_2 production with earth-abundant catalysts and low-cost materials but are unstable. In this talk I will present new strategies to understand and design electrode catalysts and ionomer-electrolyte interfaces demonstrating <10 μV/h degradation at >2 A·cm^{-2} and <2 V while operating in pure water.

LIQUID - CATALYSIS IN LIQUID, SUPERCRITICAL, AND MULTIPHASE SYSTEMS

LIQUID - SOLVENT EFFECTS AND MOLECULAR DYNAMICS

Wednesday, June 11, 2025 9:30 AM - 11:30 AM

Regency Ballroom VII

Chair: Jimmy A. Faria, University of Twente

Co-Chair: Graham Leverick, Tufts University

Functional Assessments of Solvent on Solid Brønsted Acid Catalyzed Unimolecular C–O Scission Catalysis.

__Junfeng Guo__ and Ya-Huei (Cathy) Chin
Department of Chemical Engineering and Applied Chemistry, University of Toronto, Toronto, ON, Canada

Correlative experiments across reactant-solvent and probe-solvent pairs show a probe molecule's excess adsorption free energy and its difference in charge distribution from the transition state captures the excess activation free energy during solid acid-catalyzed C-O scission, predicting solvent effect on rates and advancing understanding of acid catalysis at liquid-solid interfaces.

Impacts of pH and Surface Charge on Oxygen Reduction at Au(100)-Water Interfaces from Ab Initio Molecular Dynamics Simulations.

__Alexander von Rueden__[1], Mal Soon Lee[1], Vassiliki-Alexandra Glezakou[2], Roger Rousseau[3], and Manos Mavrikakis[4]
(1)Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA, (2)Physical and Computational Sciences Directorate and Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA, (3)ORNL, Oak Ridge, TN, (4)Department of Chemical and Biological Engineering, University of Wisconsin-Madison, Madison, WI

Our work uncovers the atomic-level participation of interfacial water and co-adsorbed OH groups in the oxygen reduction reaction on the Au(100) surface. This fundamental understanding is crucial for guiding the development of improved electrocatalysts.

Molecular Insights into the Effect of Silanol Nest Defects on Solvent Structure and Diffusion Around the Active Site in Sn-BEA..

__Woodrow Wilson__[1], John Lane[1], William Humphreys[1], Vivek Bharadwaj[2], and Neeraj Rai[1]
(1)Dave C. Swalm School of Chemical Engineering and Center for Advanced Vehicular Systems, Mississippi State University, Mississippi State, MS, (2)National Renewable Energy Laboratory, Golden, CO

Large scale reactive molecular dynamics simulations utilizing equivariant neural network interatomic potentials trained on density functional theory calculations show that multiple solvent molecules can adsorb to the active sites of Sn-BEA zeolite depending on solvent type, active site location, and presence of silanol nest defects.

Sub-Monolayer Sn Coverages on Pd Surface Promotes Catalytic Nitrate Reduction Reaction.

Janek Betting*, Leon Lefferts, and Jimmy A. Faria*
Catalytic Processes and Materials (CPM) - TNW Faculty, University of Twente, Enschede, Netherlands

In this study, the ideal composition of porous and practically non-porous SnPd catalysts prepared via in-situ controlled surface deposition are established experimentally and using DFT calculations in the context of mass transport effects in a multiphase reaction system for nitrate reduction reaction and the complexity of bimetallic catalysts.

Ammonia: A Vital Additive in the Epoxidation of Propylene over TS-1 Extrudates.

Matias Alvear[1]*, Tapio Salmi*[2]*, and Ive Hermans*[1]
(1)Department of Chemical & Biological Engineering, University of Wisconsin-Madison, Madison, WI, (2)Laboratory of Industrial Chemistry and Reaction Engineering (TKR), Åbo Akademi University, Turku, Finland

The present study aims to analyze the effect of this crucial additive on the epoxidation process. By utilizing extrudates, spectroscopy and a DFT study, it is possible to observe the challenges in achieving high selectivity with this shaped catalyst, while also allowing a clear understanding of the additive's significance.

Solvent-Manipulated C-O Elimination Reactivity of Alkanols in Beta-Type Zeolite Confinements.

Sungmin Kim[1]*, Feng Chen*[1]*, Benjamin Jackson*[2]*, Hui Shi*[3]*, Manish Shetty*[1,4]*, Mal Soon Lee*[1]*, Wenda Hu*[1,5]*, Jian Zhi Hu*[1]*, Donald M. Camaioni*[1]*, Oliver Gutiérrez-Tinoco*[1]*, and Johannes Lercher*[1,6]
(1)Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA, (2)Pacific Northwest National Laboratory, Richland, WA, (3)Technische Universität München, Muchen, Germany, (4)Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX, (5)Washington State University, Pullman, WA, (6)Department of Chemistry and Catalysis Research Center, Technische Universität München, Garching, Germany

We address how solvents, combined with the steric constraints of H-BEA micropore, influence the local organization of solvent and substrate molecules. The generalized model with the standard chemical potential at initial and transition states allows for the estimation and prediction of C-O elimination rates with different solvents.

SYNTHESIS - CATALYST SYNTHESIS AND MANUFACTURING

SYNTHESIS - MATERIAL ENGINEERING AND MANUFACTURE

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

Chair: Yeping Cai, Clariant Co.

Co-Chair: James Crawford, Montana State University

Precision Structure Engineering of High-Entropy Oxides Under Ambient Conditions.

Kevin Siniard[1]*, Zhenzhen Yang*[2]*, and Sheng Dai*[2]
(1)Chemistry, University of Tennessee, Knoxville, TN, (2)Chemical Sciences Division, Oak Ridge National Laboratory (ORNL), Oak Ridge, TN

High-entropy oxides (HEOs) are promising in catalysis for their stability and tunability but face challenges in synthesis under mild conditions. This study develops an ambient in situ lattice engineering approach to integrate HEOs into CeO_2, achieving high surface area, abundant defects, and superior catalytic performance compared to ex situ methods.

Lattice Oxygen Activation in High-Entropy Oxide Catalysts Via Li and Al Doping.

Hailing Yu[1] *and Sheng Dai*[2]
(1)University of Tennessee, Knoxville, Knoxville, TN, (2)Chemical Sciences Division, Oak Ridge National Laboratory (ORNL), Oak Ridge, TN

This study adopts a Li and Al oxide doping strategy to modify the surface structure of high-entropy oxide catalysts, significantly enhancing lattice oxygen activation. The optimized catalysts exhibit enhanced performance in oxidation reactions, showcasing a promising strategy for advancing heterogenous catalytic applications.

Multivariate Bayesian Optimization of Cobalt Oxide Nanoparticles for CO_2 Hydrogenation Catalysis.

Lanja R. Karadaghi[1]*, Emily M. Williamson*[1]*, Ahn T. To*[2]*, Allison P. Forsberg*[1]*, Kyle D. Crans*[1]*, Craig L. Perkins*[3]*, Steven C. Hayden*[3]*, Nicole J. LiBretto*[2]*, Frederick G. Baddour*[2]*, Daniel A. Ruddy*[2]*, Noah Malmstadt*[1]*,* ***Susan Habas***[2]*, and Richard L. Brutchey*[1]
(1)Department of Chemistry, University of Southern California, Los Angeles, CA, (2)Catalytic Carbon Transformation and Scale-Up Center, National Renewable Energy Laboratory, Golden, CO, (3)Materials Science Center, National Renewable Energy Laboratory, Golden, CO

We present a multivariate Bayesian optimization, coupled with a data-driven classifier, to map the synthetic design space for CoO nanoparticles and optimize them for catalytically relevant features. An optimized CoO/SiO_2 catalyst was evaluated for CO_2 hydrogenation and the high performance was attributed to particle stability and consistent H* surface coverage.

Impact of so_2 on Exsolution and Dissolution of Ni-Fe Nanoparticles from $LaFe_{0.9}Ni_{0.1}O_3$ Perovskite Oxide.

Musa Najimu[1]*, Sahanaz Parvin*[2]*, Courtney Brea*[3]*, Neelesh Kumar*[2]*, Yiqing Wu*[4]*, Zili Wu*[5]*, Jonas Baltrusaitis*[2]*, Israel Wachs*[6]*, and Kandis Leslie Gilliard-Abdulaziz*[1]

(1)Sonny Astani Civil and Environmental Engineering Department, University of Southern California, Los Angeles, CA, (2)Chemical and Biomolecular Engineering, Lehigh University, Bethlehem, PA, (3)Georgia Institute of Technology, Atlanta, GA, (4)Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN, (5)Chemical Sciences Division, Oak Ridge National Laboratory (ORNL), Oak Ridge, TN, (6)Department of Chemical and Biomolecular Engineering, Lehigh University, Bethlehem, PA

Our study shows that highly stable sulfate and sulfite species influence the number, density, and composition of exsolved NiFe nanoparticles. While NiFe catalysts enhance thermocatalytic water splitting activity, the formation of stable sulfur-adsorbed species adversely influences the surface exsolution nucleation pathway and catalyst performance.

Single-Step Syngas-to-Dimethyl Ether Synthesis on Nanoparticle-Derived Pdzn/ZnO/Mp-HZSM-5 and Pd/CeO_2/Al_2O_3 Catalysts.

Bing Wang[1], Zairan Yu[2], Shuang Chen[2], Nicola Da Roit[3], Michael Zimmermann[1], Yuemin Wang[2], and ***Silke Behrens****[1]*
(1)Institute of Catalysis Research and Technology (IKFT), Karlsruhe Institute of Technology (KIT), Eggenstein-Leopoldshafen, Germany, (2)Karlsruhe Institute of Technology, Institute of Functional Interfaces, Eggenstein-Leopoldshafen, Germany, (3)Karlsruhe Institute of Technology, Karlsruhe, Germany

The influence of the methanol and dehydration catalyst on the catalytic performance in the single-step syngas-to-dimethyl ether process is shown for different types of bifunctional model catalysts which were prepared using nanoparticle precursors. Material structure aspects are discussed.

Particle Flow, Mixing and Heat Transfer in Rotary Calcination and Drying: Effect of Wall Friction and Baffles.

William Borghard*[1], Carlin Leung[1], Marcella Raymundo Alves[1], Alberto Cuitino[2], Nina C. Shapley[1], and Benjamin Glasser[1]*
(1)Chemical and Biochemical Engineering, Rutgers University, Piscataway, NJ, (2)Mechanical and Aerospace Engineering, Rutgers, the State University of New Jersey, Piscataway, NJ

In catalyst manufacturing, rotary calciner wall friction has a significant effect on heating time and temperature uniformity. Completely smooth walls can double heating time. One baffle can remedy this. This has implications for improving the design and operation of calciners and dryers, which are known to be extremely energy intensive.

C1 - CATALYSIS OF C1 CHEMISTRY

C1 - COX ACTIVATION AND OXYGENATE PRODUCTION

Wednesday, June 11, 2025 1:00 PM - 3:20 PM
Centennial Ballroom IV

Chair: Felix Herold, Norwegian University of Science and Technology

Co-Chair: Thomas Lin, Stanford University

KEYNOTE: Tailored Materials for Engineering Activity, Stability and Selectivity in CO_2 Conversion Catalysts.

Matteo Cargnello[1] *and Chengshuang Zhou*[2]
(1)Chemical Engineering, Stanford University, Stanford, CA, (2)Molecular Foundry, Lawrence Berkeley National Lab, Berkeley, CA

We present multiple catalyst systems to tune selectivity in CO_2 hydrogenation reactions at mild pressure. We use compositionally tunable metal catalysts (Ru/In), porous polymer overlayers, and oxide supports to control metal/support and metal/ligand interactions and reaction selectivity towards the preparation of useful fuels and chemicals.

Plasma-Assisted Dry Reforming of Methane Using CeO_2 Nanorods Supported Single Atom Bimetallic Ni-Ru Catalysts.

Md Monir Hossain *and Ruigang Wang*
Chemical Engineering and Materials Science, Michigan State University, East Lansing, MI

This study investigates the impact of deposition-precipitation and hydrothermal methods on Ni-Ru bimetallic catalysts supported on CeO_2 nanorods for plasma-assisted dry reforming of methane. Preliminary results reveal differences in chemisorption behaviors. In-situ Raman and DRIFTS analyses will provide insights into structural changes and reaction mechanisms for optimizing methane reforming.

Co-Promoted Co/SiO_2 with ZnO-MnO ALD for Improved Higher Oxygenate Synthesis.

Nadine Humphrey[1]*, Stacey F. Bent*[2]*, and Simon Bare*[3]
(1)Department of Chemical Engineering, Stanford University, Stanford, CA, (2)Chemical Engineering, Stanford University, Stanford, CA, (3)Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, Menlo Park, CA

Co-promoted Co/SiO_2 with ZnO-MnO ALD increases selectivity towards higher oxygenates to 20% and enhances catalyst activity over ZnO promotion alone. This work uses ALD as a dispersed, controlled, and uniform process relating catalyst structure to performance, expanding on the promotion effects on Co in designing catalysts for higher alcohol synthesis.

2D Nanoscale MoS_2 Catalysts for Direct Conversion of Methane to Oxygenates.

Steven Farrell[1]*, Juan Jimenez*[2]*, Ayaskanta Sahu*[3]*, Sanjaya D. Senanayake*[2]*, and Eli Stavitski*[1]
(1)National Synchrotron Light Source II, Brookhaven National Laboratory, Upton, NY, (2)Chemistry Division, Brookhaven National Laboratory, Upton, NY, (3)Chemical and Biomolecular Engineering, New York University, Brooklyn, NY

Methane is difficult to transport as a gas. We present MoS_2, a low-cost material that forms 2D nanosheets, as a selective and efficient catalyst for the conversion of methane to liquid oxygenates, competitive with costly precious metals. We also probe *in situ* behavior with X-ray absorption spectroscopy under realistic conditions.

Enhancing Rh-Fe Interaction to Achieve Higher Ethanol Selectivity in CO_x Hydrogenation.

Gokce Gulfidan[1]*, Hao Xu*[2]*, Wenda Hu*[3]*, Robert A. Dagle*[4]*, Jothi Kothandaraman*[4]*, and Yong Wang*[5]
(1)Chemical Engineering, Washington State University, Pullman, WA, (2)Chemical and Bio Engineering, Washington State University, Pullman, WA, (3)The Gene and Linda Voiland School of Chemical Engineering and Bioengineering, Washington State University, Pullman, WA, (4)Pacific Northwest National Laboratory, Richland, WA, (5)Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA

The conversion of CO_x (CO and CO_2) into ethanol is essential for sustainable carbon utilization. This study demonstrates enhanced ethanol selectivity in CO_x hydrogenation using Rh-based catalysts promoted by Fe. Improved Rh-Fe interactions on silica support and co-loading boost selectivity under mild conditions, highlighting the importance of active site structure.

Evaluating Enhanced Stability of Si-Doped Methanol Synthesis Catalysts in Conventional and Sustainable Methanol Synthesis Duties.

Pauline Glen*, Norman Macleod, Monica Garcia-Dieguez, Martin Jendrlin, Mark Kent, Graham Lightfoot, and Michael Nicholson*
R&D, Johnson Matthey, Stockton-on-Tees, United Kingdom

The use of effective accelerated ageing testing protocols has allowed the development of highly stable Si-doped catalysts for methanol synthesis. These catalysts improve productivity in conventional methanol synthesis plants, increasing the useful operating life. Optimised Si-promoted catalysts for CO_2 hydrogenation allow the sustainable production of methanol via our eMERALD^{TM} technology.

CO2 - CO2 CAPTURE AND UPGRADING

CO2 - DUAL FUNCTIONAL MATERIALS FOR CO_2 CAPTURE AND CONVERSION

Wednesday, June 11, 2025 1:00 PM - 3:20 PM
Regency Ballroom VII

Chair: Marc Porosoff, University of Rochester

Co-Chair: Takashi Toyao, Hokkaido University

Self-Regenerative Ni/$CaTiO_3$/CaO Catalyst for Simultaneous CO_2 Capture and Methane Dry Reforming.

Seongbin Jo[1] *and* ***Kandis Leslie Gilliard-Abdulaziz***[2]
(1)Chemical Engineering, University of Southern California, Los Angeles, CA, (2)Sonny Astani

Civil and Environmental Engineering Department, University of Southern California, Los Angeles, CA

Integrated CO2 capture and utilization (ICCU) utilizes dual functional materials to convert CO2 into valuable fuels. A promising approach involves developing self-regenerative Ni/CaTiO3/CaO materials, enhancing multicycle stability and CO2 uptake in the Integrated CO2 Capture and Dry Reforming of Methane (ICCDRM) process, overcoming challenges like sintering and deactivation.

Bifunctional Catalysts for Sorption-Enhanced Reaction Processes.

Johannis AZ Pieterse
Energy Engineering, TNO, Petten, Netherlands

Sorption-enhanced reaction integrates adsorption with catalytic reactions to convert reactants such as CO_2, CH_3OH, and DME into fuels and chemicals within a single reactor, operating under mild conditions with high conversion. Material approaches to integrate the sorption and reaction functionalities avoid the challenging physically mixing of sorbents and catalysts.

Dual Function Materials Beyond the Lab: Industrial Applications and Material Improvements for Working with Real CO_2 Emissions.

Angie Merkouri[1], Soudabeh B. Gharamaleki[1], Luis. F Bobadilla[2], Maila Danielis[3], Juan L. Martin-Espejo[2], Anna Penkova[2], Guillermo Torres-Sempere[2], Michael Short[1], Andrea Braga[4], Alessandro Trovarelli[5], José A. Odriozola[6], Tomas Ramirez Reina[2], Sara Colussi[3], and ***Melis Duyar***[7]
(1)Chemical and Process Engineering, University of Surrey, Guildford, United Kingdom, (2)Inorganic Chemistry Department, Materials Science Institute of Seville-University of Seville-CSIC, Sevilla, Spain, (3)Polytechnic Department, University of Udine, Udine, Italy, (4)Università di Udine, Udine, Italy, (5)Polytechnic Department, Università di Udine, Udine, Italy, (6)Inorganic Chemistry Departmentnt, Materials Science Institute of Seville-University of Seville-CSIC, Sevilla, Spain, (7)Chemical Engineering, University of Surrey, Guildford, Surrey, United Kingdom

We have developed methods to collect emissions from industry sites in sealed gas bags and use these directly for our ICCU testing in the lab. We demonstrated cyclic testing with a real industrial off-gas stream, which constitutes an advancement of DFM technology readiness level to TRL 5.

Behavior of Rh-Based Dual Function Materials (DFMs) for Integrated CO_2 Capture and Methanation at Simulated Flue Gas Conditions.

Giuseppe Nava*, Alessandro Porta, Roberto Matarrese, Carlo Giorgio Visconti, and Luca Lietti*
Dipartimento di Energia, Politecnico di Milano, Milan, Italy

This work addresses DFMs behavior for CO2 capture and methanation from flue gases by operando FT-IR spectroscopy, providing insights on reaction and deactivation mechanisms, as well as guidelines for improved DFM formulations.

Metallic Phase–Free Zn-Al Mixed Oxide Dual Function Materials Enable High CO Selectivity in Reactive Carbon Capture from Dilute CO_2 Streams.

__Wilson McNeary__, Alexander Hill, Chae Jeong-Potter, Martha A. Arellano-Treviño, Daniel Ruddy, and Anh To
Catalytic Carbon Transformation and Scale-Up Center, National Renewable Energy Laboratory, Golden, CO

This work developed K-modified Zn-Al mixed oxides for reactive carbon capture (RCC) to CO with > 97% selectivity and yields up to 53% of captured CO_2 at 400 °C. *In situ* spectroscopy to elucidate the role of K-modification in improving RCC performance.

Reactive Capture and Conversion of CO_2:Catalyst and Process Development for Power-to-Gas Energy Storage.

__Matthew Yung__[1], Mathew Rasmussen[2], Sawyer Halingstad[1], Nathan C. Ellebracht[3], Melinda Jue[3], Alvina Aui[4], and Simon H. Pang[3]
(1)National Renewable Energy Laboratory, Golden, CO, (2)Bioenergy Science and Technology Department, National Renewable Energy Laboratory, Golden, CO, (3)Materials Science Division, Lawrence Livermore National Laboratory, Livermore, CA, (4)Lawrence Livermore National Laboratory, Livermore, CA

Reactive capture and conversion of CO2 to methane on TiO2-supported dual-functional materials is presented, as well as a mechanism supported by DRIFTS and control experiments and correlation between support oxygen vacancy formation and desorbed product selectivity.

Understanding Zeolitic Adsorption Sites in Which CO_2 Outcompetes Water Under Thermodynamic Control.

__Hwangho Lee__[1], Alexander Katz[2], Dan Xie[3], Stacey I. Zones[3], Ryohji Ohnishi[4], Takahiko Takewaki[4], and Shu Hikima[4]
(1)Department of Chemical and Biomolecular Engineering, University of California - Berkeley, Berkeley, CA, (2)Chemical and Biomolecular Engineering, University of California, Berkeley, Berkeley, CA, (3)Chevron Energy Technology Company, Richmond, CA, (4)Mitsubishi Chemical Corporation, Yokohama, Japan

We demonstrate K^+-exchanged double-eight-ring secondary building units in zeolites as water tolerant CO_2 adsorption sites, in which CO_2 outcompetes water under thermodynamic control. Such sites have remained a grand challenge both for combining capture & catalysis as well as enabling practical CO_2 capture from post-combustion & point-source applications.

ENVIRO AUTO - ENVIRONMENTAL AND AUTOMOTIVE CATALYSIS

ENVIRO AUTO - N_2O CONTROL USING ZEOLITE CATALYSTS

Wednesday, June 11, 2025 1:00 PM - 3:20 PM
Centennial Ballroom I

Chair: Enrico Tronconi, Politecnico di Milano

Co-Chair: Yuejin Li, BASF

Transient Response Methods for the Investigation of N_2o Decomposition on Fe/CHA Catalysts.

*Maria Elena Azzoni[1], Nicola Usberti[1], Andrea Gjetja[1], **Isabella Maria Nova**[1], Enrico Tronconi[2], Roberta Villamaina[3], Maria Pia Ruggeri[3], Veselina Georgieva[3], Loredana Mantarosie[3], and Jillian Collier[3]*
(1)Dipartimento di Energia, Politecnico di Milano, Milan, Italy, (2)Politecnico di Milano, Milan, Italy, (3)Johnson Matthey Technology Centre, Sonning Common, United Kingdom

The decomposition of N_2O, a strong greenhouse gas, is investigated on Fe/CHA catalysts using Transient Response Methods. Transient kinetic analysis of the collected data provides useful information for clarifying the nature of the Fe active sites, understanding the auto-reduction of Fe and assessing the role of the associated redox chemistry.

Interrogating the Kinetic and Mechanistic Origins of N_2o Formation during NH_3 Selective Catalytic Reduction of NO_x on Cu-CHA Zeolites.

***Bryan Cruz Delgado**[1], Raghav Saxena[2], Matthew T. Caudle[3], Vivek Vattipalli[4], Ahmad Moini[4], Subramanian Prasad[3], William Schneider[2], and Rajamani Gounder[1]*
(1)Charles D. Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN, (2)Chemical and Biomolecular Engineering, University of Notre Dame, Notre Dame, IN, (3)BASF Corporation, Iselin, NJ, (4)BASF Environmental Catalyst and Metal Solutions, Iselin, NJ

Experimental steady-state and transient kinetic measurements were combined with *in situ* and *operando* X-ray absorption spectroscopy and Density Functional Theory to provide evidence for N_2O formation pathways originating from NO_2-assisted reduction events of Cu(II) sites during low temperature ammonia-selective catalytic reduction of nitrogen oxides on Cu-exchanged zeolites.

DFT Evaluation of N_2/N_2o Selectivity during NH_3-NO_x SCR over Cu-SSZ-13 Zeolite Catalyst.

***Raghav Saxena**[1], Bryan Cruz Delgado[2], Matthew T. Caudle[3], Anthony Debellis[4], Subramanian Prasad[5], Ahmad Moini[3], Rajamani Gounder[2], and William Schneider[1]*
(1)Chemical and Biomolecular Engineering, University of Notre Dame, Notre Dame, IN, (2)Charles D. Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN, (3)BASF Environmental Catalyst and Metal Solutions, Iselin, NJ, (4)Quantum Chemistry and Hybrid Modeling Research, BASF Corporation, Tarrytown, NY, (5)BASF Corporation, Iselin, NJ

We investigate N_2O formation, a potent greenhouse gas, during NH_3-NO_x SCR over Cu-CHA catalysts. DFT and microkinetic modeling reveal NO_2 pathways on NH_3-solvated ZCuOH sites as key contributors. Reducing NO_2 and these sites provides strategies to limit N_2O emissions, advancing cleaner technologies for heavy-duty diesel engines.

Iron-Catalyzed Cooperative Red-Ox Mechanism for the Simultaneous Conversion of Nitrous Oxide and Nitric Oxide.

Filippo Buttignol[1], Jörg W.A. Fischer[2], Alberto Garbujo[3], Pierdomenico Biasi[4], Gunnar Jeschke[2], Oliver Kröcher[5], Davide Ferri[5], and ***Gabriela-Teodora Dutca**[6]*
(1)Paul Scherrer Institute, Villingen, Switzerland, (2)ETH Zurich, Zurich, Switzerland, (3)CASALE SA, Lugano, Switzerland, (4)Basic Research Department, CASALE SA, Lugano, Switzerland, (5)Paul Scherrer Institute, Villigen, Switzerland, (6)EPFL, Lausanne, Switzerland

This work demonstrates that i) the N_2O-NO-SCR reaction is a promising strategy for simultaneous conversion of N_2O and NO, ii) dynamic O*perando* spectroscopic experiments are essential to extract valuable molecular insights and iii) the reactivity of Fe centers in Fe-exchanged zeolites can be disentangled.

Intrinsic Kinetics of Disparate Redox Pathways for Nitrous Oxide Selective Catalytic Reduction over Fe-Zeolites.

***Elizabeth Brungardt**, Vaishnav Sunkireddy, and Siddarth Krishna*
Chemical and Biological Engineering, University of Wisconsin-Madison, Madison, WI

We investigated the selective catalytic reduction (SCR) of N_2O by NH_3 and NO over Fe-zeolites, which occurs via Fe^{II}-Fe^{III} redox cycle. Net rates are limited by Fe^{II} oxidation by N_2O, while reduction pathway selectivity is governed by the relative intrinsic rates of Fe^{III} reduction by NO+NH_3 versus NH_3 alone.

KEYNOTE: Catalysis for Green Hydrogen - Industry Perspective.

Aleksey Yezerets
Cummins Inc., Columbus, IN

This keynote presentation will cover various catalytic processes and applications, that are relevant to green hydrogen, ranging from its production via water electrolysis to its consumption in industrial and transportation applications.

FUNDAMENTALS - FUNDAMENTALS OF CATALYSIS AND SURFACE SCIENCE

FUNDAMENTALS - ZEOLITES AND ACID-BASE CATALYSIS 2

Wednesday, June 11, 2025 1:00 PM - 3:20 PM
Centennial Ballroom II

Chair: Rajat Subhra Ghosh, Cummins, Inc.

Co-Chair: Siddarth Krishna, University of Wisconsin-Madison

Electrically-Driven Proton Transfer Promotes Brønsted Acid Catalysis By Orders of Magnitude.

Karl Westendorff[1]*, Max J. Hülsey*[1]*, Thejas Wesley*[1]*, Yogesh Surendranath*[2]*, and Yuriy Roman*[1]
(1)Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, MA, (2)Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA

This work probes the influence of catalyst potential on heterogeneous Brønsted acid catalysis. Differences in applied potential of ~380 mV yield a 100,000-fold rate enhancement for alcohol dehydrations. Mechanistic studies indicate that the interfacial field increases the effective catalyst acidity and activity. This effect extends across acid catalysts and reactions.

First Principles Analysis of Coke Formation on Pt-Based Catalysts during Propane Dehydrogenation.

Yu-Hsiang Cheng *and Jeffrey Greeley*
Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN

Coke formation deactivates heterogeneous catalysts during hydrocarbon conversion, particularly in non-oxidative alkane dehydrogenation reactions. Here, we use DFT simulations to explore structure-sensitive coke growth on Pt surfaces, revealing higher nucleation barriers on terraces than steps. Insights from graphene nucleation models highlight strategies to develop more coke-tolerant catalysts for industrial applications.

Cattesthub: Experimental Heterogeneous Catalytic Database and Fundamental Insights.

Atharva Burte[1]*, Lars Grabow*[1]*, Paul J. Dauenhauer*[2]*, Susannah Scott*[3]*, and Omar Abdelrahman*[1]
(1)William A. Brookshire Department of Chemical and Biomolecular Engineering, University of Houston, Houston, TX, (2)Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN, (3)Department of Chemical Engineering, University of California, Santa Barbara, Santa Barbara, CA

CatTestHub is a valuable tool for chemical catalysis research, enabling a more community-wide benchmarking effort. The growth of the database promises to deepen understanding of catalytic behavior and improve the precision of experimental investigations, ultimately expediting the discovery of new, efficient catalytic materials.

Shedding Light on Catalyst Restructuring in Nitic Acid Production.

Matthew Wilson[1]*, Feng Wang*[2]*, and Jay Yan*[3]
(1)JOHNSON MATTHEY, Billingham, United Kingdom, (2)Department of Chemical Engineering, University College London, London, United Kingdom, (3)Chemical Engineering, University College London, London, United Kingdom

Platinum-based gauzes for the nitric acid industry have been studied using state of the art characterization techniques, combined with catalyst testing under industrially relevant conditions to shed light on their structural evolution. Fundamental understanding of gauze catalysts supports improved plant operation, reduced emissions and better catalyst selection.

Impact of Zeolite Pore Size on the Kinetics of Liquid-Phase Epichlorohydrin Methanolysis.

Huston Locht*, Zahra Rangoonwala, and David Flaherty*
School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA

Structural confinement within zeolites alters the organization of solvent molecules around active sites, influencing catalytic activity through both van der Waals interactions with pore walls and hydrogen-bonding interactions within the reorganized solvent network. Here, we examine the effects of zeolite pore size on the rates and regioselectivities of epichlorohydrin methanolysis.

Atomically Precise Subnanometer Cu, Pd and Cupd Cluster-Based Oxidative Dehydrogenation Catalysts: Knobs for Controlling Activity & Selectivity at the Subnanometer Scale.

Stefan Vajda
Department of Nanocatalysis, J. Heyrovsky Institute of Physical Chemistry of the Czech Academy of Sciences, Prague, Czech Republic

Results demonstrating high-fidelity control of activity (by orders of magnitude) and selectivity (switching between products) in oxidative dehydrogenation of cyclohexene on Cu, Pd and CuPd clusters, will be discussed, using tuning knobs of atomic-precision size and composition of the clusters and leveraging oxide- and carbon-based supports and optimized reaction conditions.

Interrogating the Catalytic Consequences of Extra-Framework Aluminum Species in Acid Zeolites Using Protolytic Alkane Activation.

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

Chabazite zeolites containing one T-site are interrogated to assess the catalytic consequences of extra-framework aluminum (Al_{ex}) species co-occluded within zeolitic voids near H^+ sites. Measurements of entropy-enthalpy trade-offs upon confining neutral alkanes and carbocationic alkane activation transition states indicate Al_{ex} species strengthen attractive van der Waals interactions within zeolite voids.

HYDRO ECON - CATALYSIS FOR THE HYDROGEN ECONOMY

HYDRO ECON - NH3 DECOMPOSITION

Wednesday, June 11, 2025 1:00 PM - 3:20 PM
Centennial Ballroom III

Chair: Yuanyuan Zhu, University of Connecticut

Co-Chair: Yizhi Xiang, University of Missouri Columbia

The Effect of Water Impurities on Ba-Promoted Cobalt Catalysts for the Ammonia Decomposition Reaction.

Zahra Almisbaa[1] *and Philippe Sautet*[2]
(1)Research & Development Center, Saudi Aramco, Dhahran, Saudi Arabia, (2)Chemical and Biomolecular Engineering, University of California, Los Angeles, Los Angeles, CA

DFT-based microkinetic simulations of the ammonia decomposition reaction and water dissociation were used in this study to understand oxygen poisoning on promoted and unpromoted surfaces. Our results indicate that binding energy alone does not suffice in evaluating catalytic poisoning, as a thorough understanding requires incorporating the kinetics of the reaction.

Electrified Catalytic Processes of Ammonia Decomposition for Distributed H_2 Production.

Jiachun Wu[1]*, Anthony Griffin*[2]*, Paul Smith*[2]*, Zhe Qiang*[2]*, and* ***Yizhi Xiang***[1]
(1)Department of Chemical and Biomedical Engineering, University of Missouri Columbia, Columbia, MO, (2)The University of Southern Mississippi, Hattiesburg, MS

Efficient NH_3 decomposition was achieved through Joule heating catalysis with 3D printed carbon as the heating element and catalyst support. The conversion of NH_3 in Joule-heating catalysis was higher than conventional thermal catalysis, in addition to exhibiting accelerated startup and shutdown for dynamic operations using intermittent renewable electricity.

Highly Active Cobalt Catalysts for Low-Temperature Ammonia Decomposition.

Monica Pazos Urrea[1] *and Magnus Rønning*[2]
(1)Chemical Engineering, Norwegian University of Science and Technology, Trondheim, Trøndelag, Norway, (2)Department of Chemical Engineering, NTNU, Trondheim, Norway

Bimetallic cobalt-based catalysts derived from layered double hydroxides were studied for low-temperature ammonia decomposition, focusing on the effect of the second metal on reducibility and activity. In-situ X-ray absorption spectroscopy revealed the local environment and characteristics of the metal species, supporting the development of cost-effective alternatives to ruthenium-based catalysts.

Activation of Fe, Co, and Mo Based Metal Oxides for Ammonia Decomposition.

Sahra Louise Guldahl-Ibouder[1]*, Monica Pazos Urrea*[1]*, Ingeborg-Helene Svenum*[1,2]*, and Magnus Rønning*[1]
(1)Chemical Engineering, Norwegian University of Science and Technology, Trondheim, Trøndelag, Norway, (2)SINTEF Materials and Nanotechnology, Trondheim, Norway

In situ activation of Fe, Co, and Mo based oxide catalysts in ammonia was studied by XAS-XRD. The ammonia decomposition performance of the catalysts is discussed in light of their activation, the nature of the active phase, and their low-temperature activity for ammonia decomposition.

High Throughput Testing of Ru-Based Catalysts for Ammonia Cracking.

__Ingo Graef__, Konrad Krois, Christian Breuer, Hans-Joerg Woelk, and Santiago Casu
Heraeus Precious Metals GmbH & Co. KG, Hanau, Germany

For Ru-based catalysts used in the ammonia cracking reaction, low temperature activity and stability are essential. A high throughput test campaign was performed in a single-pellet string reactor, resulting in significant performance improvements by applying the right impregnation technique and appropriate dopants.

Molybdenum Carbonitride Mxene in Catalysis of Ammonia Synthesis and Decomposition.

__Evgenia Kountoupi__[1], Diana Piankova[1], Mikhail Agrachev[2], Zixuan Chen[1], Alberto Garbujo[3], Paula M. Abdala[1], Christoph R. Müller[1], and Alexey Fedorov[1]
(1)Department of Mechanical and Process Engineering, ETH Zurich, Zurich, Switzerland,
(2)Department of Chemistry and Applied Biosciences, ETH Zurich, Zurich, Switzerland,
(3)CASALE SA, Lugano, Switzerland

H_2 pretreatment of $Mo_2(C,N)T_x$ increases the NH_3 productivity by 4-fold relative to unpretreated $Mo_2(C,N)T_x$ or the bulk β-Mo_2N. Bulk β-Mo_2N outperforms $Mo_2(C,N)T_x$ in the NH_3 decomposition, irrespective of the H_2 pretreatment. Diffusion limitations in the narrow 2D pores of multilayered $Mo_2(C,N)T_x$ inhibit the utilization of the vast MXene surface area.

Unlocking Highly Active Metal Nanoparticles Anchored on Oxide Structures for Ammonia Decomposition.

Baris Alkan, Anh Binh Ngo, Liseth Duarte, Thomas Lunkenbein, and __Annette Trunschke__
Inorganic Chemistry, Fritz Haber Institute of the Max Planck Society, Berlin, Berlin, Germany

Chemical storage of hydrogen in the form of ammonia could become an important component of a carbon-free hydrogen economy. We present a successful strategy for the synthesis of mixed oxides with nanoscale particles, from which highly active phases with efficient metal-promoter-support interactions for ammonia decomposition are generated by exsolution.

MICRO MESO - MICROPOROUS AND MESOPOROUS MATERIALS

MICRO MESO - METAL AND ZEOLITE CATALYSIS

Wednesday, June 11, 2025 1:00 PM - 3:20 PM
Hanover Hall FG

Chair: Bjorn Moden, Zeolyst International

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

Catalyzing Epoxide Ring Opening Using Tuned Lewis Acid Zeolite Sn-Beta.

Nicholas Brunelli[1], *Aamena Parulkar*[2], *Jiawei Guo*[3], *and Ambarish Kulkarni*[4]
(1)William G. Lowrie Department of Chemical and Biomolecular Engineering, The Ohio State University, Columbus, OH, (2)Chemical and Biomolecular Engineering, The Ohio State University, Columbus, OH, (3)Chemical Engineering, UC Davis, Davis, CA, (4)Chemical Engineering, University of California, Davis, Davis, CA

Site quantification experiments reveal thermodynamic titration, connecting structure to reactivity. Using organo tin precursors, the structure of highly active sites is discovered.

Designing Superior Zeolites for Hydrocracking: Improved Diffusion, Stability, and Performance.

Nilson de Paula[1], *João Monnerat*[2], *Javier García-Martínez*[3], *and Pedro Romano*[4]
(1)Federal University of Rio de Janeiro, Rio de Janeiro, Rio de Janeiro, Brazil, (2)Chemistry Institute, Federal University of Rio de Janeiro, Rio de Janeiro, Rio de Janeiro, Brazil, (3)Molecular Nanotechnology Lab, Department of Inorganic Chemistry, University of Alicante, Alicante, Spain, (4)Campus D. de Caxias, Federal University of Rio de Janeiro, Rio de Janeiro, Brazil

The present work highlights the enhanced performance and stability of surfactant-templated mesoporous Pt/HUSY zeolites in the hydrocracking of hexadecane. The findings are particularly relevant for industry offering improved activity efficiency and diffusion control, crucial for catalyst design, overcoming diffusion limitations and meeting the evolving demands on hydrocarbon processing.

The Isomerization of *M*-Xylene over Fe Modified ZSM-5: Chemical and Structural Effects.

David Lennon[1], *Christos Ballas*[1], **Charles Kanyi**[2], *Luis E. Murillo*[2], *Paul Collier*[3], *Andrew P.E. York*[4], *and Stewart Parker*[5]
(1)Chemistry, University of Glasgow, Glasgow, Scotland, United Kingdom, (2)Johnson Matthey, Savannah, GA, (3)Johnson Matthey, Sonning Common, United Kingdom, (4)Technology Centre, Johnson Matthey, Sonning Common, United Kingdom, (5)STFC ISIS Facility, Harwell, United Kingdom

The isomerisation of *m*-xylene over Fe modified ZSM-5 at 300°C is used as a test reaction to probe how different Fe concentrations may perturb the zeolite's surface chemistry. Low Fe concentrations lead to a reduction in *o*-xylene formation that is attributed to ion exchange at strong Brønsted acid sites.

Mechanisms of H_2 Reduction of Cu^{2+} Ions and Implications for Cu Site Distribution in Cu-Exchanged Zeolites.

Jose Rebolledo-Oyarce[1], *Angel Santiago-Colón*[2], *Lauren Kilburn*[2], *Rajamani Gounder*[3], *and William Schneider*[4]

(1)Chemical Engineering, University of Notre Dame, Notre Dame, IN, (2)Chemical Engineering, Purdue University, West Lafayette, IN, (3)Charles D. Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN, (4)Chemical and Biomolecular Engineering, University of Notre Dame, Notre Dame, IN

Density functional theory, kinetic simulations, and statistical titration were combined to unravel Cu reduction mechanisms in Cu-CHA zeolites and to interpret H_2-TPR data. A general framework was established for understanding and interpreting H_2-TPR data and its variations, depending on zeolite composition, to identify active sites and their distribution.

Regioselective Active Site Control in Mo-Loaded MCM-22 and ZSM-5 Zeolites for Enhanced Regeneration in Methane Dehydroaromatization.

Jong Hun Kang[1]*, Eun Ji Choi*[2]*, Yangho Jeong*[2]*, Numan Muhammad*[3]*, Do-Young Hong*[3]*,*
Jangeon Roh[2]*, and Do Heui Kim*[2]
(1)Seoul National University, Seoul, Not US or Canada, Korea, Republic of (South), (2)Seoul National University, Seoul, Korea, Republic of (South), (3)Korea Research Institute of Chemical Technology, Daejeon, Korea, Republic of (South)

This study demonstrates the importance of controlling Al siting in 10MR zeolites through combined synthesis and post-treatment methods for highly regenerable methane dehydroaromatization (MDA) catalysts. Enhanced catalyst performance, reduced coke formation, and improved regenerability achieved a near-record 10% BTX yield, showcasing its potential to advance sustainable MDA processes.

Pt and Sulfate Functionalized Uio-66 for Catalytic Hydrogenation.

Yinjie Ji[1]*, Libor Kovarik*[1]*, Shutthanandan Vaithiyalingam*[1]*, Jian Zhi Hu*[1,2]*, Radha Kishan Motkuri*[1]*, Sungmin Kim*[1]*, Huamin Wang*[1]*, and Johannes Lercher*[1,3]
(1)Pacific Northwest National Laboratory, Richland, WA, (2)The Gene and Linda Voiland School of Chemical Engineering and Bioengineering, Washington State University, Pullman, WA, (3)Technical University of Munich, Garching b. München, Germany

We developed heterogeneous MOF-based catalysts by functionalizing defect-containing UiO-66 with acidic sulfate groups and Pt nanoparticles, aiming to determine their catalytic consequences, with a specific focus on the synergy between the two functionalities in hydrogenation reactions.

Exploring the Structure and Function of Rare-Earth Elements Incorporated into Zeolite Catalysts.

Mingze Zheng[1]*, Shivangi Nandkumar Borate*[2]*, James W. Harris*[2]*, and Brandon C. Bukowski*[1]
(1)Department of Chemical and Biomolecular Engineering, Johns Hopkins University, Baltimore, MD, (2)Department of Chemical and Biological Engineering, The University of Alabama, Tuscaloosa, AL

We combined computational and experimental methods to identify stable structures for rare-earth elements incorporated into Beta Zeolites (REE-Beta). Electronic structure theory, reaction kinetics, pyridine adsorption, and spectroscopy were then combined to guide the design of selective and stable REE-Beta ethanol to olefins catalysts for synthesizing sustainable aviation fuel.

NEW COMP - NEW METHODS IN COMPUTATIONAL CATALYSIS

NEW COMP - MACHINE LEARNING

Wednesday, June 11, 2025 1:00 PM - 3:20 PM
Hanover Hall CDE

Chair: Alexander Mironenko, University of Illinois Urbana-Champaign

Co-Chair: Christian Sandoval Pauker, RICE University

Kinetic Consequences of Anharmonic Entropy Approximations Accelerated with Machine Learning Potentials.

Geet Gupta and ***Brandon C. Bukowski***
Department of Chemical and Biomolecular Engineering, Johns Hopkins University, Baltimore, MD

Quasi-harmonic entropy approximations of reactive intermediates in aluminosilicate zeolite catalysts were accelerated with machine learning potentials (MLPs). MLPs were found to have transferability to predict temperature-dependent quasi-harmonic entropies. We then investigated the kinetic consequences of quasi-harmonic entropies using microkinetic modeling.

Automated Efficient Computation of Coverage Dependent Kinetics Combining Quantum Chemistry Workflows with Active Learning.

Matthew S. Johnson *and Judit Zádor*
Combustion Research Facility, Sandia National Laboratories, Livermore, CA

We present an active learning framework fusing automated quantum chemistry and machine learning to efficiently automate the calculation of coverage dependent kinetic parameters. We validate our framework against an enumerated dataset for a single reaction and demonstrate the framework on a set of reactions important for ammonia decomposition on Pt111.

Global Optimization of Supported Nanoparticles Via Machine Learning Interatomic Potentials.

Tristan Maxson[1] *and Tibor Szilvasi*[2]
(1)Department of Chemical and Biological Engineering, The University of Alabama, Tuscaloosa, AL, (2)Department of Chemical and Biological Engineering, The University of Alabama, Department of Chbe, Tuscaloosa, AL

A methodology for efficient structure search of supported nanoparticles via machine learning interatomic potentials is developed to support work to understand catalytic descriptors resulting from structural changes induced by support. This methodology is verified by direct comparisons with state-of-the-art benchmark experiments, improving upon known idealized constructions.

Active Learning Accelerated Global Optimization of Atomic Structures.

Keishana Navodye S. a.[1], *Michael Quaynor*[2], *and Kasun Gunasooriya*[3]
(1)School of Sustainable Chemical, Biological and Materials Engineering, University of Oklahoma, Norman, OK, (2)School of Sustainable, Chemical, Biological, and Materials Engineering, University of Oklahoma, Norman, OK, (3)Chemical, Biological & Materials Engineering, University of Oklahoma, Norman, OK

A python-based software package was developed integrating DFT, genetic algorithms and on-the-fly machine learning module based on Bayesian approach to accelerate the structure optimization of surfaces and nanoclusters with different compositions and coverages. This can analyze the stable configurations of structures closely resembling the chemical environment of the real systems.

Machine Learning Perturbation Theory Makes Reference-Quality Free Energy Barriers in Catalysis Affordable.

Jérome Rey[1], *Celine Chizallet*[2], *Dario Rocca*[1], *Tomáš Bučko*[3], *and* ***Michael Badawi***[1]
(1)CNRS, Lorraine University, Nancy, France, (2)IFPEN, Lyon, France, (3)Faculty of Natural Sciences, Comenius University, Bratislava, Slovakia

Free energy barriers for catalytic reactions have been computed at an unprecendeted level of theory thanks to machine learning perturbation theory (MLPT), improving the agreement with experiments. Although MLPT is presented here for hydrocarbon conversion in zeolites, it can be directly applied to any type of chemical reaction.

Machine Learning Models for Predicting Field-Enhanced Catalysis.

Runze Zhao[1], *Qiang Li*[1], *Zhu Cheng*[2], *and Fanglin Che*[1]
(1)Chemical Engineering, University of Massachusetts Lowell, Lowell, MA, (2)Lawrence Livermore National Laboratory, Livermore, CA

This study develops a machine learning framework reducing computational costs 10^5-fold, accurately predicting local electric field effects on nanoparticle catalysis. It highlights low-coordinated sites amplifying electric fields up to four times, offering insights for designing field-enhanced catalysts.

Machine Learning-Driven Dynamical Effects in Surface Chemistry of Metal Alloy Particles.

Changzhi Ai[1,2], *Frank Abild-Pedersen*[2], *and Johannes Voss*[2]

(1)Stanford Univerisity, Menlo Park, CA, (2)SUNCAT Center for Interface Science and Catalysis, SLAC National Accelerator Laboratory, Menlo Park, CA

We report initial results for structural evolution of complex metal alloy structures and surface reaction energetics that can be correlated with catalytic activity, where we observe a complex interplay of surface compositional and structural factors resulting in a broad distribution of binding energies across different surface sites.

POLYMER - CATALYSIS FOR POLYMER SYNTHESIS, UPCYCLING, AND RECYCLING

POLYMER - HYDROLYSIS AND PYROLYSIS

Wednesday, June 11, 2025 1:00 PM - 3:20 PM
Regency Ballroom VI

Chair: Hilal Ezgi Toraman, Pennsylvania State University

Co-Chair: Lucas Ellis, Oregon State University

Interfacial Engineering for Vapor Phase Chemical Recycling of Plastic Waste.

Xiaoshen Bai and ***Kunlun Ding***
Cain Department of Chemical Engineering, Louisiana State University, Baton Rouge, LA

In this work, we first identify the long-neglected contribution from heterogeneous catalysis in metal-salt-catalyzed liquid phase PET methanolysis. We further demonstrate that the solvent-free depolymerization of PET can be achieved with the assistance of trace amounts of zinc-based catalysts deposited by different techniques.

Tandem Methanolysis and Catalytic Transfer Hydrogenolysis of Polyethylene Terephthalate to p-Xylene over Cu/ZnZrO$_x$ Catalysts.

Siddhesh Shirish Borkar[1]*, Aojie Li*[2]*, Fatima Mahnaz*[1]*, Jenna Vito*[1]*, Ashfaq Iftakher*[1]*, Faruque Hasan*[1,3]*, Srinivas Rangarajan*[4]*, and Manish Shetty*[1]
(1)Artie McFerrin Department of Chemical Engineering, Texas A&M University, College Station, TX, (2)Department of Chemical and Biomolecular Engineering, Lehigh University, Bethlehem, PA, (3)Texas A&M Energy Institute, Texas A&M University, College Station, TX, (4)Chemical and Biomolecular Engineering, Lehigh University, Bethlehem, PA

The tandem catalytic transfer hydrogenolysis (CTH) of polyethylene terephthalate (PET) to p-xylene (PX) over Cu supported on reducible metal oxide ZnZrO$_x$ using methanol for (1) the methanolysis of PET to dimethyl terephthalate (DMT) and (2) as an in-situ H_2 source for the hydrogenolysis of DMT to PX is shown.

Chemical recycling of post-consumer polyester wastes using a tertiary amine organocatalyst.

Hongfei Lin[1]*, Shaoqu Xie*[2]*, Caiqi Wang*[1]*, Wenda Hu*[1]*, and Jian Zhi Hu*[3]

(1)The Gene and Linda Voiland School of Chemical Engineering and Bioengineering, Washington State University, Pullman, WA, (2)Voiland School of Chemical Engineering and Bioengineering, Washington State University, Washington State University, Pullman, WA, (3)Pacific Northwest National Laboratory, Richland, WA

This study demonstrates the effectiveness of N-methylpiperidine (NMP) as a catalyst for PET depolymerization via methanolysis, achieving over 90% monomer yield, even from mixed and post-consumer waste. Advanced MAS NMR and AIMD analyses reveal NMP's potential for efficient, sustainable polyester recycling and high-quality monomer production from various polyesters.

Polyamide Conversion to Monomer over Metal Oxide Catalysts.

Pedro Moura[1] *and Dionisios Vlachos*[2]
(1)Chemical and Biomolecular Engineering, University of Delaware, Newark, DE, (2)Delaware Energy Institute, University of Delaware, Newark, DE

This work finds alternative metal oxide catalysts for the hydrolysis of polyamides to monomers and provides insights into their stability. These catalysts can potentially improve the industrial hydrolysis of polyamides and the findings here presented help guide the selection and design of future catalysts and reaction systems.

Influence of Pyrolysis Parameters on Catalytic Co-Pyrolysis of Plastic Mixtures Using Zeolites.

Hilal Ezgi Toraman[1]*, Sean Okonsky*[1]*, and Neil Hogan*[2]
(1)Department of Chemical Engineering, Pennsylvania State University, University Park, PA, (2)Department of Chemical Engineering, Penn State University, University Park, PA

Key findings demonstrate that the co-pyrolysis of LDPE and PET with HZSM-5 resulted in increased production of C2-C4 olefins and monoaromatics. Lower catalyst-to-feedstock ratios enhanced olefins for LDPE but reduced benzene for PET, increasing benzoic acid. Optimal conditions for target circular economy products are visualized via response surface diagrams.

Catalytic Pyrolysis of Polyethylene with Microporous and Mesoporous Materials: Assessing Performance and Mechanistic Understanding.

Johan Herber van de Minkelis[1]*, Adrian H. Hergesell*[1]*, Jan C. van der Waal*[2]*, Rinke M. Altink*[2]*, Ina Vollmer*[1]*, and Bert M. Weckhuysen*[1]
(1)Inorganic Chemistry and Catalysis, Utrecht University, Utrecht, Utrecht, Netherlands, (2)Brightsite/TNO, Geleen, Limburg, Netherlands

Testing inherent catalytic properties is hampered by low pore accessibility in plastic pyrolysis. A mesoporous material improved the accessibility, thereby decoupling microkinetics from macrokinetics, and providing new mechanistic insights on catalytic pyrolysis. This enables the development of a new generation of catalyst materials tailored towards plastic recycling.

Upcycling of Additive-Containing Waste.

Jacqueline Ngu[1], Sean Najmi[2], Esun Selvam[3], Brandon Vance[3], Piaoping Yang[1], and ***Dionisios Vlachos[4]***
(1)University of Delaware, Newark, DE, (2)Center for Plastics Innovation, University of Delaware, Newark, DE, (3)Chemical and Biomolecular Engineering, University of Delaware, Newark, DE, (4)Delaware Energy Institute, University of Delaware, Newark, DE

We investigate the resilience of chemical deconstruction technologies to additives. We compare hydroconversion, and melt catalytic pyrolysis using acid catalysts. Catalyst-additive surface interactions are studied thermogravimetrically, spectroscopically, and via reaction experiments. We uncover poisoning mechanisms and demonstrate that common hydroconversion catalysts are susceptible to most additives.

C1 - CATALYSIS OF C1 CHEMISTRY

C1 - METHENA CONVERSION, DRY REFORMING OF METHANE

Wednesday, June 11, 2025 3:40 PM - 5:40 PM
Centennial Ballroom IV

Chair: Felipe Polo-Garzon, Oak Ridge National Laboratory (ORNL)

Co-Chair: Kandis Leslie Gilliard-Abdulaziz, University of Southern California

Stable Dry Reforming of Methane Enabled By High-Entropy Oxides Via Synergistic Redox Exsolution and Strong Metal-Support Interaction.

Zhenzhen Yang[1]*, Qingju Wang[2], and Sheng Dai[1,2]*
(1)Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN, (2)Department of Chemistry, The University of Tennessee, Knoxville, TN

Stable and coking-free dry reforming of methane (conversion of CO2/CH4 to syngas) was achieved by harnessing the restructuring behaviour of alkaline earth metal-doped high entropy oxide catalysts (BaNiMgCuZnCoOx), combining synergistic redox alloy exsolution (NiCuCo alloy) and strong metal-support interaction construction (BaOx overlayer formation).

Operando **XAS-XRD of CoPt Nanoparticles Under Dry Reforming of Methane Conditions Reveals Dynamic Order-Disorder Phase Transition.**

David Niedbalka*, Marcel Janak, Diana Piankova, Paula M. Abdala, and Christoph R. Müller*
Department of Mechanical and Process Engineering, ETH Zurich, Zurich, Switzerland

We show that alloying Co and Pt, metals with low activity for dry reforming of methane (DRM), significantly enhances catalytic performance when supported on SiO_2. *Operando* XAS-XRD reveals dynamic structural transformations and electronic interactions in CoPt alloys, highlighting how their unique electronic and local structures drive superior activity and stability.

Unraveling the Influence of Interfacial Sites on Selectivity Using a Microkinetic Model for Methane Dry Reforming on Oxide Supported Ni Catalysts.

Nirenjan Shenoy Padmanabha Naveen[1], *Konstantinos Alexopoulos*[2], *Michael Janik*[2], *and Gina Noh*[3]
(1)The Pennsylvania State University, University Park, PA, (2)Chemical Engineering, The Pennsylvania State University, University Park, PA, (3)DCHAB, ETH Zurich, Zurich, CA, Switzerland

A multi-site microkinetic model is developed to explore the role of metal-support interfaces in dry reforming of methane. By quantifying the interfacial effects on activity and selectivity, this study reveals how catalyst dispersion and interfacial site tuning enhance selectivity, offering new insights for designing efficient DRM catalysts.

Improved Dry Reforming Activity, Stability, and Selectivity through Reactant Ratio Feed Tailoring.

Gabriel Otusanya, *Jonathan Lucas, and Kerry Dooley*
Cain Department of Chemical Engineering, Louisiana State University, Baton Rouge, LA

Dry Reforming of Methane (DRM) converts CH_4 and CO_2 to H_2 and CO also known as syngas. Tailoring the DRM feed by either changing the CO_2:CH_4 feed ratio or adding small partial pressures of H_2O to the feed improves the stability, selectivity and activity of DRM catalysts.

Molten Indium Alloys for CO2 and CH4 Conversion to Syngas and Carbon Fibers.

Chester Upham, *Genpei Cai, Natascha Miederhoff, and Sawyer d'Entremont*
Chemical & Biological Engineering, University of British Columbia, Vancouver, BC, Canada

We will present on methane pyrolysis using several indium alloys to selectively produce carbon fibers. When CO_2 is also used as a co-reactant, we find that high value (2:1 H_2:CO) syngas can be also be co-produced. Kinetics, the reaction mechanism, and activity trends will be discussed.

Density Functional Theory and Raman Studies of Mo/ZSM-5 Utilizing Metal Promoters for Enhancing Methane Dehydroaromatization.

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

The metal promoters enhance Mo/ZSM-5 performance in MDA. DFT was utilized to interpret Raman spectra of Mo/ZSM-5 with added promoters and to calculate binding energies of promoters and Mo species. The data reveal the surface modification with promoters and enhancing availability of specific locations in pores and ion-exchange sites.

CO2 - CO2 CAPTURE AND UPGRADING

CO2 - CO_2 CONVERSION TO METHANOL 1

Wednesday, June 11, 2025 3:40 PM - 5:40 PM
Regency Ballroom VII

Chair: Lun An, Ames National Laboratory

Co-Chair: Junjie Chen, Stanford University

Reactive Capture and Conversion of CO_2 to Methanol over Alkali Promoted $ZnZrO_2$-Mg_3alox Catalytic Sorbents.

Laura Proano[1], *Katlo Galefete*[1], *Guanhe Rim*[2], *Gabriel Gusmão*[2], *and Christopher W. Jones*[2]
(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

CO_2 reactive capture and conversion (RCC) to methanol was investigated using alkali-modified $ZnZrO_2$-Mg_3AlO_x catalytic sorbents. Na-impregnation improved CO_2 uptake and productivity. However, selectivity shifted from methanol and CO to methane under RCC conditions, revealing distinct behaviors from steady-state operation and emphasizing the interplay of material properties and dynamic reaction environments.

Insight into Structure-Activity Relationships of SiO_2 -Supported Pd-Fe Catalysts for CO_2 Hydrogenation to Methanol.

Angelo Bellia, *Christoph R. Müller, and Paula Abdala*
Department of Mechanical and Process Engineering, ETH Zurich, Zurich, Switzerland

We focus on understanding the effect of the addition of Fe to Pd-based catalysts on their geometric and electronic structure and their catalytic activity for CO_2 hydrogenation to methanol. We observed that the addition of Fe significantly enhances the methanol yield and we characterized the catalysts via a multi-technique approach.

Tuning the Support and Metal Centers in Supported Catalysts to Boost Methanol Synthesis from CO_2 Hydrogenation.

Yang He[1], *Yuanyuan Li*[2], *Felipe Polo-Garzon*[3], *De-en Jiang*[4], *and* ***Zili Wu***[2]
(1)Chemical Science Division, Oak Ridge National Laboratory, Oak Ridge, TN, (2)Chemical Sciences Division, Oak Ridge National Laboratory (ORNL), Oak Ridge, TN, (3)Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN, (4)Department of Chemical and Biomolecular Engineering, Vanderbilt University, Nashville, TN

This presentation will highlight two effective strategies in controlling the metal-support interactions via tuning the anion site (hydride) of the support as well as the synergy between metal centers to enhance CO_2 hydrogenation to the desired alcohol product.

Evaluation of Cu and Cuzn Exsolution for the CO_2 Hydrogenation to Methanol: Insights from an *in Situ* and *Operando* Study.

Eleonora Cali[1]*, Marco Pietro Mezzapesa*[1]*, William Skinner*[2]*, David J. Payne*[2]*, Saman Khayat Noroozi*[1]*, Enrico Sartoretti*[1]*, Samir Bensaid*[1]*, and Fabio A. Deorsola*[1]
(1)Department of Applied Science and Technology, Politecnico di Torino, Turin, Italy, (2)Imperial College London, London, United Kingdom

In this work, optimized catalysts for CO_2 conversion to MeOH using the novel approach of 'exsolution' have been developed. The new exsolved samples were tested for the CO_2 hydrogenation to methanol to assess their stability, activity and selectivity, and the structure-activity-selectivity correlation studied through NAP-XPS, and *operando* TEM/STEM-EDX/EELS and FTIR.

Enhancing Methanol Selectivity in CO_2 Hydrogenation through Tuning of Metal-Oxide Interfacial Sites.

Weixin Huang[1] *and Shuxuan Feng*[2]
(1)University of North Dakota, Grand Forks, ND, (2)Chemistry, Univerisity of North Dakota, GRAND FORKS, ND

By investigating Pd-supported catalysts with uniform Pd nanocrystals, we demonstrate that metal/oxide interfaces play a crucial role in determining methanol selectivity from CO_2. These findings suggest that the design of tailored metal/oxide interfaces can lead to the development of highly effective CO_2-to-methanol catalysts

Physics-Informed Techno-Economic Assessment Shows a Path to Economical CO_2 Reduction.

Shashwati da Cunha *and Joaquin Resasco*
McKetta Department of Chemical Engineering, The University of Texas at Austin, Austin, TX

Our physics-informed techno-economic assessment highlights research priorities for electrochemical CO_2 reduction. Moving away from a plug flow reactor design lowers the levelized cost from \$1.22/kg_{CO} to \$0.97/kg_{CO}. Cheap renewable electricity cannot directly drive CO_2R if it is intermittent. Intermediate current densities are optimal, even with cheap electricity.

DYNAMICS - DYNAMIC CATALYSIS

DYNAMICS - DRIVING CATALYSIS THROUGH EXTERNAL MODULATION

Wednesday, June 11, 2025 3:40 PM - 5:40 PM
Hanover Hall FG

Chair: Ming Yang, Clemson University

Co-Chair: Omar Abdelrahman, University of Houston

Making Catalysts Dance – Dynamic Stress Boosts Hydrogen Evolution on Metals.

Xiang Yu[1], Hui Wang[1], Sander Deelen[2], and ***Matteo Monai***[1]
(1)Inorganic Chemistry and Catalysis, Institute for Sustainable and Circular Chemistry, Utrecht University, Utrecht, Netherlands, (2)Utrecht University, Utrecht, Netherlands

Better catalysts are needed for a more sustainable chemical industry. Dynamically straining a catalyst can theoretically boost catalytic performance, but approaches to induce strain at high frequency are lacking. Here, we demonstrate a method to dynamically strain catalysts up to 1000 Hz, boosting hydrogen evolution reaction on metal electrodes.

Enhancing the Activity and Selectivity of Pd-Based NH_3 Oxidation Catalysts By Forced Dynamic Reactor Operation.

Thomas Häber[1], Camilo Cárdenas[2], Olaf Deutschmann[2], and ***Patrick Lott***[2]
(1)Institute of Catalysis Research and Technology, Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, Germany, (2)Institute for Chemical Technology and Polymer Chemistry, Karlsruhe Institute of Technology, Karlsruhe, Germany

Spatiotemporal investigations demonstrate that forced dynamic reactor operation promotes both the activity and selectivity of Pd-based NH_3 oxidation catalysts operated in lean conditions and uncover gradients evolving in dynamic operation. The findings of this work are relevant whenever NH_3 is used as carbon-free energy carrier, i.e. during combustion or decomposition.

Tuning Non-Equilibrium Surface Coverages for Enhanced Methane Activation during Forced Periodic Oscillations.

Fatou Baka Diop*, Cameron Armstrong, Felipe de Faria Teixeira, and Andrew R Teixeira*
Chemical Engineering, Worcester Polytechnic Institute, Worcester, MA

We herein found that feed modulation during methane oxidation enhances conversion with pre-adsorbed oxygen activating methane and promotes hydrogen production in the methane-rich cycle, with sufficiently fast pulses to optimize surface coverage. This study presents limits and conditions for optimizing activity, selectivity and catalyst lifetime beyond equilibrium using dynamic catalysis.

Dynamic Catalytic Ammonia Decomposition: A Strong Coupling between Localized Transient Heating and Reaction Kinetics.

Korawich Trangwachirachai *and Jimmy A. Faria*
Catalytic Processes and Materials, MESA+ Institute for Nanotechnology, Faculty of Science and Technology, University of Twente, Enschede, Overijssel, Netherlands

The dynamic reaction result shows the possibility in utilizing a Joule heating technique to localize heat specifically at the catalyst and enhance the reaction kinetics.

Introducing *Stimulando* Time-Resolved IR Spectroscopy to Study Resonant Catalysis in Pulsed Light-Stimulated CO_2 Hydrogenation.

Florentien Brzesowsky, *Mees R. Emond, Bert M. Weckhuysen, and Matteo Monai*
Inorganic Chemistry and Catalysis group, Institute for Sustainable and Circular Chemistry, Utrecht University, Utrecht, Netherlands

Development of high time-resolution IR spectra to study CO_2 hydrogenation under intermittent light stimulation. *Stimulando* involves delivering the stimulus to the catalyst, observing the area affected by the stimulus and correlating with performance to determine how much of the catalysis is affected by the stimulus.

Dynamic-Magnetic-Field-Enhanced Thermal Catalysis: Beyond Temperature Control for Hydrogen Production from Ammonia.

Alexander Adogwa[1] *and Ming Yang*[2]
(1)Chemical Engineering, Clemson University, Clemson, SC, (2)Chemical and Biomolecular Engineering, Clemson University, Clemson, SC

We demonstrate the far-reaching catalytic implication of dynamic-magnetic-field-enhanced thermal catalysis. Although standard thermocatalytic hydrogen recovery from ammonia is often held back by the initial *N-H scission and associative *N desorption, by inducing catalyst spin (de)magnetization under MIH, we create a favorable pathway for both steps, surpassing limitations of standard thermocatalysis.

Unveiling Dynamics of Cu/ZIF-8 Catalyst: Operando and Forced Dynamic Reactor Studies for CO_2 Hydrogenation to Methanol.

Pia Dally[1] *and Pedro Castaño*[2]
(1)KAUST, Thuwal, -, Saudi Arabia, (2)KAUST Catalysis Center, King Abdullah University of Science and Technology, Thuwal, Saudi Arabia

Our work develops an advanced workflow using forced dynamic operando reactors and high-pressure pulsing, combined with in-situ and operando techniques. This approach aims to thoroughly analyze the dynamic behavior of Cu/ZIF-8 catalyst during CO_2 hydrogenation, offering insights beyond those possible with kinetic modeling alone.

ELECTRO PHOTO - ELECTROCATALYSIS AND PHOTOCATALYSIS

ELECTRO PHOTO - MODELING ELECTROCATALYTIC SYSTEMS

Wednesday, June 11, 2025 3:40 PM - 5:40 PM
Centennial Ballroom I

Chair: Tej Choksi, Nanyang Technological University

Co-Chair: Carine Michel, ENS Lyon

Challenges in Modeling Adsorption Processes in (electro)Catalysis.

Nitish Govindarajan
School of Chemistry, Chemical Engineering, and Biotechnology, Nanyang Technological University, Singapore, Singapore

This talk will discuss the challenges in the accurate estimation of adsorption energies and the description of adsorption isotherms at (electro)catalytic interfaces. Examples of using atomistic simulations to study the impact of the various molecular interactions at interfaces on adsorption energies will be highlighted.

Understanding the Difference between Thermal and Electro-Catalysis for CH_x Species on Transition Metals.

Anwin John[1] *and Jeffrey Greeley*[2]
(1)Chemical Engineering, Purdue University, West Lafayette, IN, (2)Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN

This study compares activation barriers for hydrogenation reactions catalyzed by surfaces and proton-coupled electron transfer (PCET) processes. We use DFT simulations to establish that PCET reactions exhibit a clear Brønsted-Evans-Polanyi (BEP) relationship, while surface-mediated responses do not. These findings highlight critical thermodynamic and kinetic differences between thermal and electrocatalytic processes.

Multi-Scale Modeling Guided CO Electroreduction to Acetate.

Yuting Xu[1]*, Wanyu Deng*[2]*, Ahryeon Lee*[3]*, Hefei Li*[3]*, Yilang Liu*[1]*, Jiaqi Yang*[1]*, Feng Jiao*[2,3]*, and Fanglin Che*[1]
(1)Chemical Engineering, University of Massachusetts Lowell, Lowell, MA, (2)Energy, Environmental, and Chemical Engineering, Washington University in St. Louis, St. Louis, MO, (3)Washington University in St. Louis, St. Louis, MO

This study integrates GC-DFT and MKM simulations to identify the reaction mechanism for CORR-to-acetate under various operando conditions. The selectivity of acetate can be specifically enhanced over the catalyst with optimal binding energy of CH*. A synergetic loop between experiment and theory can allow us to make reliable predictions.

Electrolyte Effects on Electrocatalytic Reactions through Multiscale Modeling of the Electrochemical Double Layer.

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

The DFT/FF-MD multiscale approach enables modeling of both the reaction process using DFT and the local field within the EDL environment through classical MD. This facilitates the study of how surface charge density, ion concentration, and ion identity influence the stability of adsorbates in ways that were previously inaccessible.

Understanding Acid Electrolyte Adsorption and pH Effects in Oxygen Electrocatalysis.

Kasun Gunasooriya
Chemical, Biological & Materials Engineering, University of Oklahoma, Norman, OK

Understanding the solid-liquid interface, especially the effects due to acid electrolyte anions and pH is crucial in designing and optimizing existing electrocatalysts under diverse electrochemical microenvironments. We provided critical insights into the non-innocent role of acid electrolyte anions and developed new microkinetic models that can capture pH effects.

Generalized Bulk Descriptors for Predicting O and OH Adsorption Energies on Metal Oxides on Non-Octahedral Metal Oxides.

Hyeonjung Jung *and Michal Bajdich*
SUNCAT Center for Interface Science and Catalysis, SLAC National Accelerator Laboratory, Menlo Park, CA

In the search for active and stable catalysts, density functional theory (DFT) and machine learning (ML)-based models can accelerate the screening of materials, aiming to derive more accurate and useful outputs from simpler inputs.

FUNDAMENTALS - FUNDAMENTALS OF CATALYSIS AND SURFACE SCIENCE

FUNDAMENTALS - CATALYST DESIGN AND SURFACE SCIENCE 2

Wednesday, June 11, 2025 3:40 PM - 5:40 PM
Centennial Ballroom II

Chair: Rajat Subhra Ghosh, Cummins, Inc.

Co-Chair: Ari Fischer, School of Chemistry, Chemical Engineering and Biotechnology, Nanyang Technological University

KEYNOTE: Heterogeneous Atomic Catalysts: Isolated Atoms, Ensembles, Dimers.

Hyunjoo Lee
Department of Chemical & Biomolecular Engineering, Korea Advanced Institute of Science and Technology (KAIST), Daejeon, Korea, Republic of (South)

Heterogeneous atomic catalysts, whose structure is elaborately controlled and the surface reaction is better understood, can be a new paradigm with higher catalytic activity, selectivity, and durability, and used in industrial applications.

Experimental and Modeling Studies on the Impact of Promoters on Surface Oxygen Species in Ethylene Epoxidation on Ag/α-Al2O3 Catalysts.

Shiuan-Bai Ann[1]*, Shawn Lu*[1]*, Jin-Xun Liu*[1]*, and Suljo Linic*[2]
(1)Department of Chemical Engineering, University of Michigan, Ann Arbor, MI, (2)Chemical Engineering, University of Michigan, Ann Arbor, MI

We deployed first-principles density functional theory, *in operando* surface-enhanced Raman spectroscopy, kinetic measurements, and experiment-guided microkinetic modeling to investigate how Cs and Cl promoters influence oxygen intermediates and the properties of Ag/α-Al_2O_3 arriving to a picture that depicts the intricate interplay between different mechanisms of promotion depending on reactions conditions.

Ultrathin Tungstate Films on MgO(100): Model Catalysts for Chemical-Looping Oxidative Dehydrogenation (CL-ODH) of Alkanes.

Andrew Pedersen[1]*, Fanxing Li*[2]*, and H. Henry Lamb*[2]
(1)Chemical & Biomolecular Engineering, North Carolina State University, Raleigh, NC, (2)Department of Chemical and Biomolecular Engineering, North Carolina State University, Raleigh, NC

We report the growth of ultrathin WO3 films and the synthesis of monolayer Na2[W2O7] films on MgO(100). The resultant films were characterized by X-ray photoelectron spectroscopy (XPS), grazing-incidence X-ray diffraction (GI-XRD), and Raman spectroscopy to determine film composition and W oxidation state(s), crystallographic phase(s), and local structure and bonding, respectively.

Decyphering Facet-Dependent Water Impact on Alkanol Dehydration on TiO_2.

Wenda Hu[1,2]*, Jinshu Tian*[3]*, Anthony Savoy*[2]*, Fan Lin*[1]*, Zihao Zhang*[1]*, Yiqing Wu*[1]*, Junming Sun*[2]*, Huamin Wang*[1]*, Jian Zhi Hu*[1,2]*, and Yong Wang*[1,2]
(1)Pacific Northwest National Laboratory, Richland, WA, (2)Washington State University, Pullman, WA, (3)Zhejiang University of Technology, Hangzhou, Zhejiang, China

We revealed that water inhibits alkanol dehydration on TiO2(001) four times more than on TiO2(101). On TiO2(001), isopropoxide-H2O complexes raise activation barriers by 49 kJ/mol, while weakly bonded IPA-H2O on TiO2(101) increases it by 23 kJ/mol. These findings provide valuable guidance for designing catalysts for water-containing environments.

Modulation of Metal Oxide Surface Basicity Using Ppm Levels of Single Atoms of Pt on FeO_x.

Shiva Murali[1]*, Honghong Shi*[2]*, Fan Lin*[2]*, Oliver Gutiérrez-Tinoco*[2]*, Johannes Lercher*[2]*, Huamin Wang*[2]*, and Yong Wang*[1,2]
(1)The Gene and Linda Voiland School of Chemical Engineering and Bioengineering, Washington State University, Pullman, WA, (2)Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA

Small ppm loadings of reduction stable single atom Pt/FeO_x introduces new Lewis acid-base site pairs for acetone aldol condensation with greater tunability and control of individual elementary reaction steps. Base catalyzed α-H enolation activation barrier is lowered, which changes rate determining step to C-C coupling and enhances activity.

HYDRO ECON - CATALYSIS FOR THE HYDROGEN ECONOMY

HYDRO ECON - METHANE PYROLYSIS

Wednesday, June 11, 2025 3:40 PM - 5:40 PM
Centennial Ballroom III

Chair: Aayush Singh, SandboxAQ

Co-Chair: Zahra Almisbaa, Saudi Aramco

Induction Heating Impact on Catalytic Methane Decomposition to Hydrogen Beyond Thermal Effect.

Ben Ko[1]*, Erdem Sasmaz*[1]*, Henry Moise*[2]*, and Matteo Cargnello*[2]
(1)Chemical and Biomolecular Engineering, University of California, Irvine, Irvine, CA, (2)Chemical Engineering, Stanford University, Stanford, CA

This study explores catalytic methane decomposition (CMD) using induction heating (IH) to examine magnetic field effects on catalyst behavior. Results show IH enhances methane conversion by 24% at 750 ºC and stability of Fe/Al_2O_3 compared to conventional heating. The magnetic field effect on surface properties and reaction mechanisms is discussed.

Using Operando TEM to Clarify the Effect of (Earth) Alkali Additives on Ni/C Catalysts for Catalytic Methane Pyrolysis.

Daan van Eck[1]*, Suzan E. Schoemaker*[1]*, Stefan Bismeijer*[1]*, Erik Betz-Güttner*[1]*, Tom A. J. Welling*[2]*, and Petra E. de Jongh*[1]
(1)Materials Chemistry and Catalysis, Utrecht University, Utrecht, Netherlands, (2)Frontier Research Institute for Interdisciplinary Sciences, Tohoku University, Sendai, Japan

In this study, operando transmission electron microscopy is used alongside macroscopic catalytic testing to understand the influence of alkali (earth) additives to Ni/C catalysts on a microscopic scale. Slower growth of individual nanofibers in Mg-promoted catalysts contributes to a higher carbon yield and a longer lifetime on the macroscopic scale.

The Role of Hydrogen on the Kinetics of Methane Pyrolysis.

Caleb Bavlnka*, Laura Alejandra Gomez Gomez, Phuong Nguyen Thi, Daniel E. Resasco, and Steven Crossley*
School of Sustainable Chemical, Biological and Materials Engineering, University of Oklahoma, Norman, OK

Catalytic methane pyrolysis could produce industrial scale CO_2-free hydrogen by also producing base growth carbon nanotubes with in situ separation. We show hydrogen significantly impacts methane conversion rates, and utilize a kinetic model, measured barriers, and reaction orders for methane and hydrogen to explain the reaction mechanism.

Exsolution-Driven Catalytic Decomposition of Methane Via. $SrFe_xAl_{12-x}O_{19}$ Hexaaluminates for CO_x-Free Hydrogen and Carbon Nanotubes.

Samuel Portillo[1]*, Mohammadreza Kosari*[1]*, Kunran Yang*[2]*, Andrew Pedersen*[1]*, Elizabeth Nguyen*[1]*, and Fanxing Li*[1]
(1)Chemical & Biomolecular Engineering, North Carolina State University, Raleigh, NC, (2)Department of Chemical and Biomolecular Engineering, North Carolina State University, Raleigh, NC

Study demonstrates that $SrFe_xAl_{12-x}O_{19}$ hexaaluminates are active for CDM. Activity of the material is attributed to structure collapse to α-Fe supported on $SrAl_2O_4$/$FeAl_2O_4$. Differences in activity and carbon morphology depend on iron loading. Fragmentation of Fe nanoparticles causes deactivation. The roles of α-Fe and Fe_3C in iron-based CDM are explored.

Cerium-Assisted Iron Oxidation in Nickel-Catalyzed Chemical Looping Dry Reforming.

Minjung Kim[1] *and Shang Zhai*[2]
(1)Mechanical and Aerospace Engineering, The Ohio State University, Columbus, OH, (2)Department of Mechanical and Aerospace Engineering, The Ohio State University, Columbus, OH

This study explores iron-nickel oxide supported on CeO_2 for chemical looping dry reforming of methane, converting CH_4 and CO_2 into syngas. Ni facilitates CH4 pyrolysis and Fe-Ce acts as oxygen carriers. Optimal Ni loading and CeFeO3 formation ensure high methane and CO2 conversion, stability, and minimal carbon accumulation.

Turquoise Hydrogen and Carbon Nanotubes Generation By Catalytic Decomposition of Methane and Toluene.

Qian Huang*, Biswajit Saha, Sathyapal Churipard R., and Ajay Dalai*
Chemical and Biological Engineering, University of Saskatchewan, Saskatoon, SK, Canada

This study highlights that ferrocene-catalyzed decomposition of methane and toluene results in a higher quality of carbon products. This study emphasizes the dual role of toluene as both a solvent for catalyst delivery and an additional carbon source, contributing positively to the overall production of hydrogen and carbon.

NEW COMP - NEW METHODS IN COMPUTATIONAL CATALYSIS

NEW COMP - DYNAMIC SAMPLING

Wednesday, June 11, 2025 3:40 PM - 5:40 PM
Hanover Hall CDE

Chair: Judit Zádor, Sandia National Laboratories

Co-Chair: Wenshuo Hu, Texas Tech University

Data-Efficient Modeling of Catalytic Reactions Via Enhanced Sampling and on-the-Fly Learning of Machine Learning Potentials.

***Simone Perego**, Luigi Bonati, and Michele Parrinello*
Atomistic Simulations, Istituto Italiano di Tecnologia, Genova, Italy

We developed a workflow combining enhanced sampling and active learning to construct machine learning potentials requiring only ~1,000 DFT calculations per reaction. Applied to ammonia decomposition on FeCo catalysts, this approach accurately captured reaction mechanisms, free energy profiles, and dynamic surface behavior under operando conditions, enabling efficient catalytic modeling.

Unraveling Competing Catalytic Reactions Sharing a Common Transition State through Blue Moon Sampling with Path-Based Reaction Coordinate.

***Monika Gešvandtnerová**[1,2], Pascal Raybaud[3], Céline Chizallet[3], and Tomáš Bučko[2,4]*
(1)Université de Lorraine, Metz, France, (2)Faculty of Natural Sciences, Comenius University, Bratislava, Slovakia, (3)IFP Energies Nouvelles, Solaize, France, (4)Institute of Inorganic Chemistry, Slovak Academy of Sciences, Bratislava, Slovakia

Blue moon ab initio molecular dynamics with a path-based reaction coordinate combined with Bennett-Chandler theory quantified temperature-dependent pathway preferences in isobutanol dehydration. Competing pathways with a shared dynamic transition state (TS) were identified, revealing a post-TS bifurcation. This work advances the accurate determination of rates for key alcohol dehydration reactions.

A Molecular View of Methane Activation on Nickel Surfaces through Enhanced Sampling and Machine Learning Potentials.

***Yinan Xu**[1], Yezhi Jin[1], Jireh García Sánchez[1], Gustavo Perez Lemus[1], Pablo Zubieta[1], Massimiliano Delferro[2], and Juan De Pablo[3]*
(1)Pritzker School of Molecular Engineering, University of Chicago, Chicago, IL, (2)Chemical Sciences and Engineering Division, Argonne National Laboratory, Lemont, IL, (3)Tandon School of Engineering, NYU, New York, NY

Machine-learned potentials (MLPs) combined with enhanced sampling enable detailed molecular view of methane activation on Ni surfaces at experimental conditions. Iteratively refined MLPs, incorporating adaptive biasing forces and key collective variables, predict density functional theory-level energies and forces, revealing temperature-dependent thermodynamics, dynamics, and reactant-surface interactions with unprecedented efficiency and accuracy.

Integrating ML-Accelerated Estimation of Coverage Dependent Thermodynamics in Reaction Mechanism Generator (RMG) for CO Methanation.

Chao Xu *and* ***Richard West***
Department of Chemical Engineering, Northeastern University, Boston, MA

Using an ML model to reduce DFT workload for coverage-dependent microkinetic modeling, we examined how CO coverage influences CO/H binding energies on Ni(111) surfaces. We extended Reaction Mechsnism Generator to incorporate coverage-dependent thermodynamics, enabling construction of a predictive CO/H2 methanation mechanism on Ni(111) for improved heterogeneous catalysis predictions.

KEYNOTE: Bridging Length and Time Scales in Catalysis for C1 Chemistry : From the Molecule to the Catalyst Particle Level.

Veronique Van Speybroeck
Ghent University, Ghent, Belgium

C1 catalysis over zeolites involves multi-scale processes like reactions, transport, and surface barriers. New methods, leveraging machine learning and enhanced sampling molecular dynamics open perspective to understand the dynamics from the molecule to the crystal particle level. Key steps in C1 conversion will be illustrated.

POLYMER - CATALYSIS FOR POLYMER SYNTHESIS, UPCYCLING, AND RECYCLING

POLYMER - C-H ACTIVATION AND OXIDATION

Wednesday, June 11, 2025 3:40 PM - 5:40 PM
Regency Ballroom VI

Chair: Hongfei Lin, Northeastern University

Co-Chair: Hyunjin Moon, National Renewable Energy Laboratory

Upcycling Polyolefin Waste to Light Olefins with Ethylene and Base-Metal Heterogeneous Catalysts.

Alexis Bell
Department of Chemical and Biomolecular Engineering, University of California-Berkeley, Berkeley, CA

Polyethylene and polypropylene comprise 57% of polymer waste in landfills. This work demonstrates the feasibility of deconstructing PE and PP, individually or in a mixture to form propylene and isobutylene, important feedstocks for the chemical industry, using inexpensive heterogeneous catalysts in a semi-batch reactor.

Oxidative Upcycling of Polyolefins, with and without Chain Cleavage.

Costanza Leonardi[1] *and* ***Susannah Scott***[2]
(1)Chemical Engineering, University of California, Santa Barbara, Santa Barbara, CA,

(2)Department of Chemical Engineering, University of California, Santa Barbara, Santa Barbara, CA

Selective catalytic oxidation of polyethylene without chain cleavage was achieved in aqueous tBuOOH in the presence of $MnBr_2$, leading to polyketone materials. Changing the reaction conditions led to oxidative chain cleavage, resulting in polar waxes.

Effect of Dehydrogenation Catalyst and Solvent on Hydrogen-Free Tandem Heterogeneous Catalysis for Polyethylene Depolymerization Via an Olefin-Intermediate Approach.

Andrew Tran[1], Selena Moore[1], Andreas Palmateer[1], Jose Naranjo-Mendez[1], Dimitri Gatzios[2], and ***Lucas Ellis**[1]*
(1)School of Chemical, Biological, and Environmental Engineering, Oregon State University, Corvallis, OR, (2)Chemical, Biological, and Environmental Engineering, Oregon State University, Corvallis, OR

This study examines hydrogen-free tandem catalysis for polyethylene depolymerization, focusing on the dehydrogenation catalyst and solvent effects. A Pd-based catalyst achieved the highest overall rates. Key findings reveal structure-property relationships and the crucial role of solvent thermodynamics in enhancing reaction efficiency and selectivity at low temperatures.

Mechanistic Insights in the Oxidative Conversion of Polyethylene Towards Di-Carboxylic Acids with O_2/NO.

***Thomas Jan Smak**[1], Rinke M. Altink[2], Jan C. van der Waal[2], Ina Vollmer[1], and Bert M. Weckhuysen[1]*
(1)Inorganic Chemistry and Catalysis, Utrecht University, Utrecht, Utrecht, Netherlands, (2)Brightsite/TNO, Geleen, Limburg, Netherlands

The conversion of polyethylene towards di-carboxylic acids using O_2/NO has been studied. It is observed that the addition of NO increases the di-carboxylic acid yield from 7 up to 32 mol%. The reactions were followed over time using a combination of GC, IR and NMR, leading to new mechanistic insights.

Hydroformylation of Plastic Oil Model Compounds into Aldehydes Catalyzed By Unmodified Cobalt Carbonyl Under Mild Conditions.

***Houqian Li**[1], Clark Landis[2], and George Huber[3]*
(1)Department of Chemical and Materials Engineering, New Mexico State University, Las Cruces, NM, (2)Department of Chemistry, University of Wisconsin-Madison, Madison, WI, (3)Department of Chemical and Biological Engineering, University of Wisconsin-Madison, Madison, WI

This study examines hydroformylation kinetics of plastic pyrolysis oils under mild conditions (<80 bar, <453 K), focusing on isomerization-hydroformylation tandem reactions. A mechanistic model quantitatively describes aldehyde selectivity and formation rates, providing insights to enhance the conversion of waste plastics into value-added chemicals.

One-Pot Conversion of Poly(lactic acid) to 1,2-Propanediol on Cu Catalysts.

Yiqi Xu[1]*, Damilola Akinneye*[2]*, and J. Will Medlin*[3]
(1)Chemical and Biological Engineering, University of Colorado-Boulder, Boulder, CO,
(2)Chemical & Biological Engineering, University of Colorado, Boulder, Boulder, CO,
(3)Department of Chemical and Biological Engineering, University of Colorado Boulder, Boulder, CO

We developed a one-pot tandem reaction of Poly (lactic acid)(PLA) ethanolysis and ethyl lactate (EL) hydrogenation on a bifunctional Cu-based catalyst to produce 1,2-propanediol (PDO), which is widely used as a plasticizer, surfactant, and resin. The PLA can be completely depolymerized with PDO selectivity as high as ~99%.

OTHER EVENTS

WEDNESDAY POSTER SESSION

Wednesday, June 11, 2025 6:00 PM - 8:00 PM
Grand Hall

Novel Green Method for the Preparation of Supported Sub-10 Nm Non-Noble Metal (Cu, Sn and Ga) Nanoparticles.

Abdennour Benabbas, Catherine Especel, and ***Florence Epron***
CNRS, Université de Poitiers, Institut de Chimie des Milieux et Matériaux de Poitiers-IC2MP, Poitiers, France

Abundant non-noble metals such as copper, tin, and gallium are alternatives for tomorrow's sustainable industries. Herein, we have successfully developed a general, efficient, and inexpensive green method that gives rise to some fascinating physico-chemical properties of these metals, triggered at the nanoscale in both liquid and solid states.

Accelerated Catalyst and Process R&D for Conversion of Bio-Based Ethanol to Green Chemical Intermediates and Products.

Matthias Stehle
R&D Solutions, hte GmbH, Heidelberg, Germany

Catalytic valorization of bio-Ethanol into target products Ethylene and Acetaldehyde was investigated in parallel using high throughput experimentation. High quality data was acquired within short time, thus providing the right tool for process optimization and increased sustainability in chemical production.

Unlocking Superior Ethylamine Electro-Oxidation and Nitrile-like Intermediates Poisoning Resistance on Pt Enabled By Electronic and Geometric Modulation (Poster).

***Yanlin Zhu**, Jinyao Tang, and Zhenmeng Peng*
Chemical Engineering, University of South Carolina, Columbia, SC

Platinum (Pt) is active for ethylamine electro-oxidation but deactivates quickly. We developed a Pt_3Ni_1@Au catalyst, utilizing electronic effects from Pt-Ni alloying and geometric modulation via Au deposition, achieving enhanced stability. After 100 CV cycles, its activity retention is 5 times higher than pure Pt, showcasing its potential for hydrogen storage.

Regulating Lattice Oxygen Property of TiO_2 Redox Catalyst for Enhanced Oxidative Dehydrogenation of Ethane.

***Xiaoqiao Zhang**, Jianhong Gong, Lingtao Liu, and Xiaoli Wei*
Sinopec Research Institute of Petroleum Processing, Beijing, China

A systematic set of machine-learning designed catalysts were applied in ethane oxidative dehydrogenation reaction, aiming to achieve accurate regulation of catalytic performance and product distribution through the regulation of molecular oxygen on the catalyst surface.

In – Flow Catalytic Production of Levoglucosenone from Levoglucosan over Propylsulfonic Acid Functionalized SBA-15 Using γ – Valerolactone.

***Alexa Gonzalez-Rosario**[1,2], Oscar Oyola-Rivera[3], and Nelson Cardona Martinez[4]*
(1)Chemical Engineering, University of Puerto Rico - Mayagüez, Mayaguez, PR, (2)Department of Natural Sciences, University of Puerto Rico - Carolina, Carolina, PR, (3)Ketjen Corp, Pasadena, TX, (4)Department of Chemical Engineering, University of Puerto Rico - Mayagüez, Mayagüez, PR

We studied the reaction kinetics and catalytic performance of propylsulfonic acid functionalized SBA-15 for levoglucosan (LGA) conversion into levoglucosenone (LGO) in a flow reactor. We obtained a selectivity of 67% towards LGO at 57% LGA conversion. The reaction is second-order reaction for LGA with an activation energy of 37.6 kJ/mol.

Iron Catalysts for Methane Pyrolysis: Understanding the Effects of Carbon Build-up on Structure and Activity (Poster).

***Veronica Piazza**, Lidia Castoldi, Chiara Negri, Marco Orsenigo, Davide Cafaro, Matteo Maestri, Gianpiero Groppi, and Alessandra Beretta*
Laboratory of Catalysis and Catalytic Processes - Dipartimento di Energia, Politecnico di Milano, Milano, Italy

This work examines Fe-Al_2O_3 catalysts at high Fe load for methane pyrolysis. The compositional effects, the role of reduction, the transformations that follow the incipient and extensive growth of carbon are investigated to better elucidate C build-up chemism and obtain rational guidelines to scale-up and industrialization.

Catalysts for Nylon-6 Depolymerization to ε-Caprolactam: Understanding the Structure-Performance Relationship. (Poster).

Prabin Dhakal[1], *Derek Creaser*[2], *and Louise Olsson*[2]
(1)Chemistry and chemical engineering, Chalmers University Of Technology, gothenburg, Sweden, (2)Chemical Engineering, Chalmers University of Technology, Gothenburg, Sweden

We have demonstrated a heterogeneous catalytic pathway for nylon depolymerization using only hydrogen. By investigating the influence of various metal oxide support properties, we provide valuable insights for designing efficient catalysts. These findings contribute to advancing polymer recycling and upcycling, promoting more sustainable processes in a circular economy.

Microwave-Assisted Catalytic Gasification of Various Biomass with Mixed Plastic Wastes for Clean H2 Production.

Ashraf Abedin, *Duy Hien Mai, and Pranjali Muley*
NETL Support Contractor, Morgantown, WV

Catalytic gasification of biomass with plastics has been a challenge since it requires an optimal catalyst to simultaneously activate these materials with complex chemical compositions. This study highlights the roles of Fe-oxide catalyst and biochar produced in-situ during in microwave gasification of plastic-biomass to maximize product selectively towards clean H_2.

Opportunities and Challenges in Utilization of Unrefined Methanol Synthesized from Waste Methane.

Hsiang-Sheng Chen *and Paul Yelvington*
M2X Energy Inc., Rockledge, FL

M2X Energy explores hydrogen production via electrolysis using crude methanol derived from waste methane sources. While impurities increase energy consumption compared to purified methanol, potential solutions include optimizing synthesis operations or developing impurity-tolerant processes, promoting direct use of unrefined feedstock while reducing energy use and emissions from waste methane utilization.

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

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

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

Pretreatment and Catalyst Effects on Biocrude Production Via Hydrothermal Liquefaction of Canadian Lignocellulosic Residues for Renewable Transportation Fuels.

*John Churchill, Venu B. Borugadda, and **Ajay Dalai***
Chemical and Biological Engineering, University of Saskatchewan, Saskatoon, SK, Canada

Mild pretreatment and catalysts significantly influence biocrude yield and quality from lignocellulosic residues during HTL. Despite ineffective washing and steam explosion, alkaline pretreatment with Fe enhanced yields from high-lignin, while acid pretreatment with K_2CO_3 and Fe reduced biocrude oxygen in low-lignin feedstocks. Further methods to improve HTL were also identified.

Catalytic Depolymerization of Polyethylene By Induction Heating: A Continuous Flow Reactor System (Poster).

***Bernard Whajah**, Sharonda Angelle, James Dorman, and Kerry Dooley*
Cain Department of Chemical Engineering, Louisiana State University, Baton Rouge, LA

Our system combining induction heating, metal-exchanged zeolites and in particular those with BEA morphology offers a good chance of long-term catalyst operation for polyolefin depolymerization to gasoline-range products without added H_2. These results underscore the importance of both catalyst selection and operating conditions for the continuous depolymerization of LDPE.

Hydrodeoxygenation of Lignocellulosic Model Compound Using Nickel Phosphide Catalyst Supported on Mesoporous Geopolymer.

***Suraj P**[1] and Sonali Sengupta[2]*
(1)Chemical Engineering, Indian Institute of Technology, Kharagpur, Kharagpur, India,
(2)Chemical Engineering, IIT Kharagpur, Kharagpur, India

Catalytic hydrodeoxygenation is an effective route to upgrade highly oxygenated bio-oils. Herein, nickel deposited (Ni/H-GP) and nickel phosphide (Ni_2P/H-GP) deposited on mesoporous and acidic geopolymer were prepared and tested for anisole hydrodeoxygenation to cyclohexane. Ni_2P/H-GP showed high anisole conversion and selectivity to cyclohexane because of presence of moderate acid sites.

Development and Enhancement of Iron-Based Catalysts to Boost the Conversion of CO_2 to Liquid Hydrocarbons.

Florian Mai
Chair of Chemical Process Engineering, Faculty of Engineering, University of Bayreuth, Bayreuth, Germany

The focus of this research is the development of new catalysts capable of performing both reactions (RWGS + FTS) simultaneously in a single step, thereby increasing the overall efficiency.

Therefore, this study specifically investigated the effects of promoters Cu, Zn and K on sintered iron catalysts for CO_2 hydrogenation.

Utilization of Waste Biomass and Sewage Sludge for CO_2 Capture.

Sarah Stofik, *Thossaporn Onsree, Patton Courie, and Jochen Lauterbach*
Department of Chemical Engineering, University of South Carolina, Columbia, SC

Direct air capture is an emerging field that could counteract the negative impact of rising CO_2 emissions. This work utilizes waste biomass to optimize a material that can capture CO_2 from the air. Initial studies determined that wood-based biomass can capture over 8 wt% in CO_2.

Zeolites and Its Active Cations: Direct Air Capture of CO_2.

Do Yeong Kim[1], *Kyeong-Hun Ryu*[2], *Sungjoon Kweon*[3], *Min Bum Park*[3], *and Sung Bong Kang*[2]
(1)School of Environment and Energy Engineering, Gwangju Institute of Science and Technology, Gwangju, Korea, Republic of (South), (2)Department of Environment and Energy Engineering, Gwangju Institute of Science and Technology, Gwangju, Korea, Republic of (South), (3)Department of Energy and Chemical Engineering, Incheon National University, Incheon, Korea, Republic of (South)

Major findings in this study—including the DAC performance of ZSM-5 with respect to the kind of cation in real atmospheric air and the effect of humidity for DAC performance and behavior on ZSM-5—can be further explored for practical application of zeolite ZSM-5 as a feasible DAC adsorbent.

Advancing Molybdenum Carbide Catalysts for Sustainable Syngas Production in the Reverse Water-Gas Shift.

Wijnand Marquart, Michael Claeys, and ***Nico Fischer***
Department of Chemical Engineering, Catalysis Institute, University of Cape Town, Cape Town, Western Cape, South Africa

Thermodynamics of the rWGS confirm that an effective catalyst kinetically suppresses CO_x methanation and the Boudouard reaction. Mo_2C based catalysts have shown to be highly selective but at elevated pressures these side reactions are more prominent. Transient flow experiments using $^{13}CO_2$ suggest that CH_4 is predominantly formed via CO methanation.

Alkali Activated Carbons from Melamine-Resorcinol-Formaldehyde Resin: Activation Mechanism.

Shailza Sharma[1], *Selvakannan Periasamy*[2], *and Suresh Bhargava*[3]

(1)School of Science, RMIT University, Melbourne, VIC, Australia, (2)Applied Chemistry, RMIT University, Melbourne, Australia, (3)CAMIC, RMIT, Melbourne, VIC, Australia

The escalating CO_2 emissions necessitate advanced mitigation strategies. This study developed nitrogen-rich activated carbons derived from melamine-based resins via a template-assisted approach, enhancing microporosity and achieving a high surface area (2465 m^2/g) with tunable pore diameter (20.4 Å). Comprehensive characterization demonstrates their potential for efficient CO_2 capture and utilization.

Direct CO_2 Hydrogenation to *E-Crude* over a Promoted Fe-Based Catalyst.

Mattia Piacentini, *Beda Rolandi, Alessandro Porta, Luca Lietti, and Carlo Giorgio Visconti*
Dipartimento di Energia, Politecnico di Milano, Milan, Italy

A promoted iron-based catalyst was tested under conditions favoring high selectivity towards e-crude, primarily in the C_8-C_{16} range, with CH_4 and C_2-C_4 paraffins accounting for less than 15% of the products. The catalyst exhibited reversible deactivation, primarily driven by the water partial pressure.

Novel Sputtered ITO/TiO_2 Catalyst for Highly Efficient Reverse Water-Gas Shift Reaction.

Luis F. Bordini[1], *Camila P. Ferraz*[2], *João Monnerat*[3], *and* ***Pedro Romano***[4]
(1)School of Chemistry, Federal University of Rio de Janeiro, Rio de janeiro, Rio de janeiro, Brazil, (2)Chemistry Institute, Federal University of Rio de Janeiro, Rio de Janeiro, Rio de Janeiro, Brazil, (3)Chemistry Institute, Federal University of Rio de Janeiro, Rio de Janeiro, Brazil, (4)Campus D. de Caxias, Federal University of Rio de Janeiro, Rio de Janeiro, Brazil

The study highlights the industrial significance of the Reverse Water Gas Shift (RWGS) reaction for carbon capture and utilization. By employing sputtering for synthesizing ITO/TiO_2 catalysts, the research achieved near-equilibrium conversion and ~100% CO selectivity, advancing CO_2 utilization and supporting sustainable synthetic fuel production through innovative catalytic processes.

Tailoring Catalyst for CO_2 Hydrogenation: Synthesis and Characterization of NH_2-MIL-125 Frameworks.

Leidy Patricia Figueroa Quintero[1], *Tomás Cordero*[2], *Enrique V. Ramos Fernandez*[1], *Unni Olsbye*[2], *and Javier Narciso*[1]
(1)University Institute of Materials (IUMA), Inorganic Chemistry Department, University of Alicante, Alicante, Spain, (2)Department of Chemistry, University of Oslo, Oslo, Norway

This work details the innovative modification of NH2-MIL-125 with Zr, Ce, and Cu, enhancing its stability and catalytic efficiency. These advanced catalysts offer a sustainable approach to CO_2 valorization, paving the way for methanol production while contributing to environmental impact reduction.

CO_2 Hydrogenation over Cu on Early Transition Metal Carbides and Nitrides on Alumina Supports.

Siobhan Brown[1], *Justin Notestein*[2], *and Neil Schweitzer*[3]
(1)Center for Catalysis and Surface Science, Northwestern University, Evanston, IL,
(2)Department of Chemical & Biological Engineering, Northwestern University, Evanston, IL,
(3)Department of Chemical and Biological Engineering, Northwestern University, Evanston, IL

The goal of our work is to study the dynamic nature of supported early transition metal carbides and nitrides (TMNC) by varying their local environment by careful synthesis of the TMNC layer. We present a study of the impact of TMNC phases on supported-Cu for CO_2 hydrogenation to C1 products.

Cu-ZnO Bimetallic Catalyst for Industrial Relevant Production of C_{2+} Alcohols in the Alkaline CO_2 Electrolyzer.

Taha Baghban-Ronaghi[1], *Seyed Parsa Amouzesh*[1], *Sina Fazlifard*[1], *Praveen Raju*[1], *and Mohammad Asadi*[2]
(1)Chemical and Biological Engineering, Illinois Institute of Technology, Chicago, IL,
(2)Chemical and Biological Engineering, Illinois Tech, Chicago, IL

Electrocatalytic CO_2 reduction in alkaline media shows promise for carbon mitigation and sustainable alcohol production at industrial rates. However, achieving high alcohol selectivity with copper catalysts in moderate environments proves challenging. Advancing efficient catalysts to maintain high current densities and selectivity for alcohols remains a key challenge.

Direct CO_2 Hydrogenation to C_{2+} carboxylic Acids Via Heterogenous Thermo-Catalysis in Liquid Phase.

Satya Sireesha Rameswarapu[1], *Rajan Lakshman*[1], *Paul Webley*[1], *and Akshat Tanksale*[2]
(1)Chemical and Biological Engineering, Monash University, Clayton, VIC, Australia,
(2)Chemical Engineering, Monash University, Clayton, VIC, Australia

This research tackles the challenges of direct CO_2 hydrogenation to C_{2+} carboxylic acids, including low yields and high energy barriers, by employing metal organic frame work-derived catalysts. It establishes sustainable route for acetic acid production, reducing CO_2 emissions, decreasing fossil fuel dependence, and promoting green chemical synthesis for industrial applications.

Advancing CO_2 Methanation Catalysts.

Shubham Sharma and ***Sagar Sourav***
Chemical Engineering, Indian Institute of Technology Madras, Chennai, Tamil Nadu, India

A novel catalyst was designed and demonstrated for highly exothermic CO_2 methanation reaction. The core of the catalyst has a highly conductive material for effective heat dissipation, where as the surface layers have chemical functionalities to efficiently carry out the reaction.

Probing the Effects of Potassium on the Structural Properties and Reactivity of Iron-Based CO_2 Hydrogenation Catalysts.

Sinqobile Vuyisile Lusanda Mahlaba[1], *Alisa Govender*[2], *Jaco Olivier*[3], *and Eric van Steen*[1,4]
(1)Catalysis Institute, Dpt. Chemical Engineering, University of Cape Town, Rondebosch, Western Cape, South Africa, (2)Energy Operations, R&T, SASOL, Sasolburg, Free State, South Africa, (3)Centre for High Resolution Transmission Electron Microscopy, Nelson Mandela University, Gqeberha, Eastern Cape, South Africa, (4)Catalysis Institute, Dpt. Chemical Engineering, University of Cape Town, Cape Town, South Africa

The role of potassium on the performance of pre-carbided hematite in the hydrogenation of CO2 shows that the activity is hardly affected, whereas the selectivity is strongly affected by potassium. This is linked to the phase composition, and the CO2 and CO adsorptive properties.

Thermocatalytic Hydrogenation CO_2 to Methanol over Medium and High-Entropy Oxides.

Amy Knorpp[1], *Monika Mielniczuk*[1,2], *and Michael Stuer*[1]
(1)Empa, Duebendorf, Switzerland, (2)AGH University of Science and Technology, Krakow, Poland

Mesoporous high-entropy oxides (HEOs) were synthesized with 5 to 7 cations (Al, Cr, Fe, Co, In, Ga, Ce) using a solvothermal technique. Synthesized materials were active for the thermocatalytic hydrogenation of CO_2 to methanol, and differences in the selectivities were observed between samples, showing HEOs are potential tailorable hydrogenation catalysts.

Toward Understanding the Mechanism of Selective Hydrogenation of CO_2 on Rh-Based Catalysts.

*Yifeng Zhu, **Honghong Shi**, Libor Kovarik, John L. Fulton, Oliver Gutiérrez-Tinoco, and Johannes Lercher*
Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA

The multifunctional sites at the FeO_x−Rh interface exhibit significantly stronger interactions with CO_2 compared to Rh-only surfaces, presenting higher energy barriers for C−O bond cleavage while providing a barrierless pathway for the stabilization and facile-hydrogenation of methoxy species, therefore enabling the selective CO_2-to-methanol conversion process.

First-Principles Aided Understanding of Oxidative Degradation of Amines Supported on Silica during CO_2 Capture.

Neha Mehra[1], *Wilson McNeary*[1], *Gabrielle Kliegle*[1], *Wade Braunecker*[2], *and Carrie Farberow*[1]
(1)Catalytic Carbon Transformation and Scale-Up Center, National Renewable Energy

Laboratory, Golden, CO, (2)Chemistry and Nanoscience Center, National Renewable Energy Laboratory, Golden, CO

Stability of amine-based adsorbents against degradation by oxygen is critical for sustained performance over multiple regenerative CO_2 capture cycles. We perform density functional theory calculations on *N*-methyl-3-aminopropyl (MAPS), a secondary amine, to examine CO_2 binding to silica-grafted MAPS and evaluate the energetics of oxidative pathways yielding amide and imine products.

Molten Salt Upcycling of CO_2 to Diverse Carbon Architectures for Energy Storage Applications.

Shannon Mahurin[1]*, Bishnu Prasad Thapaliya*[1]*, Siyuan Gao*[1]*, Dylan Weber*[2]*, Aye Meyer*[2]*, Eric Wolfe*[3]*, and Sheng Dai*[4]
(1)Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN,
(2)Manufacturing Science Division, Oak Ridge National Laboratory, Oak Ridge, TN,
(3)Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN,
(4)Chemical Sciences Division, Oak Ridge National Laboratory (ORNL), Oak Ridge, TN

The electrocatalytic upcycling of CO_2 into value-added carbon materials with controlled microstructure in a carbonate molten salt system as a means to utilize waste CO_2 and reduce carbon emissions is reported. The effect of reaction conditions on the carbon product and a preliminary techno-economic analysis will be presented.

Zeolites-Based Dual Function Materials (DFMs) for CO_2 Capture and in-Situ Methanation: Effect of Zeolite Framework.

Galal Nasser, Shaza Yousef, and ***Jan Kopyscinski***
Catalytic & Plasma Process Engineering, Department of Chemical Engineering, McGill University, Montreal, QC, Canada

This study explores zeolites as potential Dual-Function Materials (DFMs) for integrated CO_2 capture and in-situ methanation. The synthesized cost-effective zeolites demonstrated high CO_2 adsorption. The research contributes to the advancement of efficient carbon management technologies and achieving the goal of net-zero emissions by enhancing the utilization of CO_2 and energy.

Mo-Modified Zeolites for Methane Aromatization: A Study on Metal Speciation, Distribution, and Control.

Emanuele J Hiennadi[1]*, Fateme Molajafari*[2]*, Rachita Rana*[3]*, Adam Hoffman*[4]*, Simon Bare*[4]*, Joshua D. Howe*[2]*, and* ***Sheima Khatib***[1]
(1)Chemical Engineering, Virginia Tech, Blacksburg, VA, (2)Chemical Engineering, Texas Tech University, Lubbock, TX, (3)Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, MA, (4)Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, Menlo Park, CA

Through combined experimental and computational endeavors, this work investigates what factors may govern the speciation, distribution, and evolution of Mo species supported on H-ZSM-5 for methane aromatization. Preparation technique and/or metal loading can influence the distribution of precatalytic Mo-oxide structures (MoO_2^{2+}, MoO_2OH^+, $Mo_2O_5^{2+}$) existing simultaneously.

Surface Carbon Formation and Its Impact on Methane Dry Reforming Kinetics on Rh-Based Catalysts By Operando Raman Spectroscopy.

Riccardo Colombo[1], Gianluca Moroni[1], Chiara Negri[1], Matteo Monai[2], Bert M. Weckhuysen[2], and ***Matteo Maestri***[1]
(1)Laboratory of Catalysis and Catalytic Processes - Dipartimento di Energia, Politecnico di Milano, Milano, Italy, (2)Inorganic Chemistry and Catalysis, Institute for Sustainable and Circular Chemistry, Utrecht University, Utrecht, Netherlands

A mechanism for carbon deposition and its impact on Methane Dry Reforming kinetics using rhodium-based catalysts is presented. Coupling operando Raman spectroscopy and kinetic analysis, we discovered that carbon deposition on Rh/α-Al_2O_3 catalyst follows a nucleation-growth mechanism strongly influenced by the CO_2/CH_4 ratio and the CH_4 inlet concentration.

Enhancing Surface Activity through in-Situ Exsolution of Co-Fe Nanoparticles on Co-Doped (La,Sr)FeO_3 Perovskite for Electrocatalytic Oxidative Coupling of Methane (OCM).

Serra Yesilata[1]*, Jaesung Kim[1], Yu Jin Kim[2], Matthew Ferree[1], Seval Gunduz[1], Anne Co[3], Minkyu Kim[2], and Umit Ozkan[1]*
(1)William G. Lowrie Department of Chemical & Biomolecular Engineering, The Ohio State University, Columbus, OH, (2)Yeungnam University, Gyeongsan, Geongbuk, Korea, Republic of (South), (3)Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH

Performing oxidative coupling of methane (OCM) reactions in solid oxide cells is a promising approach for converting methane into olefins. This study focuses on modifying the surface properties of Co-doped (La,Sr)FeO_3 via in-situ exsolution of CoFe alloy nanoparticles to enhance its activity for electrochemical OCM reactions.

Autothermal Dry Reforming of Methane at Kg-Lab Scale Using Ni-Ugso Catalyst Pellets at Elevated Pressures: A Parametric Study.

Nicolas Abatzoglou[1]*, Muhammad Irfan Malik[2], Esma Ines Achouri[3], and Jasmin Blanchard[4]*
(1)Chemical & Biotechnological Engineering, Université de Sherbrooke, Sherbrooke, QC, Canada, (2)Chemical & Biotechnological Engineering, UNIVERSITE DE SHERBROOKE, SHERBROOKE, QC, Canada, (3)Génie Chimique et Génie Biotechnologique, Université de Sherbrooke, Sherbrooke, QC, Canada, (4)KWI Polymenrs Inc., Sherbrooke, QC, Canada

This work presents the experimental evaluation of pelletized Ni-UGSO catalyst applied to dry catalytic reforming of methane at elevated pressures. A kg-lab scale setup was used and the reported results show that the pellets have better performances than the powder used at g-lab scale. The optimal operating conditions are presented.

Support Effects in Fischer-Tropsch Synthesis.

Truc Phung[1], *Liney Arnadottir*[2], *Gregory R. Johnson*[3], *and Konstantinos Goulas*[4]
(1)School of Chemical, Biological and Environmental Engineering, Oregon State University, Corvallis, OR, (2)Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA, (3)Chemical and Biomolecular Engineering, University of California, Berkeley, Berkeley, CA, (4)Oregon State University, Corvallis, OR

New developed generation of Fischer-Tropsch catalysts that optimizes the C_{5+} selectivity under ambient pressure condition by leveraging the electronic metal-support interaction. Our hypothesis is that by using basic oxide supports, electron can be injected into metal nanoparticles, strengthening binding of CO to the surface and driving the selectivity toward C_{5+}.

Microkinetic Modeling of the Fischer-Tropsch Synthesis over Co: Pushing Boundaries through Automated Mechanism Generation.

Bjarne Kreitz[1,2], *Kirk Badger*[1], *and C Franklin Goldsmith*[1]
(1)School of Engineering, Brown University, Providence, RI, (2)School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA

The Reaction Mechanism Generator (RMG) is extended to automatically develop detailed chemical kinetic models for the Co-catalyzed Fischer-Tropsch synthesis. RMG explores a chemical reaction space of over 170k possible reactions. Microkinetic modeling with detailed chemical kinetics provides insights into the chain growth mechanism and the role of abstraction reactions.

In-Situ XAS Investigation of Co-Based Model Catalysts for FTS.

Rabia Ilica[1,2], *Anna Zimina*[1,2], *Erisa Saraçi*[1,2], *Enrico Sireci*[1], *Felix Studt*[1], *Cherie Hsu*[1], *Moritz Wolf*[3], *and Jan-Dierk Grunwaldt*[1,2]
(1)Institute of Catalysis Research and Technology (IKFT), Karlsruhe Institute of Technology (KIT), Eggenstein-Leopoldshafen, Germany, (2)Institute for Chemical Technology and Polymer Chemistry (ITCP), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany, (3)Engler-Bunte-Institut (EBI), Karlsruhe Institute of Technology (KIT), Karslruhe, Germany

This *in-situ/operando* XAS study provides valuable insights into catalyst reduction behavior during FTS. By preparing model catalysts with two different methods, this study promotes to accelerate the identification of key parameters influencing the catalytic performance and especially, by metal-support-interaction, helping optimize catalyst design for improved efficiency and stability in FTS.

Iron Silicalite-1 for Oxidative Dehydrogenation of Ethane.

Muntaseer Bunian[1], Sungsik Lee[2], and ***Yu Lei**[3]*
(1)Paula M. Trienens Institute for Sustainability and Energy, Northwestern University, Evanston, IL, (2)X-ray Science Division, Advanced Photon Source, Argonne National Laboratory, Lemont, IL, (3)Department of Chemical and Materials Engineering, University of Alabama in Huntsville, Huntsville, AL

This work investigates the selective oxidation of ethane using silicalite-supported iron oxide catalysts. Framework iron species enhance selectivity by modulating acidity, while extra-framework species improve activity. Incorporating nickel facilitates ethane oxidative dehydrogenation with CO_2 as an oxidant, offering an environmentally friendly route to value-added chemicals.

Mechanism in Ethanol Upgrading to 1-Butanol over MgO Catalyst: Insights from Synchrotron Irradiation-Based Nanospectroscopy.

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

Synchrotron Irradiation-based Nanospectroscopy (SINS) was employed to investigate ethanol upgrading to 1-butanol over MgO catalysts. By integrating Ex situ Ethanol Temperature-Programmed Desorption and SINS, local reaction intermediates were identified. Results reveal magnesium hydride's role as a surface intermediate, advancing mechanistic understanding of the Guerbet reaction pathway for new catalysts design.

Exploiting Mo-V Catalysts in Non-Oxidative and Oxidative (CO_2- and O_2-Assisted) Propane Dehydrogenation.

***Letícia Rasteiro**[1], Victor Brandão[2], Carsten Sievers[2], and Leandro Martins[3]*
(1)Institute of Chemistry, Sao Paulo State University, Araraquara, Sao Paulo, Brazil, (2)School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA, (3)State University of Sao Paulo, Araraquara, Brazil

This study investigates catalysts for propane dehydrogenation (DHP) and oxidative dehydrogenation (ODHP) using CO_2 and O_2. V_MoO_3 showed high stability and selectivity, while MoV-N_2 exhibited higher propane conversion but rapid deactivation in CO_2-ODHP. The findings highlight the importance of reaction conditions in influencing catalyst behavior and coke formation.

Enhancing the Carbon and Energy Efficiency in SAF Production: Converting Alkenes to Aromatics and Hydrogen.

***Yang He**, Udishnu Sanyal, Junxia Wang, and Karthikeyan Ramasamy*
Pacific Northwest National Laboratory, Richland, WA

Ga- and Zn-promoted ZSM-5 catalysts boost SAF-range aromatic yields and hydrogen production from olefins, addressing by-product inefficiencies in Fischer-Tropsch synthesis. This scalable approach enhances carbon and energy efficiency in SAF production, optimizing reaction pathways via tailored zeolite acidity and metal sites to support aviation decarbonization and sustainable fuel goals.

Support Effects in Butadiene Hydrogenation over Cu and PtCu Dilute-Limit Alloys.

Ho Yi Lam[1] *and Nathaniel Eagan*[2]
(1)Chemical and Biological Engineering, Tufts University, Medford, MA, (2)Department of Chemical and Biological Engineering, Tufts University, Medford, MA

Selective hydrogenation of 1,3-butadiene to butene was studied using Cu-based catalysts supported on SiO_2, TiO_2, and CeO_2. CeO_2 showed the highest activity but reduced selectivity to form butane. Alloying Cu with Pt improved activity but reduced selectivity, especially on CeO_2, attributed to interfacial site effects and possible Pt aggregation.

Understanding the Effects of Organic Coatings on 4-Nitrostyrene Hydrogenation Selectivity over Pt Catalysts.

Jesús Meléndez Gil*, Wilson A. Smith, and J. Will Medlin*
Department of Chemical and Biological Engineering, University of Colorado Boulder, Boulder, CO

The effects of different organic coatings (thiols, phosphonic acids (PAs), and ionomers) on 1wt%Pt/TiO_2 were studied for the hydrogenation of 4-nitrostyrene. Thiol coatings shifted product selectivity towards 4-aminostyrene, while PAs and ionomers shifted towards 1-ethylnitrobenzene. These changes were attributed to the identity of adsorption sites modified by the different coatings.

Identifying and Solving the Catalytic Deactivation Problem to Improve Process Performance.

Steve Wainwright[1] *and* ***Shane Chen***[2]
(1)Johnson Matthey, Royston, United Kingdom, (2)Johnson Matthey, West Deptford, NJ

A key consideration in catalyst and process design is expected lifetime of the catalyst and the acceptable loss over time of catalytic activity and/or selectivity. By more effectively identifying the root cause of the deactivation in a process the correct mitigation can be implemented in a timely and cost-efficient manner.

Investigating the Kinetics of Ethane Hydrogenolysis over Supported Liquid Metal Catalysts.

Iklim Gokce[1]*, Kathryn MacIntosh*[2]*, and Robert Rioux*[3,4]
(1)Chemical Engineering, The Pennsylvania State University, University Park, PA, (2)Chemical

and Biomedical Engineering, The Pennsylvania State University, University Park, PA, (3)Department of Chemical Engineering, The Pennsylvania State University, University Park, PA, (4)Department of Chemistry, The Pennsylvania State University, University Park, PA

Ethane hydrogenolysis is studied over Ni-Ga liquid metal catalysts to evaluate the influence of H_2 absorption by Ga. Determination of the surface ensemble sizes and bulk partitioning of the catalytically active metals due to H_2 would allow for the application of these catalysts in combined catalytic reaction/separations.

Mesoporous Organosilica As Catalyst Support for Aqueous Phase Hydrogenation of Phenol: The Effect of Aromatic Content and Amine Loading of the Support.

***Snehal Patil**[1], James N. Gyamfi[1], Anagha Hunoor[2], Luke Gillespie[1], Paul Edmiston[3], and Umit Ozkan[1]*
(1)William G. Lowrie Department of Chemical & Biomolecular Engineering, The Ohio State University, Columbus, OH, (2)William G. Lowrie Department of Chemical and Biomolecular Engineering, The Ohio State University, Columbus, OH, (3)The College of Wooster, Wooster, OH

ABPS, a silica-based hybrid material, was used as support for Pd catalysts for aqueous phase phenol hydrogenation. Pd catalysts supported on ABPS-type supports performed significantly better than conventional Pd/SBA-15 and Pd/AC. Aromatic groups of ABPS imparted thermal stability to the support and improved Pd dispersion. Amine incorporation enhanced cyclohexanone yield.

Insights into Solvation Thermodynamics Under Different Pores and Solvent Environments in Zeolite Catalysts.

***Xiuting Chen**[1] and Rachel Getman[2]*
(1)William G. Lowrie Department of Chemical and Biomolecular Engineering, The Ohio State University, Columbus, OH, (2)Department of Chemical and Biomolecular Engineering, The Ohio State University, Columbus, OH

To clarify the influence of solvent mixtures on the stability of adsorbates, we study their solvation thermodynamics in solvent mixtures and compare them to pure water solvent. Increases (becoming more positive) of solvation entropies are observed in methanol/water mixtures compared to pure water.

Calorimetric Study of Acid-Base Interactions in Solvated Zeolite Voids.

***Jeong Hwan Lee**[1], Yanyu Mu[1], and Robert Rioux[2,3]*
(1)Chemical Engineering, The Pennsylvania State University, University Park, PA, (2)Department of Chemical Engineering, The Pennsylvania State University, University Park, PA, (3)Department of Chemistry, The Pennsylvania State University, University Park, PA

Calorimetric analysis of base molecule adsorption on acidic zeolites in gas and liquid phases helps build a Born-Haber cycle to assess solvation effects. This study aims to deepen understanding of solvent impacts on acid-base interactions in zeolites, crucial for designing liquid-phase catalytic reactions.

Mechanistic Approaches to Solvent Design for Acid-Catalyzed Biorenewable Chemical Processes.

Mohd Ussama[1]*, Gourav Shrivastav*[1]*, Rachit Khare*[2]*, Johannes A. Lercher*[2]*, and M. Ali Haider*[1]
(1)Chemical Engineering, Indian Institute of Technology Delhi, New Delhi, India,
(2)Department of Chemistry, Technische Universität München, Garching, Germany

This study explores mechanistic insights into acid-catalyzed lactone dehydration in various solvents, highlighting how solvent nature and polarity influence reaction environments. Optimizing solvent-reactant interactions, including those with Brønsted acidic protons, the study proposes solvent recipes to enhance biomass-derived oxygenate conversions, improving conversion, product selectivity, and reducing reaction free energy barriers.

O_2-Cofeed Demonstrates the Potential of Surface H-Scavenging to Boost Ammonia Decomposition on Ru-Based Catalysts.

Yi Qiu[1] *and Alessanda Beretta*[2]
(1)Politecnico di Milano, Dipartimento di Energia, Via La Masa, Milan, Milan, Italy,
(2)Politecnico di Milano, Dipartimento di Energia, Via La Masa, Milan, Italy

This work reveals that a significant improvement of NH_3 decomposition kinetics lies in the elimination of the H*-saturation. This concept (demonstrated by O_2-cofeed tests) paves the way for designing multifunctional reactors where H_2 is removed from the Ru sites by varying methods, creating an expansive field for chemical reaction engineering.

Highly Efficient Low Metal Content Ni/CeO_2 Catalysts Prepared Bymagnetron Sputtering Deposition for Ethanol Steam Reforming.

Letícia Sosa[1]*, Marco Aurélio Suller Garcia*[2]*, Augusto C. A. Silva*[1]*, Bráulio S. Archanjo*[3]*, Adriano F. Feil*[4]*, Dario Eberhardt*[4]*, Santiago J. A. Figueroa*[5]*, João Monnerat*[6]*, and Pedro Romano*[7]
(1)LIPCAT, UFRJ, Rio de Janeiro, Brazil, (2)UFRJ, Rio de Janeiro, Brazil, (3)INMETRO, Rio de Janeiro, RJ, Brazil, (4)Bluenano group, Porto Alegre, RS, Brazil, (5)CNPEM, Campinas, SP, Brazil, (6)Chemistry Institute, Federal University of Rio de Janeiro, Rio de Janeiro, Brazil, (7)Campus D. de Caxias, Federal University of Rio de Janeiro, Rio de Janeiro, Brazil

This study compares synthesis methods (sputtering deposition, SP, and incipient wetness impregnation, IWI) for Ni/CeO_2 catalysts in ethanol steam reforming. The SP catalyst exhibited superior hydrogen production, attributed to uniform Ni nanoparticle distribution, enhanced metal-support interactions, and increased oxygen vacancies, optimizing catalytic performance.

Experimental and CFD Study of CH_4 Pyrolysis over Fe-Al_2O_3 Catalyst: The Challenge of C Build-up for the Kinetic and the Reactor Studies.

*Davide Cafaro, Marco Orsenigo, **Veronica Piazza**, Chiara Negri, Lidia Castoldi, Gianpiero Groppi, Matteo Maestri, and Alessanda Beretta*
Laboratory of Catalysis and Catalytic Processes - Dipartimento di Energia, Politecnico di Milano, Milano, Italy

Thermo-catalytic methane pyrolysis is explored for CO_2-free hydrogen using Fe-Al_2O_3 catalysts. In this work, iron-based catalysts with Al_2O_3 as textural promoter were prepared and tested for CH_4 pyrolysis at different scales and reactor configurations, integrating experiments with a comprehensive reactor and kinetic modeling to guide process optimization and scale-up.

Highly Active Ru/CeO_2 Catalysts Prepared By Conventional Iwi and Novel Mechanochemistry Methods for Ammonia Cracking.

*Yi Qiu[1], Ivan Conti[1], Nicole Bendazzoli[1], Rudy Calligaro[2], Alessandro Trovarelli[2], Enzo Alessio[3], Elisabetta Iengo[3], and **Alessanda Beretta**[1]*
(1)Laboratory of Catalysis and Catalytic Processes - Dipartimento di Energia, Politecnico di Milano, Milano, Italy, (2)Dipartimento Politecnico di Ingegneria e Architettura, Università degli Studi di Udine, Udine, Udine, Italy, (3)Dipartimento di Scienze Chimiche e Farmaceutiche, Università degli Studi di Trieste, Trieste, Trieste, Italy

Ru is the preferred catalyst for NH_3 cracking, but its reaction rate is limited by Ru–H* interaction, especially at higher temperatures. The support plays a crucial role: CeO_2 offers outstanding performance and minimizes H* poisoning, and both factors are highlighted over the catalyst obtained by milling.

Electrified Ammonia Cracking Via Indirect Joule Heating of Thermally Conductive Packed Pocs.

***Federico Sascha Franchi**[1], Matteo Ambrosetti[1], Alessandra Beretta[1], Gianpiero Groppi[1], Enrico Tronconi[1], Giovanna Massobrio[2], and Matteo Lualdi[2]*
(1)Laboratory of Catalysis and Catalytic Processes - Dipartimento di Energia, Politecnico di Milano, Milano, Italy, (2)SNAM, Milano, Italy

A NH_3 cracking reactor which uses a thermally conductive aluminium POCS, packed with Ru-based catalyst and heated internally by a resistive heater in thermal contact with the POCS, enables high conversion and thermal efficiency in a compact reactor with reduced temperature gradients, while enabling fast heat up and excellent scalability.

Finding the Needle in the Haystack: Material Discovery and Design for Oxygen Electrocatalysis.

Kasun Gunasooriya
Chemical, Biological & Materials Engineering, University of Oklahoma, Norman, OK

Discovering acid-stable and active catalysts for oxygen electrocatalysis remains a challenging task. Based on our extensive theoretical work, we discuss strategies to improve the OER catalytic activity, stability, and the remaining challenges.

Enhancement of Ce^{3+} in Reduced CeO_2 Via U-Ce Charge Transfer. Implications on Hydrogen Production By the Thermochemical Water Splitting Reaction..

Carlos Morales[1]*, Rudi Tschammer*[1]*, Ingo Flege*[1]*, Thomas Gouder*[2]*, and* ***Hicham Idriss***[3]
(1)Brandenburg University of Technology, Cottbus, Germany, (2)European Commission, Karlsruhe, Germany, (3)Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

Hydrogen production via thermochemical water splitting over polycrystalline $Ce_{1-x}U_xO_2$ and single crystalline is investigated. Test reactions indicated that a small % of U (<10 %) is optimal for production hydrogen production. This is tracked down to the increase in Ce^{4+} reduction to Ce^{3+} because of the presence of U^{4+} cations.

Ni Atomically Dispersed in CeO_2 Aerogels for Unprecedented Selectivity in the Water-Gas Shift Reaction.

Travis Novak[1]*, Austin Herzog*[2]*, Matthew Buck*[3]*, Kyle Sendgikoski*[2]*, Ryan DeBlock*[1]*, Todd H. Brintlinger*[4]*, Paul A. DeSario*[5]*, and Debra Rolison*[1]
(1)Chemistry, Surface Chemistry Branch, U.S. Naval Research Laboratory, Washington, DC, (2)NRC Postdoc, Naval Research Laboratory, Washington, DC, (3)Chemistry, US Naval Academy, Annapolis, MD, (4)Materials Science and Technology Division, U. S. Naval Research Laboratory, Washington, DC, (5)Office of Naval Research, Arlington, VA

Atomically dispersing Ni in CeO_2 aerogels solves a key selectivity problem present in traditional Ni-based water-gas shift (WGS) catalysts. The 2.5% at.% Ni in CeO_2 aerogel catalyst (2.5NiCeO) combines unprecedented selectivity (< 2 ppm CH_4) with excellent activity and stability, marking a notable advance in WGS catalysts.

Novel Ni-Co/$Ca_{12}Al_{14}O_{33}$ Bimetallic Catalyst for Hydrogen Production Via Sorption-Enhanced Steam Methane Reforming Process.

Ahmad Farooqi, Muhammad Zubair Shahid, and ***Medhat Nemitallah***
King Fahd University of Petroleum & Minerals, Dhahran, Saudi Arabia

SE-SMR is the emerging technology to produce clean hydrogen and has the potential to replace the conventional SMR process. The present study has proposed an efficient catalyst/bifunctional material (Ni-Co/$Ca_{12}Al_{14}O_{33}$) that has proven excellent performance to achieve high methane conversion and low CO_2 emissions.

Mechanism of Electrochemical C=O Hydrogenation and Electroreductive C-C Coupling on Cu Cathodes.

Rachit Khare[1]*, Hongwen Chen*[1]*, and Johannes A. Lercher*[1,2]

(1)Department of Chemistry, Technische Universität München, Garching, Germany, (2)Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA

Aqueous-phase electrochemical hydrogenation of benzaldehyde on Cu leads to the formation of both benzyl alcohol and hydrobenzoin. By combining kinetic studies with molecular simulations, we present the mechanism of benzaldehyde conversion and describe the mechanistic conditions that facilitate C-C coupling between conjugated aromatic aldehyde molecules on metal surfaces.

Oxide Supported Single-Atom Catalysts for Oxygen Electrocatalysis.

Keishana Navodye S. a.[1] *and Kasun Gunasooriya*[2]
(1)School of Sustainable Chemical, Biological and Materials Engineering, University of Oklahoma, Norman, OK, (2)Chemical, Biological & Materials Engineering, University of Oklahoma, Norman, OK

Single atom catalysts (SAC) supported on acid stable SnO_2 were evaluated for the stability and activity under oxygen electrochemical conditions. We further used machine learning to identify descriptors and to predict adsorption energies. Based on these theoretical findings, rational catalyst design principles for next-generation SACs based oxygen electrocatalysts are established.

Modeling Electron-Hole Recombination in Promising Photocatalytic Magnetic Materials.

Nicholas Harmon *and David Kumi*
Physics and Engineering Science, Coastal Carolina University, Conway, SC

We develop a set of rate equations for carrier charge and spin in order to calculate electron-hole recombination in magnetically doped perovskites and other materials. Our results show that carrier decay times can be optimized by engineering the electronic structure.

Hierarchical Analysis of Transport Limitations in Gas-Diffusion Electrode Based CO_2 Electroreduction.

Kaustav Niyogi*, Mauro Bracconi, and Matteo Maestri*
Laboratory of Catalysis and Catalytic Processes - Dipartimento di Energia, Politecnico di Milano, Milano, Italy

This work explains the experimentally observed gas-diffusion electrode based CO_2 electrolyzer under-performance at high current densities, using a continuum modeling approach. Our analysis shows that the GDE diffusional resistance significantly influences the experimentally measured reaction rates, highlighting the importance of considering such limitations when benchmarking the electrolyzer performance.

Towards the Complete Mineralization of PFOA with a Pilot-Scale UV-Light, Boron-Nitride—Based Recirculating Reactor Unit.

Juan Donoso[1], *Kimberly N. Heck*[1], *Mohamed Ateia*[2], *and Michael Wong*[1]
(1)Department of Chemical and Biomolecular Engineering, Rice University, Houston, TX,
(2)Chemical and Biomolecular Engineering, Rice University, Houston, TX

Heterogeneous photocatalysis shows promise for PFAS destruction but faces challenges like low material activity and byproduct formation. This study demonstrates >99% PFOA defluorination using boron nitride (BN) in a UV flow reactor, outperforming TiO_2. BN's resilience to tap water anions highlights its potential for practical PFAS remediation.

Synthesis of High Efficiency and More Durable Pt-Ni Nanocatalysts.

Shutang Chen
Honda Research Institute USA Inc., San Jose, CA

Pt-Ni nanocatalysts demonstrated the best durability performance in acid electrolyte when compare with the state of the art.

Conductive Polymer-Coated Hydrophobic Membrane with Electrocatalyst As Robust Gas Diffusion Electrode for Long-Term Operation.

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

This first-of-its-kind gas diffusion layer (GDL) consisting of conductive polymer and hydrophobic membrane shows remarkably enhanced long-term stability at commercially relevant current regime compared to current carbon-based GDL, and represents the next generation GDL technology for various electrocatalytic reactions making the implementation of electrochemical conversion commercially viable.

V-Fe Based Photocatalysts for Oxidative Desulfurization of Dibenzothiophenes.

Luis Cedeño-Caero*, Marco A. Alvarez-Amparan, and Uriel Chacon-Argaez*
ING. QUIMICA, FAC. QUIMICA, UNAM, CDMX, DF, Mexico

Several V oxides formulations on alumina modified with Fe were evaluated on the photocatalytic oxidative desulfurization (PODS) of dibenzothiophene compounds. The structural and optical properties, and surface species of the catalysts were determined by SEM-EDS, TPR, XRD, Raman, ATR-FTIR, photoluminescence, UV-Vis diffuse reflectance, and XPS spectroscopy.

First-Principles Study of Hybrid Structure Containing Pt Clusters inside CNTs: Application As ORR Catalysts.

Hyeong Kyu Park
Department of Chemistry and Chemical Engineering, Inha University, Incheon, Korea, Republic of (South)

The overuse of fossil fuels drives global warming. PEMFCs offer clean energy but face commercialization challenges due to expensive Pt catalysts. Using DFT, we designed Pt@CNT hybrids to reduce Pt usage while enhancing ORR activity. PtM alloys further improve performance, analyzed via electronic structure studies.

Cu_2O-Pd Photocatalysts for Carbon-Carbon Coupling Reactions in Ambient Conditions.

Ravi Teja Addanki Tirumala[1], ***Shivam Kumar***[2], *and Marimuthu Andiappan*[3]
(1)Center for Environmentally Beneficial Catalysis, University of Kansas, Lawrence, KS, (2)School of Chemical, Biological, and Materials Engineering, University of South Florida, Tampa, FL, (3)Department of Chemical, Biological and Materials Engineering, University of South Florida, Tampa, FL

This work demonstrates the potential of Cu_2O-Pd hybrid photocatalysts for efficient, visible light-driven oxidative C-C coupling reactions under ambient conditions, offering a sustainable pathway for producing high-value chemicals in pharmaceutical, agrochemical, and fine chemical industries. This approach demonstrates an eco-friendly, energy-efficient method for solar-driven chemical transformations under ambient, base-free conditions.

Effects of Pt:Pd Ratios on the Activity and Stability of Pt:Pd/γ-Al_2O_3 Catalysts for Lean Methane Oxidation.

Min Wang[1], ***Haiying Chen***[2], *Yuliana Lugo-Jose*[3], *Melissa Hess*[3], *Joseph M. Fedeyko*[3], *Todd Toops*[1], *and Jacqueline Fidler*[4]
(1)Oak Ridge National Laboratory, Oak Ridge, TN, (2)National Transportation Research Center, Oak Ridge National Laboratory, Knoxville, TN, (3)Clean Air - SEC, Johnson Matthey, Audubon, PA, (4)CONSOL Energy, Canonsburg, PA

Addition of Pt to PdO/γ-Al_2O_3 catalyst has been recognized to enhance the on-stream stability of the catalyst in methane oxidation reactions. In this study, we systematically vary the Pt:Pd ratios from 1:0 to 0:1 with total (Pt+Pd) loading at 3 wt.% to investigate the effects of Pt in PtPd/γ-Al_2O_3 system.

Catalysts Based on Pt Clusters and Nanoparticles on CeO_2: Influence of the Noble Metal Size and Support Morphology in the Oxidation of CO.

Nicola Da Roit[1], *Christian Schmitt*[1], *Joachim Czechowsky*[2], *Omar Bettini*[3], *Ajai Lakshmi Nilayam*[4], *Marco Neumaier*[4], *Christian Kübel*[4], *Silvia Gross*[3], *Manfred Kappes*[4], *Maria Casapu*[2], *and Silke Behrens*[1]
(1)Institute of Catalysis Research and Technology (IKFT), Karlsruhe Institute of Technology (KIT), Eggenstein-Leopoldshafen, Germany, (2)Institute for Chemical Technology and Polymer Chemistry (ITCP), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany, (3)Department of Chemical Sciences, University of Padova, Padova, Italy, (4)Institute of Nanotechnology (INT), Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, Germany

Powder model catalysts for emission control catalysis were prepared using the "precursor" concept, where atom-precise Pt clusters and monodisperse nanoparticles were supported on ceria. We show the influence of the Pt particle size, their surface noble metal concentration and support morphology on the catalytic performance in the oxidation of CO.

Effect of CO on Alcohol Oxidation over PGM-Based Commercial Oxidation Catalysts for Control of Emissions from Lean-Burn Engines.

__Md Masudur Rahman__, Sreshtha Sinha Majumdar, and Josh A. Pihl
Oak Ridge National Laboratory, Oak Ridge, TN

Methanol oxidation was inhibited by CO on Pt DOC, Pd+Pt DOC, and MOC catalysts at temperatures below 150 °C. Ethanol formed acetate species as a partial oxidation product on the catalyst surface. Strongly adsorbed acetate species delayed CO oxidation on the Pt DOC and MOC catalysts until 200 °C.

Influence of Zirconia Loading on Pd–Pt/SBA-15 Catalysts for Methane Oxidation.

Gianni Caravaggio
CanmetENERGY-Ottawa, Natural Resources Canada (NRCan), Ottawa, ON, Canada

To address methane slip (with high GHG potential) in lean burn natural gas (LBNG) engines, where water vapor and sulfur in the exhaust deactivate conventional catalysts, Pd–Pt/SBA-15 catalysts doped with zirconia (5–15 wt%) were developed. These catalysts showed excellent methane oxidation activity under simulated LBNG exhaust

Automatically Generated Exhaust Gas Conversion Mechanism over Pt(111) Explores Chemistry between C and N Containing Adsorbates.

__Kirk Badger__, C Franklin Goldsmith, and Bjarne Kreitz
School of Engineering, Brown University, Providence, RI

Experimental data suggests that reactions between adsorbates with N and C play an important role in the conversion of exhaust gas over Pt. The open-source software RMG is extended and used to automatically generate a microkinetic model that considers such reactions in the conversion of exhaust gas over Pt(111).

Origins of the Photocatalytic NO_x Oxidation and Storage Selectivity of Mixed Metal Oxide Photocatalysts: Prevalence of Electron-Mediated Routes, Surface Area, and Basicity.

Elnaz Ebrahimi[1], Muhammad Irfan[1], Yusuf Kocak[1], Emre Erdem[2], and __Emrah Ozensoy__[1]
(1)Chemistry, Bilkent University, Ankara, Turkey, (2)Sabanci University, Istanbul, Turkey

CaO-promoted TiO_2/Al_2O_3 were utilized in photocatalytic NOx oxidation and storage reaction. An e^--scavenger suppressing the e^--mediated route, attenuated the photocatalytic selectivity by triggering NO_2(g). Superior NO_x storage selectivity was attributed to presence of e^- trapped at oxygen vacancies and superoxide species allowing direct NO oxidation to NO_3^- species.

Impact of Water on Ammonia Oxidation Performance of Coinage Metals and Their Comparison to Platinum.

Amish Chovatiya, *Hanyu Ma, and William Schneider*
Chemical and Biomolecular Engineering, University of Notre Dame, Notre Dame, IN

We use a conversion dependent mean field microkinetic model to compare ammonia oxidation activity and selectivity of coinage metals with Pt and show that the choice of catalyst is dependent on whether the feed gas is dry or wet. We then test sensitivity of our conclusions to model assumptions.

Highly Efficient Ag Single-Atom Catalyst for Selective Catalytic Oxidation of NH_3.

Kailong Ye[1], *Shaohua Xie*[2], *and* ***Fudong Liu***[3]
(1)University of California, Riverside, Riverside, CA, (2)Department of Civil, Environmental, and Construction Engineering, University of Central Florida, Orlando, FL, (3)Department of Chemical and Environmental Engineering, University of California, Riverside, Riverside, CA

Ag single-atom catalysts (SACs) with enhanced catalytic activity for the selective catalytic oxidation of NH_3 reaction were successfully developed by tailoring the Ag coordination environment and optimizing the surface density of Ag atoms within the catalysts.

Restructuring of Au-Pd Nanoparticles in the Presence of Adsorbates: Insights into Catalysis and Selectivity.

Rajeev Kumar[1,2], *Conor Waldt*[1,2], *Sucharita Vijayaraghavan*[3], *David W. Flaherty*[3], *and David Hibbitts*[1,2]
(1)Charles D. Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN, (2)Department of Chemical Engineering, University of Florida, Gainesville, FL, (3)School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA

The interaction of surface restructuring, adsorbate binding energy, and local atomic environments is crucial for stabilizing and forming intermediates during H_2O_2 production. It is essential to understand this restructuring and its impact on catalytic behavior to optimize AuPd single atom alloys for efficient and selective H_2O_2 synthesis.

Mechanistic Insights into PFOA Degradation on Covalent Organic Framework Photo-Catalysts.

Christian Sandoval Pauker[1], *Shu-Yan Jian*[2], *Liberty Tafadzwa Mutepaire*[2], *Sophia Nance*[2], *Ai-Shi Wang*[2], *Rafael Verduzco*[2], *and Thomas P. Senftle*[2]
(1)Smalley-Curl Institute, RICE University, Houston, TX, (2)Chemical and Biomolecular Engineering, Rice University, Houston, TX

We demonstrate that COF materials can photo-oxidize PFOA through defluorination. DFT calculations show PFOA binding to the –C≡C– fragment induces critical structural and electronic changes in the COF. Electron density localized around the carboxylate group facilitates PFOA photooxidation. This insight provides guidance for designing COFs for photo-catalytic PFAS removal

Identifying and Quantifying Carbon in Municipal Solid Waste Ash & Implications for Ash's Performance As a Heterogeneous Catalyst.

Kaitlyn Lawrence[1] *and Marco J. Castaldi*[2]
(1)Chemical Engineering, The City College of New York, New York, NY, (2)Chemical Engineering, City College of New York, New York, NY

This study explores waste-to-energy (WTE) ash as a low-cost NO_X reduction catalyst by characterizing its carbon forms using FTIR, TGA, and "smart" combustion. Performance testing showed promising NO conversion rates, suggesting ash's potential viability in treatment of harsh flue gases and thus, advancing circular economy practices in emissions control.

The Application of Spaci-MS on Cucha SCR Monolith Catalysts.

Aldo Lanza[1]*, Pietro De Angeli*[2]*, Nicola Usberti*[2]*, Isabella Maria Nova*[2]*,* ***Enrico Tronconi***[2]*, Tomas Hlavaty*[3]*, Petr Koci*[3]*, Djamela Bounechada*[1]*, Roberta Villamaina*[1]*, and Andrew P.E. York*[1]
(1)Johnson Matthey Technology Centre, Sonning Common, United Kingdom, (2)Laboratory of Catalysis and Catalytic Processes - Dipartimento di Energia, Politecnico di Milano, Milano, Italy, (3)University of Chemistry and Technology, Prague, Czech Republic

The development of a fast, simple and 'easy to use' analytical model represents a useful simplification in the evaluation of the probe intrusion effects when dealing with spatially resolved data. CFD validated the effectiveness of the use of this technique.

Homogeneously Distributed Heterostructure Energizes and Replenishes Oxygen Species for Boosting Toluene Degradation on Pharmaceutical Industry Park.

Bin Wang[1]*, Sunwen Xia*[1]*,* ***Bo Ning***[2]*, Kaihang Zhang*[3]*, Qiaowan Chang*[4]*, and* ***Dong Wang***[1]
(1)Shandong University, Jinan, Shandong Province, China, (2)Wenzhou Medical University, Wenzhou, China, (3)Georgia Institute of Technology, Atlanta, GA, (4)Columbia University, New York, NY

We present a scalable one-pot strategy for the in situ fabrication of a homogeneously distributed heterostructure, which brings La_2CuO_4 perovskite a 58-fold activity enhancement and robust anti-sintering/water/coke in toluene oxidation, superior to currently reported perovskite catalysts.

Advancing Pt Catalysts for the Selective Catalytic Reduction of Nitrogen Oxides with Hydrogen.

Shaohua Xie[1], *Liping Liu*[2], *Yuejin Li*[3], *Hongliang Xin*[4], *and* ***Fudong Liu***[5]
(1)Department of Civil, Environmental, and Construction Engineering, University of Central Florida, Orlando, FL, (2)Department of Chemical Engineering, Virginia Polytechnic Institute and State University, Blacksburg, VA, (3)BASF, Iselin, NJ, (4)Department of Chemical Engineering, Virginia Tech, Blacksburg, VA, (5)Department of Chemical and Environmental Engineering, University of California, Riverside, Riverside, CA

Unlike conventional strategies that focus on modifying active sites, we present a simple and versatile approach using the physical mixing of Pt catalysts with zeolites to fine-tune the surrounding environment of active sites, thereby significantly enhancing catalytic performance in the selective catalytic reduction of NO_x using H_2.

Effect of Ions on the Aqueous-Phase Adsorption of Organics on Ag.

Ankit Mathanker[1], *Gyan Sharma*[1], *Bolton Tran*[1], *Nirala Singh*[1], *and Bryan Goldsmith*[2]
(1)Department of Chemical Engineering, University of Michigan, Ann Arbor, MI, (2)Chemical Engineering, University of Michigan, Ann Arbor, MI

Ions can change the aqueous-phase adsorption strength of organics. Our main findings suggest ions can vary the adsorption of organics on Ag by up to ± 10 kJ mol^{-1}. The change in adsorption is mainly attributed to the change in the adhesion of water in the presence of ions.

Kinetic Analysis Reveals Active Sites in Heterogeneous Metathesis Catalysts: Insights from the *Cis-Trans* Isomerization of 2-Butenes.

Maria Rikaela Ilagan[1], *James Rawlings*[2], *and Susannah Scott*[3]
(1)Chemical Engineering, University of California, Santa Barbara, Santa Barbara, CA, (2)University of California, Santa Barbara, Santa Barbara, CA, (3)Department of Chemical Engineering, University of California, Santa Barbara, Santa Barbara, CA

A kinetic analysis of the *cis-trans* isomerization of 2-butene was performed using Re_2O_7/Al_2O_3, revealing active sites in heterogeneous olefin metathesis. Global curvefit analysis identified the Re ethylidene as the most abundant surface intermediate, advancing our understanding of elementary rate constants and the relative abundances of key surface intermediates.

Resolving Coverage Dependent CO and H Co-Adsorption on Pt(111).

Sifat Hossain *and Rachel Getman*
Department of Chemical and Biomolecular Engineering, The Ohio State University, Columbus, OH

The investigation of the CO*-H* system on Pt(111) using cluster expansions show H* having a 2-fold effect on CO*, evident through changes in co-adsorption saturation coverage. GCMC models connect reaction conditions to adsorbate configurations and CH_4 selectivity, providing insights to enhance selectivity for industrial CO hydrogenation processes.

Impact of Pd Single Atoms during CO Oxidation over Ceria-Supported Ni and Pt Single Atom Catalysts: Are Synergistic Effects Present?.

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

Ceria-supported Pd single atoms demonstrate ‘synergy’, arising from non-bonding influences between metal atoms mediated through the reducible support. The addition of Pd single atoms to CeO_2-supported Ni and Pt single atoms does not influence the behavior of Ni or Pt nor influence intra-atom communication between Pd atoms during CO oxidation.

Taming Complexity in Catalysis Using Transient Methods.

Christopher R. O'Connor[1]*, Eric A. High*[1,2]*, Taek-Seung Kim*[3,4]*, and Christian Reece*[1]
(1)Harvard University, Cambridge, MA, (2)Tufts University, Medford, MA, (3)Rowland Institute at Harvard, Harvard University, Cambridge, MA, (4)Korea Institute of Energy Research, Daejeon, Korea, Republic of (South)

We combine ambient pressure transient flow and spectroscopy CO oxidation experiments to probe the state of a powdered Pd/γ-Al_2O_3 catalyst and find that the kinetics and coverage dependencies measured quantitatively agree with those measured in ultra-high vacuum over model Pd/Al_2O_3/NiAl(110) and Pd(111) systems.

Sintering Resistance in Dilute-Alloy Catalysts Is Described By Decreased Surface Mobility Due to Metal Hybridization.

Audrey Dannar[1,2]*, Jordan Finzel*[3]*, Phillip Christopher*[4]*, and E Charles Sykes*[5]
(1)Rowland Institute at Harvard, Harvard University, Cambridge, MA, (2)Rowland Institute, Harvard University, Cambridge, MA, (3)Chemical Engineering, University of California Santa Barbara, Santa Barbara, CA, (4)Department of Chemical Engineering, University of California, Santa Barbara, Santa Barbara, CA, (5)Department of Chemistry, Tufts Univ, Medford, MA

Single-atom alloy (SAA) catalysts have demonstrated an unexpected and previously unexplained resistance to sintering, a major catalyst deactivation pathway. We reveal the atomic-scale processes behind sintering and SAA sintering resistance using results from supported SAA catalyst samples under high pressure environments, single crystals in UHV conditions, and computational models.

Electronic and Geometric Features Controlling the Reactivity of C_1–C_3 Alkanes on Mg-Vanadate Catalysts—a DFT+U Study.

Hansel Montalvo-Castro[1]*, Alvaro Loaiza*[2]*, Randall Meyer*[3]*, Craig Plaisance*[2]*, and David Hibbitts*[4]

(1)Department of Chemical Engineering, University of Florida, Gainesville, FL, (2)Cain Department of Chemical Engineering, Louisiana State University, Baton Rouge, LA, (3)Exxonmobil, Annandale, NJ, (4)Charles D. Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN

This work employs density functional theory (DFT) and constrained orbital (CO-DFT) to elucidate geometric and electronic features that govern initial C–H activation of C_1–C_3 alkanes on Mg-vanadate catalysts during oxidative dehydrogenation reaction.

In-Situ **Computational Design of Ni-Supported Metal Nitride Interfaces for Mild Temperature Ammonia Synthesis.**

Pranav Roy*, Weiye Qu, Chao Wang, and Brandon C. Bukowski*
Department of Chemical and Biomolecular Engineering, Johns Hopkins University, Baltimore, MD

We performed a mechanistic study of the associative Mars-van Krevelen mechanism in metal nitrides for ammonia synthesis using combined DFT and AIMD. We developed a Ni-MnN nanowire model to facilitate hydrogen adsorption on MnN. A computational workflow is presented for kinetic modeling of nanowire-metal nitride interfaces at reaction conditions.

Role of Water in the Dynamics of Active Sites in Pt-MoO_x Catalysts during Liquid-Phase Reactions.

Samir Castilla Acevedo Sr.[1]*, Ben Auer*[1]*, John Styers*[1]*, and Alan Allgeier*[2]
(1)Chemical and Petroleum Engineering, University of Kansas, Lawrence, KS, (2)Center for Environmentally Beneficial Catalysis (CEBC), University of Kansas, Lawrence, KS

The density of the active sites is strongly influenced by the presence of water in the system and ignoring these influences may lead to invalid TOF assessments.

Thermochemical Interconnectivities of Redox, Brønsted, and Lewis Sites on Metal Oxide Surfaces and Their Kinetic Consequences in C−H Scission and C−O Formation of Alkanols.

Guangming Cai *and Ya-Huei (Cathy) Chin*
Department of Chemical Engineering and Applied Chemistry, University of Toronto, Toronto, ON, Canada

The knowledge on the interconnectivities among diverse active sites on metal oxides, encompassing their thermochemical, electronic, and kinetic properties, establishes a foundation for rationalizing turnover rate couplings across multi-functional catalysts and aid in design and optimization of catalysts for alkanol ODH and DEH catalysis.

Kinetic Consequences of Surface Segregation Processes in Catalysis By Metal Alloys.

Samiha Bhat[1]*, Rong (rocky) Ye*[1]*, Jared Arkfeld*[1]*, Chenggong Jiang*[1]*, Bryan Goldsmith*[2]*, Nirala Singh*[1]*, Eranda Nikolla*[1]*, and Suljo Linic*[1]
(1)Department of Chemical Engineering, University of Michigan, Ann Arbor, MI, (2)Chemical Engineering, University of Michigan, Ann Arbor, MI

Reaction kinetics on heterogeneous bimetallic catalysts is influenced by *in situ* structural transformations, including surface segregation. This phenomenon of adsorbate-induced alloy restructuring on exposure to reaction environments is not thoroughly investigated. This study highlights the restructuring potential of Pt-Cu alloys under CO oxidation, and its effect on observed kinetics.

Unveiling the Catalytic Potential of Extra-Large Pores Zeo-1 Zeolite.

Nourrdine Chaouati[1]*, Mohammad Fahda*[2]*, Svetlana Mintova*[1]*, Ludovic Pinard*[3]*, and Valentin Valtchev*[4]
(1)Laboratoire de Catalyse et Spectrochimie, Caen, No State, France, (2)Laboratoire de Catalyse et Spectrochimie, Caen, France, (3)CNRS-ENSICaen-UniCaen, Caen, France, (4)CNRS-ENSICaen-UniCaen, Caen, Calvados, France

Our contribution focuses on the study of the fundamental catalytic properties of the recent extra-large pore zeolite ZEO-1. Results indicate that ZEO-1 has a cracking ability comparable to that of a USY, its shape selectivity is imposed by the 12 MR channels while its 16 MR channels enhance its stability.

Sterically Encumbered [(3,3'-dimethyl-2,2'-bipyridine)Ir(Cl)COE_2] Catalyst for Aromatic and Heteroaromatic Borylation.

Eric Slack*, Douglas Hartline, and Samantha Grosslight*
Life Science Technologies, Johnson Matthey, Magnolia, NJ

Experimental and computational study of iridium borylation of heteroaromatic and aromatic substrates using a sterically encumbered 3,3'-dimethyl-2,2'-bipyridine ligand for improved scope and efficiency compared to the standard process using $[Ir(OMe)COD]_2$ with 3,4,7,8-tetramethyl-1,10-phenanthroline.

Impact of Ceria Support Morphology on the Electronic Properties and Catalytic Behavior of Rh Single Atoms during CO Oxidation.

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

The study demonstrates how ceria morphology influences the electronic properties and catalytic behavior of Rh single atoms during CO oxidation. By correlating oxygen vacancy dynamics with Rh's electronic environment and performance, the findings provide critical insights for designing optimized single-atom catalysts for CO emissions control and beyond.

Transition Metal-Triazine Electrocatalysts for Carbon Dioxide Transformation and Hydrogen Storage.

Phong Huynh*, Manuel Quiroz, and Krista Kulesa*
PNNL, Richland, WA

Mitigating CO_2 emissions requires carbon capture and recycling into green energy carrier molecules. For the first time, we synthesize and characterize three transition metal-triazine (TMT) complexes. These TMT platforms are evaluated for CO2 reduction selectivity, efficiency and mechanism, introducing a promising class of molecular electrocatalysts for closing the carbon cycle.

Ambient Pretreatment Effect on Low Temperature CO Oxidation over Ni Doped Co_3 O_4 Nanocatalysts.

Zichen Wang
University of Connecticut, Storrs, CT

This study reveals that pretreatment temperature significantly impacts Ni-doped Co_3O_4 catalysts' performance in CO oxidation. Moderate pretreatment (300–600°C) enhances activity by optimizing spinel structure, while high-temperature treatment (900°C) induces phase separation, reducing effectiveness. Insights provide valuable guidance for catalyst design and environmental applications.

Synthetic Methods to Control the Siting of Trivalent Heteroatoms in MFI Zeolite Channels for Selective Toluene Methylation to p-Xylene.

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

Synthetic strategies that bias active (H^+) sites towards smaller MFI channel voids are generalizable to any trivalent heteroatoms, evidenced by regioselective toluene methylation towards less bulky para-xylene isomers. Variations in acid strength, by changing heteroatom identity, enable independent control over methylation rates while maintaining high confinement-driven selectivity in MFI zeolites.

Interplay of Local Structure and Spin State on the ORR and Oer Performance of M-N-C Catalysts.

Hyeonjung Jung *and Michal Bajdich*

SUNCAT Center for Interface Science and Catalysis, SLAC National Accelerator Laboratory, Menlo Park, CA

This study investigates the effects of z-displacement and spin states on ORR and OER performance in M-N-C catalysts using DFT. By analyzing 22 transition metals across 3d, 4d, and 5d rows, it identifies spin stability, adsorption energy trends, and dual-ligand interactions, providing insights for optimizing single-atom catalysts in energy conversion.

Toward Understanding of Oxygen Depletion Effects on Chemical Looping Propane Oxidative Dehydrogenation Using Strontium Ferrites.

***Kun Wang*[1]*, Sophie Liu*[2]*, Randall Meyer*[3]*, and Jonathan Mitchell*[1]
(1)ExxonMobil Technology and Engineering, Annandale, NJ, (2)ExxonMobil Research and Engineering Company, Annandale, NJ, (3)Exxonmobil, Annandale, NJ

Using strontium ferrites with perovskite and Ruddlesden-Popper structures as oxygen carriers for propane chemical looping oxidative dehydrogenation, we show the surfaces maintain high levels of O population and are insensitive to O depletion during the reaction. The surface reaction is limiting and the ODH performance is little impacted.

Microkinetic Modelling for Electrochemical C-N Coupling By Metal-Organic Materials.

***Yuting Xu*[1]*, Jiaqi Yang*[1]*, Gregory Foley*[2]*, Sophia Mac*[2]*, Lan On*[2]*, Sara Thoi*[2]*, and Fanglin Che*[1]
(1)Chemical Engineering, University of Massachusetts Lowell, Lowell, MA, (2)Chemistry, Johns Hopkins University, Baltimore, MD

BIFs' discrete active sites and atomic precision provide an excellent platform for advancing single-atom catalysis. This project deepens understanding of structure-reactivity relationships in single-atom electrocatalysis within cage frameworks. Integrating DFT, MKM with AI enables a fundamental approach to catalyst design, moving beyond trial-and-error.

Isomerization of Epoxides By Tris(Pentafluorophenyl)Borane (BCF): Investigation of Solvent Effects and Induction Period.

***Hiyab Mekonnen*[1]*, Guanhua Wang*[2]*, Linda Broadbelt*[3]*, and Justin Notestein*[4]
(1)Northwestern University, Evanston, IL, (2)Chemical Engineering, Northwestern University, EVANSTON, IL, (3)Department of Chemical and Biological Engineering, Northwestern University, Evanston, IL, (4)Department of Chemical & Biological Engineering, Northwestern University, Evanston, IL

This study investigates tris(pentafluorophenyl)borane (BCF) as a Lewis acid catalyst for epoxide isomerization. It examines how solvent properties, such as hydrogen bonding and coordination strength, influence reaction rates and selectivity. Kinetic experiments, in situ NMR, and DFT calculations offer insights into solvent interactions in BCF-catalyzed reactions.

Designing Strategies for the Modification of ZIF-8 for Its Optimization As an Adsorbent.

David Villalgordo Hernández *and Javier Narciso*
University of Alicante, Alicante, Spain

ZIF-8 has been post-synthetically modified with four different Triazoles aiming to tune its adsorption capacity and affinity towards CO_2 by adding a series of N sites. Incorporation of these exchanging ligands generate new coordinative systems leaving available N sites which act as anchoring points enhancing its aptitude for CO_2 capture.

Surface Brønsted Acidity Characterization of Phosphotungstic Acid.

Hyunju Lee[1] *and Brent H. Shanks*[2]
(1)Chemical and Biological Engineering, Iowa State Univeristy, Ames, IA, (2)Department of Chemical and Biological Engineering, Iowa State University, Ames, IA

Surface proton concentration and acid strength of heteropoly acid catalysts were measured by means of temperature-programmed desorption of 2,6-di-tert-butylpyridine. Also, it was found that medium level of hydration of phosphotungstic acid resulted in the highest surface proton density, as $[H_3O^+]$ showed higher mobility than H^+ and $H_5O_2^+$.

A Simple Ligand Exchange Strategy to Functionalize ZIF-8 to Improve Mercury Adsorption from Water.

Maria Karla Lopez González[1] *and Javier Narciso*[1,2]
(1)University of Alicante, Alicante, Spain, (2)Alicante Institute for Health and Biomedical Research, Alicante, Spain

This study demonstrates the power of post-synthetic modification (PSM) of ZIF-8 to enhance material functionality, offering innovative pathways for designing efficient adsorbents. The successful functionalization with 3-mercapto-1,2,4-triazole resulted in materials with high Hg^{2+} adsorption, with Int.Z2.1-0.5 excelling due to its high sulfur content.

Conversion of Low-Density Polyethylene and Waste Plastic Bottles to Fuel Grade Hydrocarbons Using Metal-Supported KIT-6 Catalysts.

Maliheh Heravi[1]*, Sathyapal Churipard R.*[1]*, Sundaramurthy Vedachalam*[1]*, Saumitra Saxena*[2]*, and Ajay Dalai*[1]
(1)Chemical and Biological Engineering, University of Saskatchewan, Saskatoon, SK, Canada, (2)CCRC, KAUST, Thuwal, Jeddah, Saudi Arabia

Efficient catalyst design enables high liquid yield and selective cracking of LDPE and plastic bottles to fuel-range hydrocarbons. Transition metals enhance KIT-6 performance by tuning pore size and creating active sites. This study highlights the potential of heteroatom introduction in KIT-6 for sustainable plastic waste conversion, advancing the circular economy.

Automation Tools As an Enabler for Zeolite Discovery and Optimization.

***Joel Schmidt**, Marat Orazov, Kurt Jensen, Nan Chen, Jilei Liu, Howard S. Lacheen, and Axel Brait*
Chevron, Richmond, CA

The use of automation tools is a necessity in a competitive R&D environment to improve on the catalyst development/commercialization cycle. This talk will give an overview of our efforts to implement these tools in Chevron's Catalytic Materials team.

Mg-MOF-74 As a Promising Precursor for Synthesizing Highly Active and Porous MgO Catalyst Towards Knoevenagel Reaction.

***Mehdi Niknam**[1] and Thomas U. Schwartz[2]*
(1)The University of Maine, Orono, ME, (2)Biology, Massachusetts Institute of Technology, Cambridge, MA

MgO catalyst can be effectively synthesized from Mg-MOF-74, with several advantages over conventional MgO. One of the key benefits is its high site density as the result of increased surface area. This enhanced surface area is critical for improving catalytic performance, as it provides more active sites for reactions.

Achieving Controllable Distribution of M Cations (Pd, Pt, Ni, Cr, Cu) As $[M\text{-}OH]^{+1}$/1Al or M^{2+}/2Al in a Zeolite Gives Mechanistic Insights for Adsorptive, Catalytic Reactions.

*Nicholas Jaegers[1], Hristiyan A. Aleksandrov[2], Eric D. Walter[3], Georgi Vayssilov[2], Dhruba Jyoti Deka[3], Janos Szanyi[3], Garam Lee[3], and **Konstantin Khivantsev**[4]*
(1)University of California at Berkeley, Berkeley, CA, (2)Faculty of Chemistry, University of Sofia, 1126 Sofia, Bulgaria, (3)Pacific Northwest National Laboratory, Richland, WA, (4)Physical and Computational Sciences Directorate and Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA

We show the first synthetic pathway for selective placement of divalent metal cations in a zeolite with the same Si/Al ratio wither as M(II)-OH/1Al or M(II)/2Al species and their divergent reactivity for important industrial catalytic and adsorption chemistries.

Metal Nanoparticle Encapsulation Strategies in MOF for Enhanced and Stabilized CO_2 Hydrogenation to Methanol.

*Vijay Velisoju[1], Enrique V. Ramos Fernandez[1,2], Jose Cerrillo[3], Rafia Ahmad[1], Hend Omar Mohamed[1], Luigi Cavallo[4], and **Pedro Castaño**[1]*
(1)KAUST Catalysis Center, King Abdullah University of Science and Technology, Thuwal, Saudi Arabia, (2)Inorganic Chemistry Department, University of Alicante, Alicante, Spain, (3)King Abdullah University of Science and Technology, Thuwal, Saudi Arabia, (4)KAUST, Thuwal, Saudi Arabia

This study demonstrates Cu and Pd catalysts embedded in ZIF-8, achieving superior activity and stability for CO_2 hydrogenation to methanol under industrial conditions. The catalysts' performance is driven by highly dispersed metal nanoparticles and metal-Zn interfaces within ZIF-8, highlighting the potential for efficient, sustainable CO_2-to-methanol conversion.

Unraveling Solvent Effects on n-Butane Cracking and Dehydrogenation in H-MFI Zeolites: A Hybrid QM/MM Approach.

Muhammad Zeeshan*, Subrata Kumar Kundu, and Andreas Heyden*
Department of Chemical Engineering, University of South Carolina, Columbia, SC

Developed an explicit solvation scheme for porous zeolites (called eSZS), which was subsequently used to study solvent effects during cracking in H-MFI.

Synthesis of a Nickel Based Nanostructured Hierarchical ZSM-5 Zeolite for Enhanced Dry Reforming of Methane to Syngas.

Yahuza Nantomah Abdulai[1], ***Khalid Alhooshani***[2,3], *and Saheed Ganiyu*[2]
(1)Chemistry, King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia, (2)Chemistry, King Fahd University of Petroleum and Minerals, Dhahran, Dammam, Saudi Arabia, (3)Chemistry, Interdisciplinary Research Center for Refining & Advanced Chemicals, King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia

This study assesses the catalytic performance of a Ni/ZSM-5-S catalyst in dry reforming of CH4 (DRM), converting CH4 and CO2 into syngas. Hierarchical ZSM-5 was synthesized hydrothermally, and Ni/ZSM-5-S via wet impregnation. The catalyst showed high syngas production (82.5% CO2,78.0% CH4 conversion) and stability for 22 hours at 700°C.

SiO_2-Coated Cu-Based Catalysts for Efficient CH_3oh Production from CO_2.

Marco A. Rossi[1], *Letícia Rasteiro*[2], *Jose Assaf*[3], *Elisabete Assaf*[1], *and* ***Luiz Vieira***[1]
(1)Sao Carlos Institute of Chemistry (IQSC), University of Sao Paulo (USP), Sao Carlos, Sao Paulo, Brazil, (2)Institute of Chemistry, Sao Paulo State University, Araraquara, Sao Paulo, Brazil, (3)Chemical Engineering Department, Federal University of São Carlos, São Carlos, Brazil

This work presents a mesoporous SiO_2 coating strategy for $Cu/In_2O_3/CeO_2$ and $Cu/In_2O_3/ZrO_2$ catalysts. This approach limited the nanoparticle size, increased metal dispersion, and resulted in higher activity and selectivity in the hydrogenation of CO_2 to methanol, with methanol yields up to 4 times higher.

Essential Insights into Electronic and Crystal Structure Modulation of Co-Catalysts By Iridium for Enhanced Fischer-Tropsch Synthesis.

Ji Won Lee*, Ji Woo Son, Seung Ju Han, Yunjo Lee, and Yang Sik Yun*

Hydrogen & C1 Gas Research Center, Korea Research Institute of Chemical Technology (KRICT), Daejeon, Korea, Republic of (South)

This work establishes Iridium as a highly effective promoter for optimizing Co-based catalysts, providing a strategic framework for the development of advanced catalysts for FTS applications.

The Effect of Buffer Electrolyte on Proton-Coupled Electron Transfer Kinetics in Electrochemical Hydrogenation Reactions.

Zhiqin Liang
School of Physical Science and Engineering, Beijing Jiaotong University, Beijing, China

Special caution must be taken when interpreting the intrinsic pH dependence in the presence of buffer species because of its potential role as a proton or oxygen carrier, which is easily overlooked in current research. We show how buffer electrolytes steer the interfacial kinetics of electrochemical hydrogenation reactions.

Molecular Catalysts Design with Massively Parallel Physics-Based Computational Workflow.

Croix Laconsay[1]*, Mathew D. Halls*[2]*, and Pavel Dub*[3]
(1)Schrödinger, Portland, OR, (2)Materials Science, Schrödinger, Inc., San Diego, CA, (3)Schrödinger, Inc., San Diego, CA

Molecular catalysts have traditionally been designed through experimental trial-and-error. We present Schrödinger's Reaction Network Enumeration Profiler module, the first fully automated computational framework capable of predicting both selectivity and turnover frequency (TOF) for dynamically generated libraries of virtual molecular catalysts, leveraging quantum mechanics.

Machine Learning-Assisted Design of Integrated Single-Atom Electrodes for Enhanced Water Oxidation.

Lingxi Zhou *and Ruitao Lv*
Tsinghua University, Asian (Including Pacific Islander), Beijing, China

The activity-stability dilemma of electrocatalysts limits their practical use, especially in OER for hydrogen production. We introduce a 'chemical steam deposition' strategy with machine learning to synthesize a Ru-Ti-Mn electrode with self-healing mechanisms, achieving high activity and stability across all pH levels. ML identified the optimal atomic metal-support ratio.

DBD Plasma Treatment on Ni/γ-Al_2O_3 for Catalytic Methane Decomposition: Effects of Pure Argon and Pure Hydrogen.

Bella -[1]*, Xun Cao*[2]*, Kang Hui Lim*[3]*, Chee Kok Poh*[1]*, Luwei Chen*[1]*, Jie Chang*[1]*, and Sibudjing Kawi*[3]

(1)Carbon Conversion and Future Energy Carriers, Institute of Sustainability for Chemicals, Energy and Environment (ISCE2), Singapore, Singapore, (2)Advanced Characterization and Instrumentation, Institute of Sustainability for Chemicals, Energy and Environment (ISCE2), Singapore, Singapore, (3)Department of Chemical and Biomolecular Engineering, National University of Singapore, Singapore, Singapore

DBD plasma was used to decompose Ni precursor on γ-Al_2O_3 where the effects of using different pure gases (Ar and H2) were studied on low temperature catalytic methane decomposition reaction to co-produce hydrogen and carbon nanotubes. Surface characterizations were conducted to understand the effects of different gases on the catalysts.

Machine Learning Driven Catalyst Optimization for Biomass to H_2-Rich Syngas with Experimental Validation.

Kaushik Kundu[1], *Avan Kumar*[2], *Hariprasad Kodamana*[1], *and Kamal Pant*[3]
(1)Chemical Engineering Department, Indian Institute of Technology Delhi, New Delhi, India, (2)School of Sustainability, Arizona state university, Tempe, AZ, (3)Chemical Engineering, Indian Institute of Technology Roorkee, Roorkee, India

Transforming biomass into hydrogen-rich syngas tackles fossil fuel depletion and environmental harm. Machine learning optimization, validated experimentally, ensures reliable, scalable industrial applications. This research supports the shift to a low-carbon economy, promoting sustainability and energy independence while addressing critical global energy and environmental challenges.

Immobilization of Endoxylanase Onto Functionalized SBA-15 for Xylooligosaccharides Production.

Parasuraman Selvam
Department of Chemistry & NCCR, IIT-Madras, CHENNAI, India

Enzymatic methods are eco-friendly while the immobilization of the enzyme enhances stability, rigidity and reusability, therefore the immobilized enzymes are more suitable as catalysts for the industrial production of xylooligosaccharides from xylan.

Step-Wise Activation of CH_4 and CO_2 over Partially Oxidized Surfaces of MoO_xC_y.

Nurul Farhana Binti Abd Ghaffar[1], *Tej Choksi*[1], *Wen Liu*[1], *and Mingwu Tan*[2]
(1)School of Chemistry, Chemical Engineering and Biotechnology, Nanyang Technological University, Singapore, Singapore, (2)4Agency for Science, Technology and Research (A∗STAR), Singapore, Singapore

We study the evolution of Mo_2C surface structure upon exposure to different reactive environments, viz., 1) CO_2; 2) H_2 and (3) CH_4. We demonstrate 20 cycles of chemical looping DRM with a steady increase of methane conversion from 74 % to 93 % with no obvious sign of deactivation.

The Influence of Strong Metal Support Interaction Phenomena on the Rates and Selectivity of Formic Acid Decomposition.

Luan Q. Le[1], Chuhong Lin[1], Hui Ling Tan[1], Lavie Rekhi[1], Renhong Li[2], Wen Liu[1], and ***Tej Choksi**[1]*
(1)School of Chemistry, Chemical Engineering and Biotechnology, Nanyang Technological University, Singapore, Singapore, (2)National Engineering Lab for Textile Fiber Materials and Processing Technology, Zhejiang Sci-Tech University, Hangzhou, China

Noble metals like Pd supported on TiB_2 exhibit a first-of-its-kind strong metal support interaction phenomena, that yields sinter-resistant metal catalysts. Using first principles microkinetic modelling and experimental characterization, we elucidate how dynamically formed TiB_2 overlayers on Pd nanoparticles modify the reaction mechanism, rates, and selectivity, for formic acid decomposition.

Modeling Dynamic Activation of Single Atom Catalysts: Conversion of Formic Acid on Rh/Fe3O4 (001).

***Benjamin Jackson**[1], Christopher Lee[1], Marcus Sharp[1], Mausumi Mahapatra[1], Simone Raugei[1], Liney Arnadottir[1,2], Mal Soon Lee[1], Bruce D. Kay[1], and Zdenek Dohnalek[1]*
(1)Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA, (2)School of Chemical, Biological and Environmental Engineering, Oregon State University, Corvallis, OR

Supported single-atom catalysts (SACs) have emerged as a frontier in fundamental catalytic research. This study demonstrates how thermally stable octahedral Rh single atoms incorporated in the Fe_3O_4(001) surface are dynamically released to form Rh adatoms catalytically active Rh adatoms due to surface hydroxyl recombination to water during reaction conditions.

Conversion of Bio-Ethanol into Olefins and Other Products for the Production of Sustainable Aviation Fuel.

Svetlana Tungatarova
Chemistry and Chemical Technology faculty, al-Farabi Kazakh National University, Almaty, Kazakhstan

Integrated technology for the catalytic conversion of bioalcohols is a solution to the growing global energy needs and ensures the creation of environmentally friendly technologies.

Synthesis of a Magnetic Fe-Cu-Zn Trimetallic Catalyst for CO2 Hydrogenation to Value-Added Chemicals.

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

This project focuses on converting CO_2 to light olefins via hydrogenation, addressing global warming and advancing green energy. The catalyst's novelty lies in tailored Fe-Cu-Zn interactions, enabling efficient conversion and high selectivity. Preliminary results show excellent catalytic performance and structural stability under reaction conditions.

One Step Dimethyl Ether Synthesis from CO_2 Hydrogenation over Hybrid Cu-ZnO-Al_2O_3/ Desilicated ZSM-5 Catalysts.

Dominique A. DAniel[1], Amanda Guimarães[1,2], Lícia Ranni F. Coelho[1,3], Andressa Andrade Alves da Silva[1], Gabriel L. CAtuzo[4], Elisabete Assaf[4], and ***Lisiane Veiga Mattos***[1]
(1)Fluminense Federal University, Niteroi, Brazil, (2)Rio de Janeiro State University, Rio De Janeiro, Rio de Janeiro, Brazil, (3)Military Institute of Engeneering, Rio De Janeiro, Rio de Janeiro, Brazil, (4)Instituto de Química de São Carlos/Universidade de São Paulo, São Carlos, Brazil

This work evaluates the performance Cu-ZnO-Al_2O_3/desilicated ZSM-5 catalysts for direct DME synthesis from CO_2 hydrogenation. The 6CZA/ZSM-5 catalyst achieved optimal performance (240°C, 28 bar, 2,400 mL h^{-1} g^{-1}), demonstrating high CO_2 conversion and DME selectivity, highlighting the potential of this hybrid system as an efficient solution for CO_2 utilization.
4o

A Unique Magnetic FeCo Bimetallic Catalyst for Carbon Dioxide Conversion to Value Added Chemicals.

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

Addresses climate change by advancing CO_2 utilization through innovative catalysts. Synthesized iron and cobalt organometallic complexes, oxidized to produce magnetic Fe_3O_4 and Co_3O_4, achieved efficient CO_2 hydrogenation. The process yielded valuable chemicals, including light olefins, with high selectivity and conversion rates, showcasing potential for sustainable energy and greenhouse gas mitigation.

Role of Carbon Species in Dry Reforming and Pyrolysis of Methane: Insights from Molten in-Sn and in-Ni Alloys.

Nikil Surya R[1], Genpei Cai[2], Chester Upham[2], and ***Vishal Agarwal***[3]
(1)Department of Chemical Engineering, Indian Institute of Technology, Kanpur, India, (2)Chemical & Biological Engineering, University of British Columbia, Vancouver, BC, Canada, (3)Department of Chemical Engineering, Indian Institute of Technology Kanpur, Kanpur, India

This study presents a comparative analysis of the impact of accumulated carbon on the surface of molten In-Sn and In-Ni alloys, emphasizing its role in modulating catalyst surface properties and altering reaction pathways during methane dry reforming and pyrolysis reaction.

Quantitative TPR for Spillover and Surface Vacancy Determination on Reducible Oxide Supported Metal Catalysts.

Greg Barber[1]*, Griffin A. Canning*[2]*, and Robert Rioux*[1,3]
(1)Department of Chemical Engineering, The Pennsylvania State University, University Park, PA, (2)Chemical Engineering, The Pennsylvania State University, University Park, PA, (3)Department of Chemistry, The Pennsylvania State University, University Park, PA

A methodology for quantifying total spilled over hydrogen and estimating surface vacancies on metal supported reducible oxide catalysts by closing the H mass balance utilizing the captured water from temperature programmed reduction was developed and applied to a Cu/TiO_2 catalyst to demonstrate the role of spillover hydrogen in alkene hydrogenation.

Catalytic Activity of Iron-Doped Molybdenum Oxide on Cyclohexane Oxidation.

Nishamini Ruwanthika Jayasekara[1]*, Inosh P. Perera*[1]*, Isaac Olowookere*[1]*, Yasas Wickramathilaka*[1]*, Santiago T. Salamanca*[1]*, Sami Dursun*[2,3]*, and Steven L. Suib*[1,2]
(1)Department of Chemistry, University of Connecticut, Storrs, CT, (2)The Institute of Materials Science, University of Connecticut, Storrs, CT, (3)Department of Metallurgical and Materials Engineering, Konya Technical University, Konya, Turkey

Cyclohexane oxidation produces important key monomers which are crucial for nylon synthesis. In this study, iron-doped molybdenum oxide materials were synthesized and used as a promising candidate for the oxidation of cyclohexane due to its higher conversion and better selectivity towards desired products under ambient conditions.

The Relation between Energy Transfer and Chemical Production during Ultrasound-Induced Cavitation..

Ari Fischer*, Tej Choksi, and Robert Maligon Querimit*
School of Chemistry, Chemical Engineering and Biotechnology, Nanyang Technological University, Singapore, Singapore

Ultrasound waves drive aqueous chemical reactions through bubble cavitation. We show that the reaction energy generated during cavitation, not the total work applied on the bubble, controls chemical production. These findings rationalize the effects of acoustic (e.g., wave amplitude) and solution properties (e.g., density) on chemical yields.

Dynamic Behavior of Oxide Overlayer on Supported Metal Catalysts.

Seyeon Park*, Daeyeon Lee, Raymond Gorte, and John Vohs*
Department of Chemical and Biomolecular Engineering, University of Pennsylvania, Philadelphia, PA

We investigate the dynamics of WO_x overlayers on Pt/SBA-15 and Pt/Al_2O_3. Its impacts on Pt coverage and catalytic activity are evaluated. Characterization reveals that WO_x migrates onto Pt

on SBA-15, suppressing gas adsorption, but remains on Al_2O_3, partially covering Pt. Atomically thin WO_x maintained Pt reactivity in cyclohexane dehydrogenation.

Ragchem: Unlocking Chemical Knowledge.

Damian Camilo Martinez Martinez[1] *and Hui Fang*[2]
(1)Electical and Computer Engineering, University of Delaware, Newark, DE, (2)University of Delaware, Newark, DE

RAGChem, an innovative search engine designed to provide accurate and citable answers to chemistry questions. This system integrates our proposed RAG pipeline. Additionally, it extracts property-related entities from scientific literature in the field of catalysis

Development of Pt-Based Catalysts for the Dehydrogenation of Liquid Organic Hydrogen Carriers.

Musbau Gbadamosi[1]*, Kaveh Shariati*[2]*, Yanjiao Yi*[3]*, John Meynard Tengco*[3]*, Thossaporn Onsree*[2]*, Azadeh Mehrani*[2]*, Jagoda M. Urban-Klaehn*[4]*, John Monnier*[3]*, Jochen Lauterbach*[2]*, and Donna Chen*[5]
(1)Chemistry and Biochemistry, University of South Carolina, Columbia, SC, (2)Department of Chemical Engineering, University of South Carolina, Columbia, SC, (3)Chemical Engineering, University of South Carolina, Columbia, SC, (4)Idaho National Laboratory, Idaho Falls, ID, (5)Chemistry, University of South Carolina, Coulmbia, SC

Pt catalysts supported on SiO_2, Al_2O_3, TiO_2, and ZrO_2 were studied for methylcyclohexane dehydrogenation. Pt/Al_2O_3 showed highest activity and stability, while Pt/SiO_2 deactivated due to carbon fouling and pore blockage. Findings support improved hydrogen release in LOHC systems.

Chen et al., *Fuel*, 360, 130607, 2024

Direct Visualization of Metal–Support Interactions during CO_2 Hydrogenation Via in Situ Gas-Cell TEM.

Hongkui Zheng[1]*, Pritam K. Chakraborty*[2]*, Ronald Spruit*[3]*, Yevheniy Pivak*[1,3]*, Hongyu Sun*[1,3]*, Shibabrata Basak*[2]*, Rüdiger-A Eichel*[2]*, and Hugo Pérez Garza*[1,3]
(1)DENSsolutions, Irvine, CA, (2)Forschungszentrum Jülich GmbH, Jülich, NA, Germany, (3)DENSsolutions, Delft, Netherlands

We use in situ gas-cell TEM to visualize nanoparticle exsolution from a perovskite catalyst during CO_2 hydrogenation at 800 °C. Time-resolved imaging reveals dynamic migration, nucleation, and anchoring of particles, offering nanoscale insights into metal–support interactions critical for designing stable, high-performance catalysts under realistic conditions.

Mechanistic Insights into Crotyl Alcohol Isomerization over Cu/CeO_2 Catalysts.

Haiting Cai[1], *Shiva Murali*[1,2], *Huamin Wang*[1,2], *and Yong Wang*[1,2]
(1)Pacific Northwest National Laboratory, Richland, WA, (2)The Gene and Linda Voiland School of Chemical Engineering and Bioengineering, Washington State University, Pullman, WA

Controlling isomerization of crotyl alcohol is critical for the selective crotonaldehyde hydrogenation. The finding that the reaction preferentially occurs on the Cu^0-Ce^{n+}-O^{2-} active site ensembles, with the rates limited by the α-C-H cleavage, can shed light on the rational catalyst design for improving product selectivity during the selective crotonaldehyde hydrogenation.

Comparison Study on the NH_3 Cracking Catalysts Depend on the Manufacturing Methods for Commercialization.

Noh-Hyun Park
Ceracomb Co.,LTD., Asan-Si, Korea, Republic of (South)

For commercialization, nickel-based catalysts were prepared by coating, extrusion, and tablet methods, then evaluated for ammonia decomposition. The coating catalyst exhibited the highest ammonia conversion, attributed to the abundant of active materials on the surface. This result indicated the importance of catalyst structure in enhancing ammonia conversion performance.

Can in Situ TEM Identify Dynamic Active Sites?.

Gbolagade Olajide[1], *Tristan Maxson*[2], *and Tibor Szilvasi*[2]
(1)Chemical and Biological Engineering, University of Alabama, Tuscaloosa, AL, (2)Department of Chemical and Biological Engineering, The University of Alabama, Tuscaloosa, AL

Using DFT-trained machine learning interatomic potentials and TEM simulations, we show that active site formation and elimination occurs too quickly to be captured by *in situ* TEM. Consequently, relying only on *in situ* TEM for active site identification risks overlooking transient structures that may be crucial for catalytic performance.

CO_2 Direct Conversion to Methanol on Novel Membrane Reactor.

Yiqing WU[1], *Matthew Seabaugh*[1], *Anna Lee Tonkovich*[2], *Eric Daymo*[2], *Yong Wang*[3], *and Wei Liu*[4]
(1)Nexceris, Lewis Center, OH, (2)Tonkomo LLC, Gilbert, AZ, (3)The Gene and Linda Voiland School of Chemical Engineering and Bioengineering, Washington State University, Pullman, WA, (4)Molecule Works Inc., Richland, WA

In this poster, our Nexceris team will present a novel reactor design that integrates a water-removal membrane into a CO_2-to-methanol reactor. This innovative membrane reactor design addresses two major challenges in the commercial development of CO2-to-methanol techniques: low CO2 single pass conversion and limited catalyst hydrothermal stability.

Development of Testing Methodology and Characterization Methods for Chromium Getters for Solid Oxide Fuel Cells.

Melissa Hess[1]*, Kevin Doura*[1]*, Nicole Garcia*[1]*, Joseph M. Fedeyko*[1]*, and Prabhakar Singh*[2]
(1)Clean Air - SEC, Johnson Matthey, Audubon, PA, (2)Materials Science and Engineering, University of Connecticut, Storrs, CT

The development of a chromium getter can lead to extended lifetimes for SOFC components, speeding adoption of new, environmentally friendly technologies. Testing these new technologies can be difficult, expensive, and unsafe, but the reactor systems described here allow development to occur in a safe, efficient manner.

Copper Based Nitride Nanoparticles for Efficient Electrochemical Carbon Dioxide Reduction Under Low Overpotential.

Junrui Li[1]*, Oluwaseun Olarinde*[1]*, Rihana Burciaga*[1]*, Chaochao Dun*[2]*, Uhart Bradnock*[3]*, and Kayla Crawford*[1]
(1)Department of Chemistry, Clark Atlanta University, Atlanta, GA, (2)The Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, CA, (3)Williams College, Williamstown, MA

Current catalysts for CO_2 reduction suffer from low activity, poor selectivity, or limited stability. Herein, Cu-based nitride nanoparticles were precisely synthesized. Operando XAS study revealed the co-exisiting Cu^0 and Cu^+ that are believed to be active sites for ethanol production, emphasizing the importance of precise synthesis of catalysts.

Machine Learning Assisted Design of Metal-Nitrogen-Carbon Dual-Atom Catalysts for the Oxygen Reduction Reaction.

Prajeet Oza *and Guoxiang (Emma) Hu*
Georgia Institute of Technology, Atlanta, GA

Our ML-assisted computational framework employs the percentage of catalytically active structures, a more reliable descriptor than single structural configurations, to design stable, high-performing M1M2–N–C dual atom catalysts (DACs) for oxygen reduction reaction. This approach captures experimental trends and provides actionable guidance for rational design of DACs.

Choosing the Right Computational Model for Electrochemical Interfaces: Insights from MoS_2.

Ankit Bansal[1] *and Guoxiang (Emma) Hu*[2]
(1)Material Science and Engineering, Georgia Institute of Technology, Atlanta, GA, (2)Georgia Institute of Technology, Atlanta, GA

Accurate modeling of the electrochemical interface is critical for understanding catalytic mechanisms. Three main computational approaches are commonly employed: the computational hydrogen electrode (CHE) model, capacitance-based corrections, and grand canonical density functional theory (GC-DFT). These methods are investigated in this study using molybdenum disulfide (MoS_2) as a model system.

Dynamic Electrification Steers CO_2 Hydrogenation Selectivity Via Transient Surface Intermediates.

Kewei Yu[1], *Sagar Sourav*[2], ***Weiqing Zheng***[3], *and Dionisios Vlachos*[4]
(1)Chemical and Biomolecular Engineering, University of Delaware, Newark, DE, (2)Department of Chemical Engineering, Indian Institute of Technology Madras, Chennai, Tamil Nadu, India, (3)Delaware Energy Institute, University of Delaware, Newark, DE, University of Delaware, Newark, DE, (4)Delaware Energy Institute, University of Delaware, Newark, DE

Rapid pulse heating of CO_2 hydrogenation over Ni/Al_2O_3 enhances CO selectivity by dynamically modulating *CO and *H surface coverages. Operando spectroscopy reveals that temperature pulsing promotes *CO desorption over hydrogenation, enabling non-equilibrium pathways. This strategy offers a low-cost route to steer selectivity without altering catalyst composition or structure.

Copper-Doping and Surface Activation in Atomically Precise Au_{42}

Nanorods for Carbon Dioxide Reduction.

Rahul Somni *and Guoxiang (Emma) Hu*
Georgia Institute of Technology, Atlanta, GA
Change in potential-determining steps operando causes copper doping to hinder catalytic activity for CO_2RR for atomically precise Au_{42} nanoclusters (APNCs), a deviation from the norm for copper-based materials. This work highlights the importance of operando characterization of structure transformation, for which APNCs offer unique advantages.

Engineering the Nature of Rh Catalyst for Integrated CO_2 Capture and Utilization Via Dry Reforming of Methane: Effect of CeO_x and FeO_x Promoters on HAP.

Aybala Topcu[1], *Ayse D. Erdali*[2], *Erdem Deniz*[1], *Yusuf Kocak*[2], *Kaan Karaca*[2], *and Zafer Say*[1,3]
(1)Micro and Nanotechnology, TOBB University of Economics and Technology, Ankara, Turkey, (2)Chemistry, Bilkent University, Ankara, Turkey, (3)Material Science and Nanotechnology Engineering, TOBB University of Economics and Technology, Ankara, Turkey

This study develops Rh-based dual functional materials (DFMs) for integrated CO_2 capture and dry reforming of methane over HAP supports with CeO_x and FeO_x promoters. The tailored systems show enhanced stability and coke resistance, offering a promising pathway for syngas production aligned with net-zero and circular carbon strategies.

Dimensional Energy: Converting CO_2 into Chemicals Via Reverse Water Gas Shift and Fischer-Tropsch Catalysts.

Bradley Brennan *and Sam Garncarz*
Dimensional Energy, Ithaca, NY

Dimensional Energy has developed a two-step process to convert CO_2 into chemicals and fuels, providing a scalable and sustainable alternative to fossil-based feedstocks. The Reverse Water Gas Shift thermocatalyst shows thermodynamic maximum conversion and high selectivity under wide boundary conditions, and the Fischer-Tropsch catalyst designed for high liquid/wax output.

Predicting Acid Pka at Catalyst-Solution Interfaces Using O-H Vibrational Frequency.

Bolton Tran*, Dean Sweeney, Yifei Liu, Jean-Patrick Selo, Mad Lindsey, and Bryan Goldsmith*
Chemical Engineering, University of Michigan, Ann Arbor, MI

We developed a computational approach to compute the O-H vibrational frequency of acids at catalyst-solution interfaces, from which the acid pKa value can be inferred. Our results advance fundamental understanding of the relationship between acid dissociation and the hydration environment.

Enhancing Dual Reforming Via Electric Field-Assisted Nanocomposite Catalysts.

Jung-Il Yang
Clean Fuels Laboratory, Korea Institute of Energy Research, Daejeon, Korea, Republic of (South)

Electric field-assisted nanocomposite catalysts demonstrated high CH_4 and CO_2 conversions and excellent coke resistance in low-oxidant dual reforming. The observed performance is attributed to internal electric fields formed within nanopore structures. The results suggest a promising pathway toward catalytic reforming electrification at lower temperatures for stable hydrogen production.

Enhancing Durability and Activity Toward Oxygen Evolution Reaction Using Single-Site Re-Doped Nifeox Catalysts at Ampere-Level.

Xiang Lyu *and Alexey Serov*
Oak Ridge National Laboratory, Knoxville, TN

Herein, we prepared a NiFeReOx catalyst with single-site Re dopants and observed that the single-site Re dopants could significantly enhance the durability without compromising the activity. A low degradation rate is observed with NiFeReOx catalyst in anion-exchange membrane water electrolyzer, which outperforms the NiFeOx and commercial IrOx catalysts.

Nanoporous Metal Oxide-Carbon Hybrid Materials Synthesized By Biomass Pyrolysis for Carbon Dioxide Capture.

Hong Je Cho *and Md Razaul Karim*
Chemical Engineering, Oklahoma State University, Stillwater, OK

We present one-step, facile synthesis of metal oxide-carbon (MO-C) hybrid materials via metal precursor-activating pyrolysis of spent coffee grounds (SCG) as carbon precursors, and elucidate how structure and properties of MO-C materials tailored by the control of synthetic factors affect their CO_2 adsorption performance.

Catalytic $SnSe_2$@Mxene Composite Separators for Superior Polysulfide Regulation in Lithium–Sulfur Batteries.

Amirhossein Mirtaleb*, Ruigang Wang, and* ***Md Monir Hossain***
Chemical Engineering and Materials Science, Michigan State University, East Lansing, MI

Lithium–sulfur batteries offer high energy density but face issues like polysulfide shuttling and poor cycling stability. This study introduces $SnSe_2$@MXene composites as functional interlayers to enhance LiPSs adsorption, catalysis, and conductivity, thereby improving redox kinetics and stability for high-performance lithium–sulfur batteries.