PLENARY LECTURES

2025 PAUL H. EMMETT AWARD PLENARY LECTURE BY PHILLIP CHRISTOPHER

Tuesday, June 10, 2025 8:00 AM - 9:00 AM
Centennial Ballroom

Chair: Suljo Linic, University of Michigan, Ann Arbor

Atomically Dispersed Pt-Group Metal Catalysts: Active Site Structure, Function and Design.

Phillip Christopher
Department of Chemical Engineering, University of California, Santa Barbara, Santa Barbara, CA

I will highlight efforts focused on: (1) the synthesis and characterization of uniform atomically dispersed Pt active sites, (2) the development of structure-function relationships, (3) the local restructuring of these active sites due to changes in environmental conditions and (4) atomically dispersed Rh based catalysts for alkene hydroformylation.

AI - AI-DRIVEN CATALYSIS

AI - APPLICATION-DRIVEN AI CATALYST DESIGN

Tuesday, June 10, 2025 9:30 AM - 11:30 AM
Regency Ballroom VII

Chair: Long Qi, Ames Laboratory

Co-Chair: Nancy M. Washton, Pacific Northwest National Laboratory

Catalyst Discovery for Ammonia Synthesis Using Active Learning.

Jochen Lauterbach[1] *and Withana A R Jayarathna*[2]
(1)Department of Chemical Engineering, University of South Carolina, Columbia, SC, (2)University of South Carolina, Columbia, SC

Literature data for heterogeneous catalysts make it a great source for AI searches, and selectively adding experimental data via Active Learning allows for the efficient discovery of novel catalysts. We employ this framework for heterogeneous catalyst development for ammonia synthesis, reporting previously unknown formulations.

Autonomous AI-Driven Discovery of Multicomponent Oxides for CO_2 Utilization in Chemical Looping.

Anders Hellman
Competence Centre for Catalysis, Chalmers University of Technology, Göteborg, Sweden

Utilizing a self-learning cycle, we discover several new multi-component oxygen carriers for CO_2 splitting in chemical looping. The study demonstrates the self-learning cycle's scalability and effectiveness in accelerating material discovery while contributing to advancements in carbon utilization and hydrogen production processes.

Accelerated Discovery of Heterogeneous Catalysts Using Machine Learning Approach.

Ken-ichi Shimizu[1] *and* ***Takashi Toyao***[2]
(1)Institute for Catalysis, Hokkaido university, Sapporo, Japan, (2)Hokkaido University, Sapporo, Japan

We demonstrate a ML approach to develop new multi-elemental reverse water-gas shift catalysts. By performing 44 cycles of the closed loop discovery system (ML prediction + experiment), we experimentally tested 300 catalysts and identified more than 100 catalysts with superior activity compared to those of the previously reported high-performance catalysts.

Atomistic Evolution of Active Sites in Multi-Component Heterogeneous Catalysts.

Cameron Owen[1]*, Lorenzo Russotto*[1]*, Christopher O'Connor*[2]*, Nicholas Marcella*[3]*, Anders Johansson*[1]*,* ***Albert Musaelian***[1]*, Ralph G. Nuzzo*[3]*, Anatoly I. Frenkel*[4,5]*, Christian Reece*[1]*, and Boris Kozinsky*[1,6]
(1)Harvard University, Cambridge, MA, (2)Rowland Institute at Harvard, Harvard University, Cambridge, MA, (3)University of Illinois Urbana-Champaign, Urbana, IL, (4)Stony Brook University, Stony Brook, NY, (5)Brookhaven National Laboratory, Upton, NY, (6)Robert Bosch LLC Research and Technology Center, Watertown, MA

This work studies PdAu metal nanoparticle catalysts using machine learning force field techniques to conduct simultaneously accurate and scalable atomic-scale simulations. Among other results, we provide direct atomistic evidence that verifies existing experimental hypotheses for bimetallic catalyst deactivation under reaction conditions, namely that Pd preferentially segregates into the Au bulk.

Accelerating Material Discovery in Syngas Hydrogenation Via Open-Access Feature Engineering and Semantic Standardization.

Mohammad Khatamirad[1]*, Tiago Goncalves*[2]*, Edvin Fako*[2]*, Sandip De*[2]*, Raoul Naumann d'Alnoncourt*[1]*, Michael Geske*[1]*, Stephan A. Schunk*[2,3]*, Sonja Schimmler*[4]*, and Frank Rosowski*[1,2]
(1)BasCat - UniCat BASF JointLab, Berlin, Germany, (2)Group Research, BASF SE, Ludwigshafen, Germany, (3)hte GmbH, Heidelberg, Germany, (4)Open Communication Systems, Fraunhofer FOKUS, Berlin, Germany

This work presents a data-driven approach to accelerate multi-component catalyst discovery for the syngas-to-ethanol reaction. By leveraging open-access descriptors, predictive modeling, and semantic standardization, this study identifies novel catalyst compositions, enhancing ethanol yield without time-intensive computations, and establishes a reusable framework for machine-actionable catalytic data.

Development of Improved Promoted Pt Catalysts for Propane Dehydrogenation through Bayesian Optimization with Uncertainty Quantification.

Harsh Darji[1], *Unni Kurumbail*[1], *Matias Alvear*[2], *Siying Chen*[2], *and Ive Hermans*[1,2,3]
(1)Department of Chemical & Biological Engineering, University of Wisconsin-Madison, Madison, WI, (2)Department of Chemistry, University of Wisconsin - Madison, Madison, WI, (3)Wisconsin Energy Institute, University of Wisconsin - Madison, Madison, WI

This study presents a Bayesian optimization strategy to identify highly active and stable multi-metallic heterogeneous catalysts within a large design space of ~1.4MM possible formulations of Pt/γ-Al_2O_3 catalysts for propane dehydrogenation. The approach employs a two-tiered optimization process, incorporating finer variations in metal loadings and integrating uncertainty into surrogate models.

BIOMASS - BIOMASS AND WASTE VALORIZATION CATALYSIS

BIOMASS - BIOMASS CONVERSION

Tuesday, June 10, 2025 9:30 AM - 11:30 AM
Regency Ballroom VI

Chair: Yomaira Pagan Torres, University of Puerto Rico at Mayaguez

Co-Chair: Mike Griffin, National Renewable Energy Laboratory

An Electrobiomanufacturing Strategy for the Production of Renewable Adipic Acid.

Prathamesh T. Prabhu[1,2], *Deep M. Patel*[1,2], *Marco Nazareno Dell'Anna*[1,2], *Devanshi Mistry*[1,2], *Luke T. Roling*[1,2], *and* ***Jean-Philippe Tessonnier***[1,2]
(1)Center for Biorenewable Chemicals (CBiRC), Ames, IA, (2)Department of Chemical and Biological Engineering, Iowa State University, Ames, IA

Biobased *cis,cis*-muconic acid is converted to adipic acid, a Nylon monomer, using an electrobiomanufacturing approach that leverages biomass as renewable carbon feedstock, water as a hydrogen source, and green electricity to drive the transformation. Outer-sphere and surface-mediated electrohydrogenation pathways are controlled by the nature of the metal catalyst and pH.

Developing Nanoscale Catalysts for Biomass Electro-Valorization through Structure-Property Relationships.

Nicholas Bedford[1] *and Yuwei Yang*[2]
(1)Colorado School of Mines, Golden, CO, (2)University of New South Wales, Sydney, Australia

This contribution summarizes our group's recent work in implementing electrocatalytic approaches toward the valorization of biomass-derived substrates. This will include electrooxidation and electrocoupling reactions and will showcase the importance of understanding structure-property relationships to help elucidate catalytic properties.

Characterization of Catalyst Performance for Conversion of Bio-Derived Oxygenates Using Dual-Column GC.

Christopher P. Nicholas*, Benjamin R. Hoekstra, and Lyle Monson*
Lakril Technologies Corporation, Chicago, IL

The dual-column GC method uses a single injection to analyze samples containing high levels of water, organic acids, oxygenates, and permanent gases (CO, CO2, and C2H4) using a single injection. This method has been utilized to investigate reaction pathways during lactate dehydration and the impact of feedstock impurities on catalysis.

Role of Phosphorous in Transition Metal Phosphides for Selective Hydrogenolysis of Hindered C–O Bonds.

Conor Waldt[1,2]*, Hansel Montalvo-Castro*[1]*, Justin Atlas*[1]*, Angela Aguirre*[1,2,3]*, Alvaro Loaiza*[4]*, Craig Plaisance*[4]*, and David Hibbitts*[1,2]
(1)Department of Chemical Engineering, University of Florida, Gainesville, FL, (2)Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN, (3)Chemical Engineering, University at Buffalo, Buffalo, NY, (4)Cain Department of Chemical Engineering, Louisiana State University, Baton Rouge, LA

Adding P to Ni and other transition metals generally leads to an increase in selectivity for cleaving hindered C–O bonds. These shifts in selectivity are resultant of electronic modifications of the M atoms by P and to a lesser degree changes in the size of the continuous M atom ensembles.

Selective Production of Biobased Primary Amines By Reductive Amination over Atomically Dispersed Pt_1/S-C.

Yangming Ding*, Guanna Li, Tomas Haasterecht, van, and Johannes Hendrik Bitter*
Wageningen University, Wageningen, Netherlands

Reductive amination of furfural is a sustainable strategy towards primary amine synthesis. The electronic effect of Pt has a significant influence on the selectivity. Pt single atom and nanoparticles supported on carbon doped S was prepared for proof of concept. The highest yield to furfural amine was achieved over Pt_1/S-C.

Catalytic Lactide Production from Renewable Alkyl Lactates over Ti MWW-Type Zeolite Catalysts.

Haerin Lee, ***Seung Hyeok Cha****, and Dong Won Hwang*
Korea Research Institute of Chemical Technology (KRICT), Daejeon, Korea, Republic of (South)

Ti-MWW catalysts demonstrate superior lactide productivity in the gas-phase conversion of methyl lactate, outperforming TiO_2/MCM-41 and TS-1. Accessible tetrahedral TiO_4 active sites on 12-ring cup-shaped external surfaces enhance catalytic activity, doubling the turnover frequency compared to other catalysts, highlighting Ti-MWW's efficiency and selectivity for lactide production.

C2+ - CATALYSIS OF C2+ CHEMISTRY

C2+ | ETHANE DEHYDROGENATION AND AMMOXIDATION REACTIONS

Tuesday, June 10, 2025 9:30 AM - 11:30 AM
Hanover Hall CDE

Chair: Nathaniel Eagan, Tufts University

Co-Chair: Stephen Purdy, Oak Ridge National Laboratory

Kinetic Consequences of Oxygen Vacancies in Cobalt-Molybdenum Oxides on C−H Activation of Ethane.

Guangming Cai[1]*, Gregory Novotny*[2]*, Alyssa Hensley*[3]*, Prashant Deshlahra*[2]*, and Ya-Huei (Cathy) Chin*[1]
(1)Department of Chemical Engineering and Applied Chemistry, University of Toronto, Toronto, ON, Canada, (2)Department of Chemical and Biological Engineering, Tufts University, Medford, MA, (3)Chemical Engineering and Materials Science, Stevens Institute of Technology, Hoboken, NJ

This work highlights the kinetic consequences of O-vacancies in ethane C−H bond activation, emphasizing the necessity of considering in situ defect dynamics to accurately establish structure-reactivity relationships.

Modeling Particle Size Effect for Ethane Dehydrogenation over Pt Catalysts.

Mubarak Bello[1]*, Bhawana Rayamajhi*[1]*, Olajide Bamidele*[1]*, Wenqiang Yang*[1]*, and Andreas Heyden*[2]
(1)Chemical Engineering, University of South Carolina, Columbia, SC, (2)Department of Chemical Engineering, University of South Carolina, Columbia, SC

A new particle-based microkinetic modeling approach was used to investigate the effect of Pt particle size on ethane dehydrogenation (EDH) kinetics and mechanism. Better kinetic agreement with experiment was achieved and new insights into the EDH mechanism uncovered.

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

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

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

Subtle Changes to the Active Sites of Zeolite-Supported Metals during Reaction: Understanding the Promotional Effect of Parallel CO_2 Reduction on Ethane Dehydrogenation.

*Wenqi Zhou, Ron Runnebaum, and **Coleman Kronawitter***
Chemical Engineering, University of California, Davis, CA

Co-feeding CO_2 has a promotional effect on the rate of ethane dehydrogenation for many catalyst material systems, but the mechanism is not understood. This work leverages a zeolite-based catalyst with well-defined active sites, combined with operando X-ray absorption spectroscopy, to understand the impact of parallel CO_2 reduction on ethane dehydrogenation.

CO_2 Oxidative Ethane Dehydrogenation on CeO_2/SiO_2 Supported $NiFe_3$ Catalysts.

***Rachel Spurlock**[1,2], Ezgi Erdem[1,2], Sang-Won Lee[1,2], Junjie Chen[1,2], Alessandro Gallo[1,2], Adam Nielander[2], and Thomas Jaramillo[1,2]*
(1)Chemical Engineering, Stanford University, Stanford, CA, (2)SUNCAT Center for Interface Science and Catalysis, SLAC National Accelerator Laboratory, Menlo Park, CA

Supporting $NiFe_3$ on a mixed CeO_2 on SiO_2 support system allows the creation of a solid solution of Fe-doped CeO_2 crystals. The solid solution results in high ethylene production rate, as well as high ethylene selectivity; a marked improvement over a CeO_2-only supported $NiFe_3$, which shows poor ethylene selectivity.

Influence of Metal Identity on Acetonitrile Selectivity in Ethane Ammoxidation.

***Jieun Lee**[1], Yongwoo Kim[1], Jing Luo[2], Ida (xue) Chen[3], and David W. Flaherty[1]*
(1)Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA, (2)Engineering and Process Science, The Dow Chemical Company, Midland, MI, (3)Dow, Inc., Manvel, TX, 77578, TX

We synthesize, characterize, and kinetically examine catalysts formed by ion exchange of metal cations (M-BEA) to beta zeolites for ethane ammoxidation to acetonitrile. Co and Ni-BEA show higher acetonitrile selectivity, likely because Co and Ni bind with NH_3 to form a stable metal-amine complex required for acetonitrile formation.

ELECTRO PHOTO - ELECTROCATALYSIS AND PHOTOCATALYSIS

ELECTRO PHOTO - ORGANIC ELECTROCHEMICAL TRANSFORMATIONS 2

Tuesday, June 10, 2025 9:30 AM - 11:30 AM
Centennial Ballroom I

Chair: Jason Bates, University of Virginia

Co-Chair: Robert Warburton, Case Western Reserve University

Elucidating the Influence of Potassium Addition in Ru/TiO_2 on Charge-Carrier Dynamics for Photocatalytically Enhanced Ammonia Synthesis.

Carissa Yim[1], *Anna Klinger*[2], *Hannah R. Faustyn*[3], *Alondra M. Ortiz-Ortiz*[4], *Daniel Penley*[4], *Daniel O. Delgado Cornejo*[4], *Sijun Seong*[1], *Xiwen Gong*[1], *Neil P. Dasgupta*[5], *Galen Fisher*[1], *Johann Schwank*[1], *and Andrej Lenert*[1]
(1)Chemical Engineering, University of Michigan, Ann Arbor, MI, (2)Chemical Engineering, University of Michigan, Ann Arbor, Ann Arbor, MI, (3)Mechanical Engineering, University of Michigan, Ann Arbor, Ann Arbor, MI, (4)Mechanical Engineering, University of Michigan, Ann Arbor, MI, (5)Mechanical Engineering and Materials Science, University of Michigan, Ann Arbor, MI

We study the crystallographic structure, Ru nanoparticle (NP) size, and charge-carrier lifetime (τ) in 1 and 4 wt.% Ru/TiO_2 catalysts with 0.2, 4, or 8 wt.% K (y wt.% Ru/ x wt.% K-TiO_2), aiming to inform the design of efficient photocatalysts to help address the demand for distributed NH_3 synthesis.

Selective Formation and Reaction of Surface Oxygen Species to Promote Alkene Epoxidation over Oxygen Evolution on Au Anodes.

Richa Ghosh, *Jordan W. Lu, Geoffrey Hopping, and David Flaherty*
School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA

Previous attempts to promote epoxidation on electrodes focused on catalyst development. Oscillation of electrode potentials may increase Faradaic efficiencies for alkene epoxidations through O_2 evolution inhibition. Here, we use transient open circuit potential transients and *operando* surface enhanced Raman spectra to develop potential oscillation programs for epoxidation Faradaic efficiency optimization.

Enhancing the Electrooxidation of Furfural with Metal/Oxide Interfaces and Low Loading Catalyst.

Emma Hollis, *Marc Manye Ibanez, and Adam Holewinski*
Chemical and Biological Engineering, University of Colorado Boulder, Boulder, CO

Metal oxides interfaces and low loading catalyst were explored to enhance reaction efficiency of furfural oxidation in acid. Pt/ATO oxidizes furfural 0.2V lower than Pt/C, leading to sustained current with less decay in rate over time. Further kinetics implies that ATO donates OH to the strongly bound intermediates on Pt.

Complete Electrocatalytic Aqueous Defluorination of PFAS with Nonprecious Materials.

Astrid Müller
Chemical Engineering, University of Rochester, Rochester, NY

PFAS are persistent pollutants requiring effective remediation strategies. We developed a cost-effective electrocatalytic method using nonprecious nanocatalysts and deep ultraviolet light for

complete mineralization of PFOS, PFOA, and GenX. This approach minimizes energy use and prevents anode fouling, demonstrating significant advancements in PFAS destruction technologies.

KEYNOTE: Electrified Olefin Epoxidation Via Water Activation.

Karthish Manthiram
Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, CA

We present methods of epoxidizing olefins using water-derived oxygen atoms at ambient conditions. Water is activated at the anode, generating oxygen-containing intermediates that convert olefins into epoxides, while generating hydrogen at the cathode. Spectroscopy unveils structural features of the most active catalysts, acting as design principles for future work.

ENVIRO AUTO - ENVIRONMENTAL AND AUTOMOTIVE CATALYSIS

ENVIRO AUTO - MECHANISTIC INSIGHTS ON SELECTIVE CATALYTIC REDUCTION (SCR) OVER CU-ZEOLITES

Tuesday, June 10, 2025 9:30 AM - 11:30 AM
Hanover Hall FG

Chair: Rohil Daya, Cummins Inc.

Co-Chair: Isabella Maria Nova, Politecnico di Milano

Fundamental Insight from Decoupling RHC and OHC in the Standard-SCR Redox Mechanism over Cu-CHA Catalysts.

Andrea Gjetja[1], Nicola Usberti[1], Nicole Daniela Nasello[1], Umberto Iacobone[1], Isabella Maria Nova[1], ***Enrico Tronconi**[1]*, *Roberta Villamaina[2], Maria Pia Ruggeri[2], Djamela Bounechada[2], Andrew P.E. York[2], and Jillian Collier[2]*
(1)Dipartimento di Energia, Politecnico di Milano, Milan, Italy, (2)Johnson Matthey Technology Centre, Sonning Common, United Kingdom

Decoupling RHC and OHC of the Standard-SCR redox mechanism by transient response methods provides novel insight into the effects of reaction variables and catalyst parameters on NH_3-SCR over Cu-CHA. Such effects are often opposite for the two redox half cycles: they would remain unclear if focusing just on steady-state data.

H2O-Assisted Oxidation Half-Cycle of Low Temperature NH3-SCR over Cu-CHA.

***Gabriele Contaldo**, Isabella Maria Nova, Matteo Maestri, and Enrico Tronconi*
Laboratory of Catalysis and Catalytic Processes - Dipartimento di Energia, Politecnico di Milano, Milano, Italy

H_2O dissociates over dimeric Cu(I) species to form H_2O_2, a strong oxidant that completes the oxidation of a second pair of Cu(I) moieties in adjacent CHA cages. Such results describe the reaction mechanism of OHC of NH_3-SCR and clarify the active role of H_2O in promoting the kinetically relevant step.

NH_3-SCR Redox Kinetics Monitored By Operando UV Spectroscopy.

*Nicola Usberti[1], Gabriele Contaldo[2], Mauro Bracconi[2], **Chiara Negri**[2], Isabella Maria Nova[2], Matteo Maestri[2], and Enrico Tronconi[3]*
(1)Dipartimento di Energia, Politecnico di Milano, Milan, Italy, (2)Laboratory of Catalysis and Catalytic Processes - Dipartimento di Energia, Politecnico di Milano, Milano, Italy, (3)Politecnico di Milano, Milan, Italy

We demonstrated the possibility to extract kinetic relevant data from operando UV-Vis spectroscopy to monitor Cu redox chemistry, during NH3-SCR. By combining a packed bed reactor with a high temperature UV-Vis probe we monitored the evolution of Cu oxidation state, extracting kinetic relevant data aligned with gas phase quantification data.

Insights into NH_3 Inhibition of SCR on Cu-CHA Catalysts.

***Dhruba Jyoti Deka**[1], Mingyu Wan[2], Garam Lee[1], Eric D. Walter[1], Fanglin Che[2], Kenneth Rappe[1], Janos Szanyi[1], and Yong Wang[1,3]*
(1)Pacific Northwest National Laboratory, Richland, WA, (2)Chemical Engineering, University of Massachusetts Lowell, Lowell, MA, (3)Washington State University, Pullman, WA

Excess NH_3 in selective catalytic reduction on Cu-CHA hinders NO_x conversion by reducing Cu ion mobility, impacting low-temperature performance. This study provide fundamental insights into NH_3 inhibition mechanism and suggests optimizing Si/Al ratios, Cu loading, and NH_3-to-NO_x ratios to enhance SCR efficiency and guide better urea dosing in diesel engines.

Collective Effects and Aluminum Distribution Control Diffusion and Pairing of $[Cu(NH_3)_2]^+$ Complexes in Cu-CHA.

***Joachim Bjerregaard**[1], Martin Votsmeier[2], and Henrik Grönbeck[1]*
(1)Department of Physics and Competence Centre for Catalysis, Chalmers University of Technology, Göteborg, Sweden, (2)Umicore, Hanau-Wolfgang, Germany

Copper exchanged chabazite (Cu-CHA) is state-of-the-art catalyst for removal of NO_x from lean burn engines. The pairing of mobile $[Cu(NH_3)_2]^+$ complexes is crucial for sustaining a high activity. Here we utilize machine learning forcefield to investigate the influence of diffusion mechanisms and zeolite compositions on the pairing of $[Cu(NH_3)_2]^+$ complexes.

Role of HTA and Cu Speciation in NH_3-SCR Reactions over Cu-SSZ-13 Catalysts.

***Andrea Gjetja**[1], Nicola Usberti[1], Isabella Maria Nova[1], Enrico Tronconi[2], Rohil Daya[3], Lai Wei[3], Hongmei An[3], and Krishna Kamasamudram[3]*
(1)Dipartimento di Energia, Politecnico di Milano, Milan, Italy, (2)Politecnico di Milano, Milan, Italy, (3)Cummins Inc., Columbus, IN

Mild Hydrothermal Aging (HTA) of Cu-SSZ-13 catalysts causes a DeNOx performance loss in NH_3-SCR. A clear effect over the mechanism of the different SCR reactions is still not understood. This work delves into these aspects, understanding the role of the different Cu species.

FUNDAMENTALS - FUNDAMENTALS OF CATALYSIS AND SURFACE SCIENCE

FUNDAMENTALS - CATALYST DESIGN AND SURFACE SCIENCE

Tuesday, June 10, 2025 9:30 AM - 11:30 AM
Centennial Ballroom II

Chair: Benjamin Jackson, Pacific Northwest National Laboratory

Co-Chair: Konstantin Khivantsev, Pacific Northwest National Laboratory

Structure-Activity Relationship of Transition Metal Carbide Catalyst for Hydrodeoxygenation Reaction.

Raghavendra Meena[1], Johannes Hendrik Bitter[2], and ***Guanna Li***[2]
(1)Wageningen University and Research, Wageningen, Netherlands, (2)Wageningen University, Wageningen, Netherlands

The reaction mechanism and structure-activity relationship of Mo_2C towards hydrodeoxygenation reaction was rationalized by integrating multiple modeling approaches of DFT, molecular dynamics, microkinetic modeling, and machine learning method. The key descriptors correlating to the barrier of the rate-determining step were identified. The in-situ-generated molybdenum oxycarbide is the most active catalyst.

Impacts of Titania Phase on H_2 Adsorption and Spillover on Au/TiO_2 Catalysts.

Audrey Battiste[1] *and Bert Chandler*[2]
(1)Chemistry, Pennsylvania State Univerisity, State College, PA, (2)Chemical Engineering, Pennsylvania State Univerisity, State College, PA

H_2 adsorption and spillover on Au/TiO_2 catalysts is strongly dependent on TiO_2 phase. Au/rutile exhibits adsorption quantities more than an order of magnitude higher than Au/anatase catalysts. Adsorption thermodynamics also change dramatically with TiO_2 phase and metal identity (e.g. replacing Au with Pt).

Diverse Active Sites on CuO_x Nanoparticles and Their Catalytic Consequences in Oxidation Catalysis.

William Broomhead[1], Maarten Nachtegaal[2], Peng Zhang[1], Yuechang Wei[3], and ***Ya-Huei (Cathy) Chin***[1]
(1)Department of Chemical Engineering and Applied Chemistry, University of Toronto, Toronto, ON, Canada, (2)Paul Scherrer Institute, Villigen, Switzerland, (3)College of Science, China University of Petroleum, Beijing, China

This study highlights the diverse catalytic roles of Cu in alkanol (oxidative) dehydrogenation and CO oxidation. Cu speciation and its immediate microenvironment (with reactive oxygen species) mediate the stability of the kinetically relevant transition states as well as their ability to bind to the hydroxyl species, thus affecting catalyst stabilities.

Designing the Cu-ZnO Interfacial Structure By Atomic Layer Deposition for Methanol Synthesis from CO_2 Hydrogenation.

Junjie Chen[1,2]*, Nadine Humphrey*[1,2]*, Anshuman Goswami*[1,2]*, Ezgi Erdem*[1,2]*, Rachel Spurlock*[1,2]*, Andrzej Rogala*[1,2]*, Alessandro Gallo*[1,2]*, Frank Abild-Pedersen*[1,2]*, Stacey F. Bent*[1,2]*, and Thomas Jaramillo*[1,2]
(1)Department of Chemical Engineering, Stanford University, Stanford, CA, (2)SUNCAT Center for Interface Science and Catalysis, SLAC National Accelerator Laboratory, Menlo Park, CA

In this work, we utilized model catalysts (Cu/SiO_2, $Cu/ZnO/SiO_2$, $ZnO/Cu/SiO_2$) with uniform Cu nanoparticles synthesized by colloidal chemistry and controllable ZnO overlayer prepared *via* atomic layer deposition to investigate the impact of the original structure of Cu-ZnO interface and ZnO overlayer thickness on CO_2 hydrogenation performance.

Selective Hydrogenation of Aromatic Hydrocarbons over Noble Metal Catalysts.

Yue Qi, Ziyu Tang, and ***Simon Podkolzin***
Department of Chemical Engineering and Materials Science, Stevens Institute of Technology, Hoboken, NJ

Reaction mechanisms for selective hydrogenation of aromatic hydrocarbons to cycloolefins and cycloalkanes over noble metal catalysts were studied at the molecular level. Reactive intermediates were identified by combining experimental IR and Raman spectroscopic measurements with DFT calculations and related to catalytic activity and selectivity differences. Improved catalyst formulations were developed.

Adsorption of Alcohols Allows Defining Hydrophilic and Hydrophobic Interactions in Tectosilicates.

Ruixue Zhao[1]*, Sungmin Kim*[2]*, Mal Soon Lee*[2]*, Fuli Deng*[1]*, Xiaomai Chen*[1]*, Yue Liu*[1]*, and Johannes Lercher*[1,2]
(1)Technical University of Munich, Garching b. München, Germany, (2)Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA

Investigating the interaction of water and alcohols with zeolite pores provides a fundamental insight into molecular interactions and differentiates these from macroscopic properties such as “hydrophilicity” and “hydrophobicity”. This understanding will be critical for using intermolecular forces, surface interactions, and confinement effects, to aid sorption and catalysis.

REACTOR - REACTION ENGINEERING AND REACTOR DESIGN

REACTOR - MODELING AND SCALE-UP OF REACTORS FOR INDUSTRIAL APPLICATIONS

Tuesday, June 10, 2025 9:30 AM - 11:30 AM
Centennial Ballroom III

Chair: Nicholas Thornburg, National Renewable Energy Laboratory

Co-Chair: Weijian Diao, Villanova University

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

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

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

Model-Based Reactor Design and Process Optimization for Scaling up Direct CO_2 Hydrogenation to Dimethyl Ether Production.

Canan Karakaya[1]*, Dylan Weber*[1]*, Aye (pimphan) Meyer*[1]*, and Hai-Ying Chen*[2]
(1)Manufacturing Science Division, Oak Ridge National Laboratory, Oak Ridge, TN,
(2)National Transportation Research Center, Oak Ridge National Laboratory, Knoxville, TN

This study uniquely combines a multi-scale reactor model with TEA and LCA analyses to assess the viability of the CO_2-to-DME process. The results underscore the importance of process optimization to enhance reactor design, maximizing yield, catalyst lifespan, and energy efficiency.

Imposing Atom Conservation on Physics-Informed Neural Networks for Catalytic Reactor Model Surrogates.

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

Physics-informed neural networks (PINNs) leverage *a priori* physical knowledge to provide highly performant, yet physically plausible surrogates of catalytic reactors or derive kinetic models from integral reactor data. However, most works on PINNs ignore the fundamental law of atom conservation. Here, we develop atom conserving PINNs to guarantee physical consistency.

Accelerating Catalyst Discovery Utilizing Nanoparticle Mega Libraries & Compositionally Controlled Thin Films: Development of a Spatially Resolved Scanning Probe Reactor.

Muntaseer Bunian[1], *Neil Schweitzer*[2], *and Selim Alayoglu*[3]
(1)Paula M. Trienens Institute for Sustainability and Energy, Northwestern University, Evanston, IL, (2)Department of Chemical and Biological Engineering, Northwestern University, Evanston, IL, (3)Department of Chemical & Biological Engineering, Northwestern University, Evanston, IL

In the space of continuous and parallel catalyst discovery, a scanning probe reactor system was developed to spatially detect and analyze local catalytic activity across domains ranging from thin films to nanoparticles with the goal of achieving detection at the single particle level.

Effects of POCS design on the intensification of heat transfer in FT structured reactors: a pilot plant experimental study.

Martino Panzeri[1], *Carlo Giorgio Visconti*[2], ***Gianpiero Groppi***[2], *and Enrico Tronconi*[1]
(1)Politecnico di Milano, Milan, Italy, (2)Dipartimento di Energia, Politecnico di Milano, Milan, Italy

We have studied experimentally the effect of the geometry of conductive POCS with skin for heat management of the FT synthesis. Our data identify the relative density RD as the most important parameter. This work shows that structured internals are a promising solution for the intensification of FT reactors.

Scaleup of Additively Manufactured Microchannel Reactor for Single-Step Conversion of Ethanol into n-Butene-Rich Olefins for Alcohol-to-Jet Application.

Austin Winkelman[1], *Johnny Saavedra-Lopez*[1], *Matthew Coblyn*[2], *Patrick Mcneff*[1], *Michael Hubbard*[1], *Kwangtae Son*[2], *Goran Jovanovic*[2], *Brian Vincente*[3], *Ralph Gillespie*[3], *Brian Paul*[4], *and Robert A. Dagle*[1]
(1)Pacific Northwest National Laboratory, Richland, WA, (2)School of Chemical, Biological and Environmental Engineering, Oregon State University, Corvallis, OR, (3)LanzaTech, Skokie, IL, (4)School of Mechanical, Industrial & Manufacturing Engineering, Oregon State University, Corvallis, OR

Sustainable aviation fuel production pathways from renewable ethanol that can be deployed at scale are of substantial interest. This work leverages microchannel technology to enable a 400x scaleup of our catalytic ethanol to n-butene system, demonstrating potential to reduce capital and operating expenditures compared to the current state-of-the-art alcohol-to-jet process.

SYNTHESIS - CATALYST SYNTHESIS AND MANUFACTURING

SYNTHESIS - INNOVATIVE CATALYST MATERIALS AND SYNTHESIS ROUTES

Tuesday, June 10, 2025 9:30 AM - 11:30 AM
Centennial Ballroom IV

Chair: Gianni Caravaggio, Natural Resources Canada (NRCan)

Co-Chair: Jason Wu, Honeywell UOP

KEYNOTE: Development of Soluble and Reusable Polymer-Based Catalysts with Brønsted and Lewis Acidity.

Ibeh S. Omodolor[1]*, Subhash Kalidindi*[1]*, Nkem O. Ofole*[1]*, Sarah A. Walz*[1]*, Maria R. Coleman*[1]*, Sridhar Viamajala*[1]*, Ravikumar Gogar*[1]*, Manuel López Granados*[2]*, Francielle Candian Firmino Marcos*[3]*, and* ***Ana C. Alba-Rubio***[1,3]
(1)Department of Chemical Engineering, The University of Toledo, Toledo, OH, (2)Institute of Catalysis and Petrochemistry (ICP-CSIC), Cantoblanco, Madrid, Spain, (3)Department of Chemical and Biomolecular Engineering, Clemson University, Clemson, SC

We developed a series of soluble and reusable polymer-based catalysts with Brønsted and Lewis acidity. These catalysts were studied in the one-pot synthesis of hydroxymethylfurfural from glucose and potato starch. The best catalyst presented similar catalytic activity as a combination of H_2SO_4 and $AlCl_3$ with the advantage of being reusable.

SiC with High Specific Surface Area for Use in Catalysis.

Adrian Ortega[1]*, Mario Caccia*[2]*, and* ***Javier Narciso***[1]
(1)University of Alicante, Alicante, Spain, (2)Alfred University, Alfred, Spain

In this work, a new synthetic route for SiC is presented. Hierarchical SiC with a surface area of 200 m^2/g has been obtained. This SiC has been used as a support for Pt, and the Pt-SiC interaction has been studied and how it affects the reaction for obtaining crotyl alcohol.

Rapid Crystallization of Zeolites with Controllable Defects: Disentangling Fluoride Concentration and pH Using Ammonium Fluoride.

Muhammad Shah[1]*, Taras Nagornyy*[1]*, Success Aiwekhoe*[1]*, Seungbo Hong*[1,2]*, Nhan Huu Huy Tran*[1]*, Song Luo*[1]*, Zhu Chen*[1]*, Scott M. Auerbach*[1,2]*, and Wei Fan*[1]
(1)Department of Chemical Engineering, University of Massachusetts Amherst, Amherst, MA, (2)Department of Chemistry, University of Massachusetts Amherst, Amherst, MA

Zeolite synthesis in neutral fluoride-media produces fewer defects, however, this often requires significantly longer crystallization times and involves handling dangerous HF. In the present study, by disentangling fluoride concentration and pH using NH_4F as a safer alternative, we found that the crystallization rate can be significantly improved with fewer defects.

SSZ-43 Zeolites: A Comparative Study of Synthesis Routes and Catalytic Applications.

Taekyung Ryu[1]*, Jesús Pascual*[1]*, Marat Orazov*[1]*, Joel Schmidt*[1]*, C.Y. Chen*[2]*, and Stacey I. Zones*[1]
(1)Chevron, Richmond, CA, (2)Chevron Energy Technical Center, Richmond, CA

Here, we provide an overview of the synthesis and post-synthetic treatment of borosilicate SSZ-43 (B-SSZ-43) zeolites crystallized via different synthesis routes: direct, seed-assisted, and interzeolite conversion. The physicochemical and catalytic characterization of these SSZ-43 materials will be discussed.

Raspberry-Colloid-Templating As a Model Thermocatalytic Platform.

Kang Rui Garrick Lim[1] *and Joanna Aizenberg*[2]
(1)Chemistry and chemical biology, Harvard University, Cambridge, MA, (2)John A. Paulson School of Engineering and Applied Sciences, Harvard University, Cambridge, MA

The performance of heterogeneous catalysts depend on descriptors related to the nanoparticles, support, and their interactions. However, current methods do not permit independent changes to these parameters. To unequivocally derive structure-property relationships, we developed a raspberry-colloid-templating strategy that enables independent combinatorial variations of the material's building blocks and their organization.

AI - AI-DRIVEN CATALYSIS

AI - USING AI TO NAVIGATE LARGE CATALYST DESIGN SPACES

Tuesday, June 10, 2025 1:00 PM - 3:20 PM
Regency Ballroom VII

Chair: Tibor Szilvasi, The University of Alabama, Department of Chbe

Co-Chair: Tej Choksi, Nanyang Technological University

Digital Catalysis: Accelerated Discovery through Human in the Loop.

Charles Pare[1]*, Aybike Terzi*[2]*, Christian Kunkel*[1]*, Frederik Rüther*[2]*, Frederic Felsen*[1]*, Raoul Naumann D'Alnoncourt*[2]*, Christoph Scheurer*[1]*, Karsten Reuter*[1]*, and Frank Rosowski*[2]
(1)Fritz Haber Institute of the Max Planck Society, Berlin, Germany, (2)BasCat - UniCat BASF Joint Lab, Technische Universität Berlin, Berlin, Germany

Promoters are indispensable for the optimized performance and lifetime of industrial catalysts, with modern catalysts mostly benefiting from only a small number of promoters. Here we present an accelerated discovery approach that globally explores a high-dimensional multi-promoter design space with only a few experiments and identify promising new catalyst chemistries.

Expanding the Synthesis Window of Zeolites Containing *Lta* Cavities through Rational Design of Structure-Directing Agents and Ionic Environment.

Soonhyoung Kwon[1] *and Yuriy Roman*[2]
(1)Charles D. Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN, (2)Department of Chemical Engineering, Massachusetts Institute of Technology, Cambridge, MA

We employed high-throughput simulations to design optimal organic structure-directing agents and ionic environments for synthesizing high-silica small-pore zeolites with *lta* cavities. This approach achieved unprecedented Si/Al ratios, superior hydrothermal stability, and phase selectivity in **LTA**, **UFI**, **RHO**, and **KFI** frameworks, expanding the synthesis window for tailored zeolitic materials.

Understanding Metal-Support Interactions By Interpretable Machine Learning.

Chenggong Jiang[1]*, Bryan Goldsmith*[2]*, and Suljo Linic*[1]
(1)Department of Chemical Engineering, University of Michigan, Ann Arbor, MI, (2)Chemical Engineering, University of Michigan, Ann Arbor, MI

Using physics-informed machine learning and molecular dynamics simulations, we identified key oxide support features governing metal-support interactions in Pt nanocatalysts. Surface energy, oxygen bond order, dipole, and work function predict Pt-oxide interaction strength. This enables screening of 10,000+ oxide surfaces for sinter-resistant supports, accelerating stable nanocatalyst discovery.

Micro-Kinetic Modeling of Temporal Analysis of Products Data Via Kinetics-Informed Neural Networks.

Dingqi Nai[1]*, Gabriel Gusmão*[2]*, Zachary Kilwein*[1]*, Fani Boukouvala*[3]*, and Andrew Medford*[2]
(1)Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA, (2)School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA, (3)School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA

We utilize kinetics-informed neural networks to efficiently model TAP data. KINNs can fit transient data, retrieve kinetic parameters, and interpolate unseen pulse behavior even when thin-zone information is unavailable. KINNs outperform traditional methods in noise tolerance and computational efficiency, offering a promising alternates for interpreting transient kinetics in catalysis research.

Advantages in the Use of AI-Based Regressions for the Kinetic Modelling of Industrial Catalysts.

Hugo Pétremand[1]*, Andrea Pappagallo*[1]*, and Emanuele Moioli*[2]
(1)Paul Scherrer Institute, Villigen, None, Switzerland, (2)Politecnico di Milano, Milano, None, Italy

This papers shows the potential of using AI-based regressions (artificial neural networks, random forests) for kinetic models of industrial catalysts, comparing them with standard LHHW-based approaches

Representation Learning for Predicting Shape Selectivity in Nanoporous Zeolites.

Yachan Liu[1]*, Ping Yang*[1]*, Aaron Sun*[2]*, Zezhou Cheng*[2]*, Gustavo Perez*[2]*, Wei Fan*[1]*, Subhransu Maji*[2]*, and* ***Peng Bai***[1]
(1)Department of Chemical Engineering, University of Massachusetts Amherst, Amherst, MA, (2)College of Information and Computer Sciences, University of Massachusetts Amherst, Amherst, MA

ZeoNet, a representation learning framework based on 3D convolutional neural networks and a new volumetric representation, was developed for capturing shape selectivity in zeolites. ZeoNet was found to significantly outperform other popular materials representations including graph networks, vision transformers, and point clouds in predicting Henry's constants of long-chain hydrocarbon isomers.

Investigating the Sulfur Poisoning Characteristics of High-Entropy Alloys Using a Multi-Property Graph Neural Network.

Gaurav Deshmukh[1]*, Madison Bird*[2]*, and Jeffrey Greeley*[3]
(1)Chemical and Biological Engineering, Northwestern University, Evanston, IL, (2)Charles D. Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN, (3)Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN

Sulfidation stability of high-entropy alloy catalysts was explored using a multi-property graph neural network (SlabGCN) trained on a Pt-Pd-Rh-Cu quaternary alloy dataset. Sulfur coverage as a function of reaction conditions was visualized using surface phase diagrams. An optimal quaternary alloy composition was discovered using a Monte Carlo-inspired optimization scheme.

BIOMASS - BIOMASS AND WASTE VALORIZATION CATALYSIS

BIOMASS - FURANS

Tuesday, June 10, 2025 1:00 PM - 3:20 PM
Regency Ballroom VI

Chair: Silvia Morales de la Rosa, Instituto de Catálisis y Petroleoquímica, Spanish National Research Council (CSIC)

Co-Chair: Thomas Schwartz, University of Maine

Reductive Amination of Acetal-Protected 2,5-Diformylfuran to 2,5-Bis(aminomethyl)Furan Using Co_2p Nanorod (NR) Catalyst.

Nirupama Sheet[1]*, Ryota Osuga*[1]*, Satoshi Suganuma*[1]*, Takato Mitsudome*[2]*, and* ***Kiyotaka Nakajima***[1]
(1)Institute for Catalysis, Hokkaido University, Sapporo, Japan, (2)Graduate School of Engineering Science, Department of Materials Engineering Science, Osaka University, Toyonaka, Osaka, Japan

A stepwise reaction system was designed to synthesize 2,5-bis(aminomethyl)furan (BAMF) by the reductive amination of acetal-protected 2,5-diformylfuran (DFF) with 1,3-propanediol (PD) using a state-of-the-art Co_2P nanorod (NR) catalyst. The current system realized the production of BAMF in high yields (> 90%) even using concentrated solutions (10-20 wt%).

Catalytic Upgrading of Furfural Using Hierarchical ZSM-5 Zeolite.

Sancler C. Vasconcelos[1]*, Thiago Lima*[1]*, and* ***Fabio B. Passos***[2]

(1)Institute of Chemistry, Universidade Federal Fluminense, Niteroi, Brazil, (2)Department of Chemical and Petroleum Engineering, Universidade Federal Fluminense, Niteroi, Brazil

This work presents the use of hierarchical ZSM-5 zeolites for lignocellulosic biomass upgrading in liquid phase catalysis, in particular the conversion of furfural . Furfural conversion increased along with materials acidity, and the alkaline treatment lead to higher conversion.

Synthesis of a Jet Fuel Precursor By Hydroxyalkylation-Alkylation of 2-Methylfuran with Furfural Using Hierarchical H-Y Zeolites.

Odiri Siakpebru[1,2]*, Lakshmiprasad Gurrala*[1,2]*, Anoop Uchagawkar*[1,3]*, Oliver Norris*[1,2]*, Jared Bartlett*[1,2]*, and Ana Colaco Morais*[1,2]
(1)Chemical and petroleum Engineering, University of Kansas, Lawrence, KS, (2)Wonderful Institute for Sustainable Engineering, Department of Chemical and Petroleum Engineering, The University of Kansas, Lawrence, KS, (3)Center for Environmentally Beneficial Catalysis, University of Kansas, Lawrence, KS

We described the production of jet fuel precursor through the hydroxyalkylation-alkylation of 2-methylfuran with furfural using hierarchical H-Y zeolites synthesized from Na-Y (Si/Al = 2.6) via surfactant templating technique. Hierarchical H-Y-mod-1 zeolite demonstrated high reactant conversion and jet fuel precursor yield due to its strong Brønsted acidity and improved mesoporosity.

Modification of Gold Catalysts for the Selective Oxidation of 5-Hydroxymethyl Furfural to 2,5-Furandicarboxylic Acid.

Hidde Nolten[1] *and Petra E. de Jongh*[2]
(1)Utrecht University, Utrecht, Netherlands, (2)Inorganic Chemistry and Catalysis, Utrecht University, Utrecht, Netherlands

Oxidation of 5-hydroxymethylfurfural facilitates plastics production from biomass. We improve this important reaction by tuning the particle size and composition of a Au/TiO_2 catalyst, visualized with atomic-resolution electron microscopy. Our results show that adding Ag or increasing the particle size to 4 nm massively increases the desired product yield.

Hydrodeoxygenation of Tetrahydrofuran 2,5-Dicarboxylic Acid to Adipic Acid Driven By Pt-MoO_x Interfacial Sites.

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

The proximity of Pt and Mo is a critical factor for AA selectivity since it ensures the optimal degree of reduction of the oxyphilic metal and activate pathways where catalytic bifunctionalities are essential.

Sustainable Cu-Fe/Al_2O_3 Bimetallic Catalyst Synthesis Using Extract of Aged *Rosa Chinensis Jacq* Petals and Its Use in Furfural Hydrogenation..

Barbara Lino Galarza[1,2]*, Javier Rivera De la Rosa*[1]*, Carlos Enrique Escarcega González*[1]*,*
Carlos Javier Lucio Ortíz[1]*, Ladislao Sandoval*[3]*, Diana Bustos Martínez*[1]*, and Antonia Infantes-Molina*[2]
(1)Facultad de Ciencias Químicas, Universidad Autónoma de Nuevo León, Monterrey, NL, Mexico, (2)Química Inorgánica, Cristalografía y Mineralogía, Universidad de Malaga, Malaga, Malaga, Spain, (3)Escuela De Ingeniería y Ciencias, Instituto Tecnológico y de Estudios Superiores de Monterrey, Monterrey, NL, Mexico

Aged *Rosa Chinensis Jacq* petals, extracted with green solvents, were used to synthesize Cu-Fe/Al_2O_3 catalysts at low temperature. These catalysts, particularly contained the Cu_4Fe phase, showed high efficiency in the hydrogenation of furfural, a key step in biorefinery processes.

Selective Hydrogenation of Biomass-Derived Furans over Cu Catalysts: Experiments and Theory.

Evangelos Smith*, Michael Rebarchik, Hochan Chang, James A. Dumesic, and Manos Mavrikakis*
Department of Chemical and Biological Engineering, University of Wisconsin-Madison, Madison, WI

Herein, we combine reaction kinetics experiments with density functional theory (DFT) calculations to investigate the selective hydrogenation of HAH, a biomass-derived platform molecule, over copper catalysts. These findings may assist in the rational design of transition metal catalysts for the hydrogenation of compounds containing both aliphatic and aromatic double bonds

CO2 - CO2 CAPTURE AND UPGRADING

CO2 - CO_2 CONVERSION TO METHANE

Tuesday, June 10, 2025 1:00 PM - 3:20 PM
Centennial Ballroom IV

Chair: Haruka Nishiyama, SEKISUI CHEMICAL CO.,LTD

Co-Chair: Matteo Monai, Utrecht University

Elucidating the Crucial Role of Ta Dopant in Enhanced Selectivity of CO_2 Methanation Reaction over Ru/CeO_2 Catalyst at Lower Temperature.

Jose Rodriguez and ***Deboshree Mukherjee***
Chemistry, Brookhaven National Laboratory, Upton, NY

Ru/CeO_2 catalyst prepared with varying wt.% of Ta (0, 2.5, 11, and 18 wt.%) dopant, and applied for CO_2 Methanation reaction. At lower temperature, a consistent increase in methane

selectivity was observerved with increasing Ta wt.%. In-situ DRIFTS and EXAFS were perfomed to explain the findings.

Deciphering Effects of Nanoparticles Shape and Size on the Structure Sensitivity of CO_2 Methanation Reaction on Ni.

Gabriele Spanò[1], *Matteo Ferri*[1], *Raffaele Cheula*[1], *Matteo Monai*[2], *Bert M. Weckhuysen*[2], *and* ***Matteo Maestri***[1]
(1)Laboratory of Catalysis and Catalytic Processes - Dipartimento di Energia, Politecnico di Milano, Milano, Italy, (2)Inorganic Chemistry and Catalysis, Institute for Sustainable and Circular Chemistry, Utrecht University, Utrecht, Netherlands

Nickel nanoparticle shape critically influences turnover frequency (TOF) in CO2 methanation, but conflicting trends in TOF are reported. In this study we reveal that shape, not just size, governs the overall catalytic activity. Therefore, we offer a framework that reconciles highly debated discrepancies in the experimental literature

Mechanistic Insights and Selectivity Control in CO_2 Hydrogenation on Dispersed Ru, Co, and Ni Nanoparticles.

Wenshuo Hu[1], *Gregory Tate*[2], *and Enrique Iglesia*[3]
(1)Chemical Engineering, Texas Tech University, Lubbock, TX, (2)Chemical Engineering, University of California, Berkeley, Berkeley, CA, (3)University of California at Berkeley, Berkeley, CA

This study elucidates mechanistic elementary steps mediating CO_2-H_2 reactions on dispersed Ru, Co, and Ni nanoparticles, which are similar in identity and kinetic relevance. These mechanism and kinetic formalisms demonstrate that the presence of CO at specific inlet pressures enables the exclusive formation of CH_4 from CO_2-H_2 reactants.

Promoting Ni-Catalyzed CO_2 Methanation Via Gd Doping.

Majed Alam Abir[1] *and* ***Madelyn Ball***[2]
(1)Chemical and Biomedical Engineering, West Virginia University, Morgantown, WV, (2)Chemical Engineering and Materials Science, Michigan State University, East Lansing, MI

We have demonstrated enhanced performance for CO_2 methanation by doping Ni/SiO_2 catalysts with Gd at varied ratios. The addition of Gd impacts performance by changing the nature of the surface species under reaction conditions, enabling development of structure-performance relationships.

Advanced Biogas Methanation Catalysts for Generating Renewable Natural Gas.

Mathew Rasmussen[1], *Sawyer Halingstad*[2], *Dipesh Adhikari*[3], *Weijie Zhang*[4], *Robert Davis*[5], *Sen Zhang*[6], *and Matthew M. Yung*[7]
(1)Bioenergy Science and Technology Department, National Renewable Energy Laboratory,

Golden, CO, (2)National Renewable Energy Laboratory, Golden, CO, (3)university of virginia, charlottesville, VA, (4)Chemical Engineering, chemistry, university of Virginia, Charlottesville, VA, (5)Chemical Engineering, University of Virginia, Charlottesville, VA, (6)Chemistry, University of Virginia, Charlottesville, VA, (7)National Bioenergy Center, National Renewable Energy Laboratory, Golden, CO

In this work, we have compared the performance of Ni-based catalysts for converting biogas, a 50:50 mixture of CO_2 and CH_4, into renewable natural gas (RNG). We have demonstrated the feasibility of this technology by converting raw biogas from a wastewater treatment facility into pipeline-compliant RNG continuously for 100 hours.

Catalytic Methanation of CO_2 over Ni Nanoparticles for Production of Renewable Natural Gas from Biogas.

Dipesh Adhikari[1]*, Robert Davis*[2]*, Colby Whitcomb*[2]*, Weijie Zhang*[3]*, Matthew M. Yung*[4]*, Mathew Rasmussen*[5]*, Sen Zhang*[6]*, Sawyer Halingstad*[7]*, Bryan Schmerber*[8]*, and Lisa M. Colosi*[9]
(1)university of virginia, charlottesville, VA, (2)Chemical Engineering, University of Virginia, Charlottesville, VA, (3)Chemical Engineering, chemistry, university of Virginia, Charlottesville, VA, (4)National Bioenergy Center, National Renewable Energy Laboratory, Golden, CO, (5)Bioenergy Science and Technology Department, National Renewable Energy Laboratory, Golden, CO, (6)Chemistry, University of Virginia, Charlottesville, VA, (7)National Renewable Energy Laboratory, Golden, CO, (8)South Platte Renew, Englewood, CO, (9)Civil and Environmental Engineering, University of Virginia, Charlottesville, VA

This work investigates the roles of Ni particle size and support composition in the catalytic CO_2 methanation reaction for biogas upgrading to renewable natural gas. Life cycle analysis and techno-economic assessment of catalytic methanation utilizing renewable H_2 compared to conventional pressure swing adsorption reveal improvements in environmental and economic outcomes.

Reaction Pathways and Site Requirements for H-Assisted CO_2 Activation at Ni-Ce Interfaces.

Suchetana Samanta*, Jeffrey D. Rimer, and Praveen Bollini*
William A. Brookshire Department of Chemical and Biomolecular Engineering, University of Houston, Houston, TX

This work elucidates the reaction pathways and intermediates mediating methanation turnovers at the Ni-Ce interface. Kinetic, in-situ spectroscopic, and isotopic measurements provide evidence for hydrogen-assisted CO_2 activation routes at these interfaces, with hydrogen-assisted C-O bond scission of bidentate carbonates being the rate-determining step and bidentate formates acting as spectators.

ENVIRO AUTO - ENVIRONMENTAL AND AUTOMOTIVE CATALYSIS

ENVIRO AUTO - SUPPORTED METAL-OXIDES FOR EMISSION CONTROL CATALYSIS

Tuesday, June 10, 2025 1:00 PM - 3:20 PM

Hanover Hall FG

Chair: Krishna Gunugunuri, Cummins Inc.

Co-Chair: Sreshtha Sinha Majumdar, Oak Ridge National Laboratory

Developing the Science of Self-Healing Catalysts.

Abhaya Datye[1], *Hien N. Pham*[1], *Andrew T. DeLaRiva*[1], *Chase Thompson*[1], *Stephen Porter*[1], *Hao Xu*[2], *Konstantin Khivantsev*[3], *Yipeng Sun*[4], *Holmes Ahari*[5], *and Yong Wang*[6]
(1)Department of Chemical and Biological Engineering and Center for Micro-Engineered Materials, University of New Mexico, Albuquerque, NM, (2)Chemical and Bio Engineering, Washington State University, Pullman, WA, (3)Physical and Computational Sciences Directorate and Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA, (4)BASF, Iselin, NJ, (5)Fiat Chrysler Automobile US, Auburn Hills, MI, (6)The Gene and Linda Voiland School of Chemical Engineering and Bioengineering, Washington State University, Pullman, WA

Emission control catalysts are subjected to accelerated aging at temperatures ~1000 C where the catalytically active metals (Pt, Pd and Rh) are emitted to the vapor phase. Here we describe how catalyst supports allow these catalysts to function over their full useful life, a process we describe as self-healing.

Tuning Support Lattice Oxygen Activity for Emission Control Catalysts.

Hao Xu[1], *Weixin Huang*[2], *Hien N. Pham*[3], *Andrew T. DeLaRiva*[3], *Abhaya Datye*[3], *and Yong Wang*[4]
(1)Chemical and Bio Engineering, Washington State University, Pullman, WA, (2)Department of Chemical Engineering, Washington State University, Pullman, WA, (3)Department of Chemical and Biological Engineering and Center for Micro-Engineered Materials, University of New Mexico, Albuquerque, NM, (4)Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA

Here, we develop strategies for synthesizing catalyst supports and demonstrate that the modulation of support lattice oxygen greatly benefits catalyst efficiency for emission control purposes.

The Reducibility of Ce, Pr and Tb Containing Mixed Oxides Have Been Studied and Trends with Composition Determined and the Effect on Twc Transient Catalytic Activity Shown..

David Thompsett, *Amy Kolpin, and Janet Fisher*
Johnson Matthey Technology Centre, Sonning Common, United Kingdom

Ce and Pr fast and total reducibility have been determined as a function of CeZr and PrZr mixed oxide composition. Ce oxides show limited reduction which improve with Zr content while Pr

oxides show opposite trends. These differences in redox behaviour show benefit during TWC transients.

Influence of Nanoparticle Structure in Bimetallic PtPd/Al_2O_3 Catalysts on Activity and Stability during Emission Control Applications.

Joachim Czechowsky[1], *Paolo Dolcet*[1], *Carina B. Maliakkal*[2], *Silke Behrens*[3], *Michael Türk*[4], *Moritz Wolf*[3], *Jan-Dierk Grunwaldt*[1,3], *and Maria Casapu*[1]
(1)Institute for Chemical Technology and Polymer Chemistry (ITCP), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany, (2)Institute of Nanotechnology (INT), Karlsruhe Institute of Technology (KIT), Eggenstein-Leopoldshafen, Germany, (3)Institute of Catalysis Research and Technology (IKFT), Karlsruhe Institute of Technology (KIT), Eggenstein-Leopoldshafen, Germany, (4)Institute for Technical Thermodynamics and Refrigeration (ITTK), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

By using various synthesis methods, different initial states of PtPd/Al_2O_3 catalysts were obtained, which allowed to derive robust structure-activity correlations during lean CO-/NO-oxidation. Hydrothermal aging and extensive characterization were used to identify the factors responsible for structural changes and deactivation such as size effects, alloying and particle segregation during use.

Enhanced NH_3-SCO Performance through Synergistic Effects of PtCu Intermetallics and $PtCuO_x$ Clusters.

Jiaxing Li, *Yue Peng, and Junhua Li*
State Key Joint Laboratory of Environment Simulation and Pollution Control, Tsinghua University, Beijing, China

This work highlights the electron-rich effect of PtCu intermetallic compounds in lowering NH_3 activation temperature and the tandem role of CuOx clusters in enhancing N_2 selectivity, achieving efficient NH_3-SCO catalysis.

Decomposition and Hydrolysis of Sulfonamides on CeO_2(111).

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

Sulfonamides are widely used to treat bacterial and fungal infections in humans and livestock. They accumulate in the environment resulting in antibiotic resistance in bacteria. DFT calculations are performed to investigate the ability of ceria to catalyze the hydrolysis of sulfonamides and shed light on factors that affect its efficacy.

Controlling Rh-CeO_2 Interaction Enhances N_2o Decomposition.

Yi Liu[1,2], *Hao Xu*[2], *Wenda Hu*[3], *Chia-Yu Chang*[4], *Bing Joe Hwang*[4], *and Yong Wang*[5]
(1)CHEMICAL ENGINNERING, Washington State University, pullman, WA, (2)Chemical and

Bio Engineering, Washington State University, Pullman, WA, (3)The Gene and Linda Voiland School of Chemical Engineering and Bioengineering, Washington State University, Pullman, WA, (4)Chemical Engineering, National Taiwan University of Science and Technology, Taipei, Taiwan, (5)Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA

By tuning the Rh coordination environment through calcination temperature, a signficant self-promotion effect is observed for 0.5 wt.%Rh/CeO_2-1000 sample after reaction with N_2O, attributed to abundant active oxygen species and higher Rh-O coordination number. It provides crucial insights into optimizing Rh/CeO_2 interaction for more effective N_2O abatement technology.

FUNDAMENTALS - FUNDAMENTALS OF CATALYSIS AND SURFACE SCIENCE

FUNDAMENTALS - CHARACTERIZATION TECHNIQUE FOCUSED

Tuesday, June 10, 2025 1:00 PM - 3:20 PM
Centennial Ballroom II

Chair: Steven Chavez, University of California, Los Angeles

Co-Chair: Andrew Palermo, Johnson Matthey

Revealing Kinetics of Pt Exsolution Phenomenon and High Reactivity: Combining Operando X-Ray Absorption Spectroscopy and Graph Neural Network.

Yunkyung Kim[1], *Wonjun Lee*[1], *and Jeong Woo Han*[2]
(1)Department of Materials Science and Engineering, Seoul National University, Seoul, Korea, Republic of (South), (2)Department of Materials Science and Engineering, Research Institute of Advanced Materials, Seoul National University, Seoul, Korea, Republic of (South)

Operando XAS was employed to study the exsolution dynamics of Pt, providing real-time insights into Pt coordination and identifying optimal conditions to minimize sintering while enhancing stability. The resulting Pt-exsolved catalysts demonstrated superior reactivity and durability, with GNN-DFT modeling and DRIFTS highlighting the role of strain effects near interfaces.

Quantifying Ambient Pressure Charge Transfer: NH_3 on Ru.

Jesse Canavan[1], *Rajat Daga*[1], *Justin Hopkins*[1], *Ulrick Gaillard*[1], *Matthew Neurock*[1], *Alon McCormick*[1], *Omar Abdelrahman*[2], *and Paul J. Dauenhauer*[1]
(1)Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN, (2)William A. Brookshire Department of Chemical and Biomolecular Engineering, University of Houston, Houston, TX

The extent of charge transfer due to NH_3 adsorption on a Ru thin film has been measured and quantified at temperatures and pressures typical of heterogeneous catalysis. This technique can

be used to study trends in the affinity of adsorbates to different metal surfaces at reaction conditions.

Dynamic Transformations of Heterogeneous Catalysts Under Operando Conditions.

Umberto Raucci[1], *Axel tosello Gardini*[2], *Manyi Yang*[3], *Francesco Mambretti*[2], *and Michele Parrinello*[2]
(1)Italian Institute of Technology, Genova, Italy, (2)Atomistic Simulations, Italian Institute of Technology, Genova, Italy, (3)Nanjing University, Nanjing, China

Traditionally considered static entities, catalysts were mainly thought to maintain fixed active sites during reactions. However, our work challenges this view, demonstrating that catalysts undergo profound structural transformations when exposed to industrial reaction conditions, such as high temperatures, pressures, and reactant flows.

Effects of Microwave Heating on Atomically Dispersed Fe-N-C Catalysts.

Takatoshi Murakami[1], *Yusaku Yamazaki*[1], *Shin R. Mukai*[2], *and* ***Isao Ogino***[2]
(1)Graduate School of Chemical Sciences and Engineering, Hokkaido University, Sapporo, Japan, (2)Faculty of Engineering, Hokkaido University, Sapporo, Japan

Despite significant advances in the activity of Fe-N-C catalysts for the electrochemical oxygen reduction reaction (ORR), rapid deactivation persists as a challenge. Brief microwave heating enhances their $4e^-$ ORR selectivity and reduces H_2O_2formation, a key deactivation factor. We report how microwave heating modifies catalyst properties, enabling improved selectivity.

In-Situ Characterization of Pt-Cu Single-Atom Alloy Catalysts: Pt Mobility Under Reaction Conditions.

Francisco Zaera
Chemistry, University of California-Riverside, Riverside, CA

Bimetallic $CuPt_x$/SBA-15 catalysts were tested for the selective hydrogenation of unsaturated aldehydes. Catalysts with x = 0.001 to 0.05 proved quite selective toward the desired unsaturated alcohol. However, *in situ* spectroscopy experiments found the Pt atoms embedded at the metal/silica interface. The role of Pt is remote and indirect.

Measuring Dispersion of Zr-SiO_2 with *in Situ* Titration.

Emily Chase[1] *and Justin Notestein*[2]
(1)Northwestern University, Evanston, IL, (2)Department of Chemical & Biological Engineering, Northwestern University, Evanston, IL

In situ titration with methylphosphonic acid was used to quantify and describe kinetically relevant Zr species on Zr-SiO_2 materials for the MPV reduction of cyclohexanone. Two distinct

active species were identified: titratable, isolated Zr with higher intrinsic activity and non-titratable Zr with lower intrinsic activity.

In Situ Measurement of Nanoparticle-Support Interactions in Supported Bimetallic Catalysts.

Andrew Baker[1], Sai Vishnubohtla[1], Sanjana Karpe[2], Yahui Yang[2], Tevis Jacobs[1], and ***Götz Veser[2,3]***
(1)Materials Science, University of Pittsburgh, Pittsburgh, PA, (2)Department of Chemical and Petroleum Engineering, University of Pittsburgh, Pittsburgh, PA, (3)Mascaro Center for Sustainable Innovation, University of Pittsburgh, Pittsburgh, PA

Adhesion of nanoparticles critically impacts their performance and stability. However, scientific advances are currently hampered by a lack of experimental accessibility. We present a novel in situ technique for the direct measurement of adhesion of individual nanoparticles, which enables first insight into the impact of alloying for bimetallic systems.

MICRO MESO - MICROPOROUS AND MESOPOROUS MATERIALS

MICRO MESO - HYDROCARBON REACTIONS ON ZEOLITIC MATERIALS

Tuesday, June 10, 2025 1:00 PM - 3:20 PM
Hanover Hall CDE

Chair: Michele Sarazen, Princeton University

Co-Chair: Stephen Schuyten, Johnson Matthey Inc.

Toluene Alkylation with Ethylene on Acidic Mordenite Zeolite: The Role of Proton Location in Catalysis.

Kemakorn Ithisuphalap*, Michelle Nolen, and Stephanie Kwon*
Colorado School of Mines, Golden, CO

This study demonstrates that protons in the small 8-membered ring (8-MR) pores of Mordenite (MOR) zeolites can facilitate alkylation reactions of toluene (C_7H_8) with ethylene (C_2H_4), despite steric restrictions. This challenges conventional assumptions about zeolite catalysis and introducing a new perspective on "pore mouth" catalysis.

Quantifying Deactivation Phenomena during Low-Temperature Toluene Methylation on Brønsted Acid Zeolite Catalysts.

Sopuruchukwu Ezenwa[1]*, Andrew Norfleet[1], David Hibbitts[1,2], and Rajamani Gounder[1]*
(1)Charles D. Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN, (2)Department of Chemical Engineering, University of Florida, Gainesville, FL

We investigate the deactivation mechanism and influences of zeolite properties and reaction conditions on deactivation rate during low-temperature toluene methylation. We show that deactivation rates predominantly reflect the rate of accumulation of bulky polymethylated

aromatics within intracrystalline domains, which depend on their rates of formation and diffusion within zeolite crystallites.

Atypical Reactivity of Mesoporous Silicalite-1 in Alkene Oligomerization.

Nibras Hijazi[1], *Alla Dikhtiarenko*[2], *Rushana Khairova*[1], *Jose Cerrillo*[1], *and Jorge Gascon*[1]
(1)KAUST Catalysis Center, King Abdullah University of Science and Technology, Thuwal, Saudi Arabia, (2)KAUST Core Labs, King Abdullah University of Science and Technology, Thuwal, Saudi Arabia

This work demonstrates that accessible H-bonded silanol groups are highly reactive towards propene oligomerization, which leads to a reconsideration of the origins of reactivity in zeolites in the context of alkene oligomerization.

KEYNOTE: Conversion of Short-Chain Alcohols over Hierarchical Zeolites and the Dependence of Their Porosity and Composition on the Formed Coke Species.

Leandro Martins
State University of Sao Paulo, Araraquara, Brazil

The study shows how structural and chemical modifications of zeolite catalysts and the associated operational conditions impact coke speciation and, consequently, the distribution of compounds from converting short-chain alcohols, methanol, ethanol, and glycerol.

Impact of Al Distribution on Methane Activation over FER-Type Aluminosilicate Zeolite.

Peipei Xiao, Kengo Nakamura, Hiroto Toyoda, Yong Wang, and ***Toshiyuki Yokoi***
Institute of Integrated Research, Institute of Science Tokyo, Yokohama, Kanagawa, Japan

FER zeolites with different Al distributions were prepared using 1,4-dioxane as the pore-filling agent or pyrrolidine as the OSDA. We have found the significance of the distribution and arrangement of Al atoms in FER zeolite for methane oxidation over FER-type aluminosilicate zeolite.

Process Intensification at the Nanoscale: Embedding SiC in Zeolites for Energy-Efficient Catalysis.

Alexandre Young[1], *Julia de Souza*[2], *Antonio Mario Leal Martins Costa*[1], *Pedro Romano*[3], *Javier García-Martínez*[4], *and* ***João Monnerat***[5]
(1)LIPCAT (UFRJ), Rio de Janeiro, Rio de Janeiro, Brazil, (2)LIPCAT, Rio de Janeiro, Brazil, (3)Campus D. de Caxias, Federal University of Rio de Janeiro, Rio de Janeiro, Brazil, (4)Molecular Nanotechnology Lab, Department of Inorganic Chemistry, University of Alicante, Alicante, Spain, (5)Chemistry Institute, Federal University of Rio de Janeiro, Rio de Janeiro, Rio de Janeiro, Brazil

Incorporating SiC nanoparticles into FER zeolite during synthesis enhanced catalytic activity by 2.5 times for Friedel-Crafts alkylation under microwave heating, with over 40% energy savings compared to the physical FER/SiC mixture. This novel synergy, optimizing SiC-FER interaction for sustainable catalysis, represents a previously unreported advancement in microwave-assisted catalysis.

NITRO CHEM - NITROGEN CHEMISTRY

NITRO CHEM - SUSTAINABLE AMMONIA SYNTHESIS

Tuesday, June 10, 2025 1:00 PM - 3:20 PM
Centennial Ballroom I

Chair: Nirala Singh, University of Michigan

Co-Chair: Andrew Medford, Georgia Institute of Technology

Recent Findings and Open Questions on the Fundamental Chemistry and Practical Realization of Photocatalytic Nitrogen Fixation.

Andrew Medford[1]*, Po-Wei Huang*[1]*, Nianhan Tian*[2]*, and Marta Hatzell*[3]
(1)School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA, (2)School of Chemical & Biomolecular Engineering, Georgia Tech, Atlanta, GA, (3)George W. Woodruff School of Mechanical Engineering, Georgia Institute of Technology, Atlanta, GA

Ammonia is important for producing synthetic fertilizers to sustain the growing global population, and photocatalytic ammonia synthesis is a promising strategy for sustainable ammoina. Although widely reported, there are open debates on the detailed molecular mechanism of photocatalytic ammonia synthesis, and conflicting reports on the reliability of measured rates.

Electrochemical Nitrate Reduction to Ammonia on Cu(111): Potential Dependent DFT Study.

Adyasa Priyadarsini[1] *and Shyam Kattel*[2]
(1)Physics, Florida A&M University, Tallahassee, FL, (2)Department of Physics, University of Central Florida, Orlando, FL

Our work provides an atomistic insight into the stability of Cu catalysts at experimental conditions and importantly, can be extended to study other catalytic surfaces. Furthermore, the reaction pathways, reaction energetics and kinetics of NO_3RR on Cu(111) will provide key insight into the design of selective catalysts.

Ru/PrO_x Catalysts for Mild Ammonia Synthesis.

Samuel Drummond*, Jennifer Naglic, Alexis Allegro, Thossaporn Onsree, and Jochen Lauterbach*
Department of Chemical Engineering, University of South Carolina, Columbia, SC

Here we have produced multiple new, more efficient, promoted ruthenium-based catalysts to reduce emissions from ammonia synthesis. After screening and optimization, the new catalyst produced more than three times the best previous catalysts on a per-ruthenium basis. Further, in situ spectroscopy led to determination of the mechanism of these catalysts.

Earth-Abundant Manganese Nitride Catalysts for Mild-Condition Ammonia Synthesis.

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

We developed a ζ-phase $MnN_{0.43}$ catalyst for low-temperature NH_3 synthesis. This catalyst exhibits high NH_3 synthesis activity at 250-350 °C, surpassing the conventional noble metal-based Ru/MgO catalyst. Our work offers fundamental insights into the NH_3 synthesis mechanisms on earth-abundant transition metal nitrides, highlighting their significant potential for NH_3 synthesis.

Metal Hydride/Carbon-Based Nanocomposites As Catalysts for Ammonia Synthesis at Moderate Conditions.

***Juliette Verschoor**[1]*, *Petra E. de Jongh[1,2], and Peter Ngene[1]*
(1)Materials Chemistry and Catalysis, Utrecht University, Utrecht, Netherlands, (2)Inorganic Chemistry and Catalysis, Utrecht University, Utrecht, Netherlands

Alkali hydride–graphite nanocomposites were prepared via mechanochemical synthesis, i.e. ball milling (BM), and tested for thermal ammonia synthesis. Both potassium and sodium based catalysts are active without the presence of transition metals and adding small amounts of iron to these catalysts resulted in a significant increase in catalytic activity.

Mechanochemical Ammonia Synthesis over Transition Metal Nitrides.

***Jacob A. Dewitt**[1]*, *Erin V. Phillips[2], Karoline L. Hebisch[1], Andrew W. Tricker[3], and Carsten Sievers[4]*
(1)School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA, (2)Chemistry & Biochemistry, Georgia Institute of Technology, Atlanta, GA, (3)AAAS/NSF, Washington, DC, (4)School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA

In an effort to reduce the environmental cost of modern ammonia production, ambient-conditioned mechanochemical ammonia synthesis represents a promising pathway for improving sustainability. This work investigates the catalytic activity of transition metal nitride catalysts titanium, molybdenum, zirconium, vanadium, and niobium, by demonstrating catalytic performance and analysis of phase behavior.

Fundamental Chemistry in Lithium-Mediated Nitrogen Reduction Reaction Revealed By First-Principles Simulations.

Chengyu Zhou[1] *and Qing Zhao*[2]
(1)Northeastern University, Boston, MA, (2)Department of Chemical Engineering, Northeastern University, Boston, MA

Lithium-mediated nitrogen reduction reaction (Li-NRR) is a sustainable and feasible approach for ammonia electrosynthesis. We apply advanced computational tools based on electronic structure theory to elucidate fundamental chemistry in Li-NRR, including elementary reaction mechanisms of N_2 activation and reduction and microenvironments of the active solid-electrolyte interface layer.

REACTOR - REACTION ENGINEERING AND REACTOR DESIGN

REACTOR - REACTOR DESIGN FOR EMERGING APPLICATIONS

Tuesday, June 10, 2025 1:00 PM - 3:20 PM
Centennial Ballroom III

Chair: Ali Hussain Motagamwala, Shell

Co-Chair: Sungmin Kim, Pacific Northwest National Laboratory

Inductively Heated Structured E-Reactors for Dry Reforming of Methane.

Mohammad Raihan Arfin, ***Akshat Tanksale****, and Hamza Asmat*
Chemical and Biological Engineering, Monash University, Clayton, VIC, Australia

The double pancake coil improves magnetic flux density, enhancing current and temperature distribution. Gyroid monoliths achieve higher temperatures than octet monoliths due to efficient heat propagation through interconnected channels. These findings highlight the critical role of coil configuration and lattice geometry in understanding strucutred e-reactor design for chemical processes.

Catalyst Discovery and Bench-Scale Reactor Design for Ammonia Autothermal Reforming As a Route to Net-Zero-Carbon Hydrogen.

Kathleen D. Brown[1]*, Gabrielle Kliegle*[1]*, Jacob H. Miller*[1]*, Adam Yonge*[1]*, Carrie A. Farberow*[1]*, Justin M. Bracci*[1]*, Alexander J. Hill*[1]*, Matthew Yung*[1]*, and* ***Nicholas Thornburg***[2]
(1)National Renewable Energy Laboratory, Golden, CO, (2)Center for Energy Conversion & Storage Systems, National Renewable Energy Laboratory, Golden, CO

This presentation encompasses several years of efforts by NREL reaction engineers to develop multifunctional supported ruthenium catalysts and to establish a unique fixed bed reactor capability leveraged to investigate an underappreciated autothermal strategy for ammonia conversion to hydrogen. These insights enable advantaged catalyst formulation and commercially relevant reformer design strategies.

Kinetic Study for CO_x Methanation Based on in-Situ Spatially Resolved Measurements in a Catalytic Plate Reactor..

Pakpong Roongruangsree, Varun Surendran, and ***Jan Kopyscinski***
Catalytic & Plasma Process Engineering, Department of Chemical Engineering, McGill University, Montreal, QC, Canada

With our novel catalytic plate reactor, a significantly larger set of data for the kinetic parameter estimation can collected than by use of a typical steady-state reactor with concentration measurements at the outlet only, which makes this setup very suitable for studying the kinetics of heterogeneous catalyzed reactions.

Enabling syngas production with negative CO_2 emissions via intensified and electrified Reverse Water Gas Shift: an experimental study..

Federico Nicolini[1]*, Francesca Zaio*[1]*, Matteo Ambrosetti*[2]*, Alessanda Beretta*[1]*, Gianpiero Groppi*[1]*, Enrico Tronconi*[3]*, Mariasole Cipolletta*[4]*, and Alessia Marini*[4]
(1)Dipartimento di Energia, Politecnico di Milano, Milan, Italy, (2)Decarbonization unit, SNAM, San Donato Milanese, Italy, (3)Politecnico di Milano, Milan, Italy, (4)Rosetti Marino SpA, Ravenna, Italy

Syngas production is the building block of several chemical processes, but its production heavily contributes to the emission of green-house gases. In this work we present an innovative concept of electrified reactor aimed at the production of green syngas via Reverse Water Gas Shift.

Enabling High-Pressure Ammonia Reforming: Reactor Design,Validation, and Kinetic Insights.

Ceyhun Ege Köseoglu[1]*, Michael Geske*[1]*, Grigorios Kolios*[2]*, Jan Pottbacker*[2]*, Sophie Hund*[3]*, Martin Lerch*[3]*, Michael Kraemer*[2]*, and Frank Rosowski*[2]
(1)BasCat - UniCat BASF Joint Lab, Technische Universität Berlin, Berlin, Germany, (2)Group Research, BASF SE, Ludwigshafen, Germany, (3)Anorganische Chemie/Festkörperchemie, Technische Universität Berlin, Berlin, Germany

A novel reactor for high-pressure ammonia reforming enables precise thermal control up to 50 bar and 750°C. Initial tests with Ni/Al_2O_3 and Fe_3Mo_3N catalysts demonstrate high hydrogen productivity and provide kinetic insights, advancing sustainable hydrogen production and supporting techno-economic evaluations of small-scale reforming plants.

KEYNOTE: Sustainable Catalysts with Membranes or Plasma for Energy and Environmental Applications.

Sibudjing Kawi
Department of Chemical and Biomolecular Engineering, National University of Singapore, Singapore, Singapore

In this presentation, I will address how our research group has avoided catalyst issues by systematically developing efficient non-noble metal catalysts to tackle CO_2, CH_4 and H_2

challenges (such as for CO_2 methane reforming, biomass tar reforming, water gas shift, CO_2 methanation, CO_2 hydrogenation to methanol, methane pyrolysis, methane coupling).

ADV CHARAC - NEW AND ADVANCED METHODS IN CATALYST CHARACTERIZATION

ADV CHARAC - MECHANISTIC INSIGHTS FROM ADVANCED CHARACTERIZATION TOOLS

Tuesday, June 10, 2025 3:40 PM - 5:40 PM
Hanover Hall FG

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

Co-Chair: Amrit Venkatesh, University of Virginia

Learning from Failure: Advanced Characterizations on SPA Catalysts.

__Renqin Zhang__, Seif Yusuf, and Greg Korynta
Clariant, Louisville, KY

In the journey of understanding the characteristics of catalyst performance, we learned from failure. To predict the performance of solid phosphoric acids catalysts, in-situ characterization on catalysts under practical condition is necessary due to its dynamic nature, as well as the fact that it has hygroscopic property.

N_2o and CH_4 Utilization Via a Site-Specific Fe^{2+}/Fe^{3+} Redox Couple in Fe-Exchanged Zeolites.

__Daniel Camilo Cano Blanco__[1,2], Jörg W.A. Fischer[3], Daniele Bonavia[1,4], Gabriela-Teodora Dutca[1,2], Gunnar Jeschke[3], Oliver Kröcher[1,2], and Davide Ferri[1]
(1)Paul Scherrer Institute, Villigen, Switzerland, (2)EPFL, Lausanne, Switzerland, (3)ETH Zurich, Zurich, Switzerland, (4)ESRF, Grenoble, France

We employed advanced operando techniques with modulated-excitation to determine the nature of active Fe sites in Fe-SSZ-13 during N_2O activation and CH_4 hydroxylation. Site-specific monomeric Fe undergoes reversible Fe^{2+}/Fe^{3+} redox, with temperature-dependent contributions from species. We highlight the advantage of combining multiple spectroscopic techniques to interrogate complex catalysts

Surface Anchoring Requirements for Vanadia Clusters on Titanium Oxide Surface and Their Impact on Activity for Oxidative Dehydrogenation of Ethanol..

__Dongmin Yun__[1], Jose Herrera[2], Nicholas Jaegers[3], Jian Zhi Hu[4], Adrian Hucal[2], and Yong Wang[5]
(1)SK Innovation, San Francisco, CA, (2)Department of Chemical and Biochemical Engineering, Western University, London, ON, Canada, (3)University of California at Berkeley, Berkeley, CA, (4)Pacific Northwest National Laboratory, Richland, WA, (5)The Gene and Linda Voiland School of Chemical Engineering and Bioengineering, Washington State University, Pullman, WA

By using oxygen doped TiN as support for vanadia clusters, we carry a detailed study of the relationship between support oxygen content, vanadia dispersion, and catalytic performance for ethanol partial oxidation. Lattice oxygen from the titania support play a critical role in the catalytic activity of the vanadia species.

Advancing Spectrokinetics in Heterogeneous Catalysis: From Bulk to Surface Species and Beyond.

Juan Bravo-Suarez[1], *Alejandra Torres Velasco*[1,2], *Hashim Alzahrani*[1,2,3], *Bhagyesha Patil*[1,2], *Yue Qi*[4], *Simon Podkolzin*[4], *and Hongda Zhu*[2]
(1)Chemical & Petroleum Engineering, The University of Kansas, Lawrence, KS, (2)Center for Environmentally Beneficial Catalysis, The University of Kansas, Lawrence, KS, (3)Chemical and Materials Engineering Department, King Abdulaziz University, Jeddah, Saudi Arabia, (4)Department of Chemical Engineering and Materials Science, Stevens Institute of Technology, Hoboken, NJ

This work proves the feasibility of utilizing steady state and transient in situ/operando spectroscopy to extract mechanistic information that reduces and leads to robust kinetic models. It also opens new avenues to explore kinetics and mechanisms with charge transfer data in heterogeneous catalysis.

Good Practices for Pulse Chemisorption.

Benjamin Le Monnier *and Katie A. Cychosz-Struckhoff*
Anton Paar Quantatec, Boynton Beach, FL

This presentation discusses optimizing pulse chemisorption parameters for accurate catalyst characterization. Key factors like carrier gas flow, temperature, and detector settings are explored using examples from propane dehydrogenation and carbon capture. These optimizations enhance repeatability and accuracy, providing practical guidance for researchers in applied catalysis.

Elucidating the Origin of Electrocatalytic Phenomena Using Steady State Isotopic Transient Kinetic Analysis.

Abigail Circelli[1] *and Ezra L. Clark*[2]
(1)Chemical Engineering, The Pennsylvania State University, University Park, PA, (2)Chemical Engineering, Penn State, University Park, PA

This presentation will demonstrate electrochemical SSITKA for the first time using DEMS and methanol oxidation over Pt as a test reaction to understand the rise and decline of the methanol oxidation activity in the low overpotential regime. This general analytical method will accelerate understanding of a variety of electrocatalytic phenomena.

AI - AI-DRIVEN CATALYSIS

AI - DEVELOPMENT OF NEW AI-DRIVEN METHODOLOGIES

Tuesday, June 10, 2025 3:40 PM - 5:40 PM

Regency Ballroom VII

Chair: Siddharth Deshpande, University of Rochester

Co-Chair: Christian Sandoval Pauker, RICE University

Text Mining Experimental Heterogeneous Catalysis Literature with Large Language Models.

Benjamin Walls[1] *and Suljo Linic*[2]
(1)Department of Chemical Engineering, University of Michigan, Ann Arbor, Ann Arbor, MI, (2)Chemical Engineering, University of Michigan, Ann Arbor, MI

We programmed a computational workflow to extract catalyst names, properties, and operating conditions from heterogeneous catalysis research papers using large language models. We identified model choices and prompting strategies that maximized performance and then used the workflow to extract 2773 measurements from 423 papers on the oxidative coupling of methane.

Hybrid Generative AI – Quantum Chemistry Feedback for Catalyst Discovery.

Mariefel Olarte
Pacific Northwest National Laboratory, Richland, WA

This work reports the first chemical descriptor-driven search algorithm for catalyst discovery that incorporates LLM knowledge space with quantum-chemical feedback. We will present experimental and DFT validation results for carbon monoxide conversion to methanol as use case.

Agentic Artificial Intelligence (AI) for Accelerating Catalytic Materials Research.

Hongliang Xin
Department of Chemical Engineering, Virginia Tech, Blacksburg, VA

Agentic AI accelerates catalysis research by autonomously tackling tasks like knowledge queries and active site optimization. Using multimodal large language models, it identifies metallic nanostructures for nitrate reduction, addressing pollution and enabling net-zero ammonia synthesis. This scalable framework advances reproducibility and sustainability in energy and environmental science.

AI-Driven Analysis of Solvation Thermodynamics of Adsorbates at Catalyst Surfaces and Liquid Water Interfaces.

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

This study uses machine learning (ML) models to predict solvation thermodynamic properties of adsorbates at catalytic surfaces, achieving high accuracy while reducing computational costs compared to DFT. By using advanced data representations, these models show strong potential for automating high-throughput catalyst screening and analyzing diverse catalytic environments.

Metric Robustness in Catalysis Reproducibility and Machine Learning Model Development.

Selin Bac[1], *Seunghwa Hong*[1], *Emily K. Schroeder*[1], *Adam Hoffman*[2], *Jake A. Heinlein*[3], *Greg Barber*[4], *Simon Bare*[2], *Robert Rioux*[4], *Matteo Cargnello*[5], *and Phillip Christopher*[1]
(1)Department of Chemical Engineering, University of California, Santa Barbara, Santa Barbara, CA, (2)Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, Menlo Park, CA, (3)Department of Chemical Engineering, Stanford University, Stanford, CA, (4)Department of Chemical Engineering, The Pennsylvania State University, University Park, PA, (5)Chemical Engineering, Stanford University, Stanford, CA

This study examines the importance of mitigating intra- and inter-lab variability in catalysis, especially when multiple institutions contribute data for machine learning models. We highlight challenges in using common metrics and propose a robust approach that distinguishes experimental errors from variations in catalytic parameters like metal loading.

Generation of Catalysis Testing Data Via Uncertainty Sampling to Build Machine Learning Models for Catalyst Durability.

Dongjae Shin[1,2], *Jake A. Heinlein*[1], *Emily K. Schroeder*[3], *Seunghwa Hong*[4], *Selin Bac*[3], *Anastassiya Khan*[5], *Adam Hoffman*[2,5], *Phillip Christopher*[4], *Matteo Cargnello*[6], *Simon Bare*[2,5], *Christopher J. Tassone*[5], *and Kirsten Winther*[2]
(1)Department of Chemical Engineering, Stanford University, Stanford, CA, (2)SUNCAT Center for Interface Science and Catalysis, SLAC National Accelerator Laboratory, Menlo Park, CA, (3)Department of Chemical Engineering, University of California, Santa Barbara, Santa Barbara, CA, (4)Chemical Engineering, University of California, Santa Barbara, Santa Barbara, CA, (5)Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, Menlo Park, CA, (6)Chemical Engineering, Stanford University, Stanford, CA

Evaluating the long-term stability of catalysts is crucial to determine their potential for commercialization. However, current methods for long-term stability testing rely on expensive on-stream studies. Thus, we efficiently generated testing data with the navigation by uncertainty sampling (US) algorithm, resultant data being used for machine-learned (ML) durability models.

CO2 - CO2 CAPTURE AND UPGRADING

CO2 - CO_2 CONVERSION VIA RWGS

Tuesday, June 10, 2025 3:40 PM - 5:40 PM
Centennial Ballroom IV

Chair: Wilson McNeary, National Renewable Energy Laboratory

Co-Chair: Melis Duyar, University of Surrey

Tuning Ru Catalyst for Enhanced CO Production from CH_4 in CO_2 Hydrogenation.

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

By precisely controlling Ru structures and local environments, the CO_2 hydrogenation pathways on Ru-based catalysts have been clearly elucidated. Moreover, strategies such as creating dual Ru structural sites, engineering Ru-CeO_2 interfaces, and optimizing Ru coordination environments have proven effective in enhancing CO yields.

Intermediate-Temperature Reverse Water-Gas Shift Under Process Relevant Conditions Catalyzed By Dispersed Alkali Carbonates.

Kesha Tamakuwala, *Robert Kennedy, and Matthew Kanan*
Department of Chemistry, Stanford University, Stanford, CA

Alkali carbonate catalysts(K_2CO_3/Na_2CO_3) dispersed on γ-Al_2O_3 enable selective reverse water-gas shift reaction at intermediate temperatures (400-700°C) and elevated pressure, achieving equilibrium CO_2 conversion with 100% CO selectivity. These low-cost, transition metal-free catalysts demonstrate long-term stability, hydrocarbon tolerance, and maintain performance in commercially-relevant form-factors, advancing sustainable fuel and chemical production.

Ceria-Supported Metal-Oxide (MO_x/CeO_2) Catalysts Developed By a One-Pot Chemical Vapor Deposition (OP-CVD) Technique: Structure and Reverse Water Gas Shift Reaction Study.

Amol Pophali[1], *Ryuichi Shimogawa*[2,3], *Lihua Zhang*[4], *Gihan Kwon*[5], *Kwangsuk Yoon*[6], *Jangeon Roh*[7], *Do Heui Kim*[7], *Hocheol Song*[6], *Anatoly I. Frenkel*[2,8], *and Tae Jin Kim*[1]
(1)Materials Science and Chemical Engineering, Stony Brook University, Stony Brook, NY, (2)Stony Brook University, Stony Brook, NY, (3)Mitsubishi Chemical Corporation, Science and Innovation Center, Yokohoma, Japan, (4)Center for Functional Nanomaterials, Brookhaven National Laboratory, Upton, NY, (5)National Synchrotron Light Source II, Brookhaven National Laboratory, Upton, NY, (6)Department of Resource and Environmental Engineering, Hanyang University, Seoul, Korea, Republic of (South), (7)Seoul National University, Seoul, Korea, Republic of (South), (8)Brookhaven National Laboratory, Upton, NY

A novel one-pot chemical vapor deposition (OP-CVD) technique was developed for the synthesis of wide range of MO_x/CeO_2 catalysts. Structural characterizations validated this development and reverse water gas shift (RWGS) reaction tests showed the effectiveness of the prepared catalysts. In-situ DRIFTS and XRD showed reaction mechanisms and structural changes, respectively.

Accelerating Decarbonization By Representing Catalysts with Natural Language.

Mayk C. Ramos, Shane Michtavy, Andrew White, and ***Marc Porosoff***
Department of Chemical Engineering, University of Rochester, Rochester, NY

Representing reverse water-gas shift catalysts with the text of synthesis procedures and reaction conditions enables Bayesian optimization, leading to accelerated catalyst discovery.

Demonstration of Innovative CO_2 to CO Transformation Technology for Carbon Neutrality.

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

SEKISUI has been developing technologies to efficiently convert CO_2 to CO with Reverse Water Gas Shift by Chemical Looping. Over 90% CO generation yields and 80% H_2 conversion was achieved in the demonstration with actual gas from blast furnace. The details of demonstrations and dissemination plans will be explained.

Mechanistic and Kinetic Relevance of Hydrogen and Water in CO_2 Hydrogenation on Cu-Based Catalysts.

Ting Lin[1]*, Michelle Nolen*[2,3]*, Carrie Farberow*[3]*, Stephanie Kwon*[2]*, and Aditya Bhan*[1]
(1)Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN, (2)Chemical and Biological Engineering, Colorado School of Mines, Golden, CO, (3)Catalytic Carbon Transformation & Scale-Up Center, NREL, Golden, CO

Kinetic effects of H_2, H_2O, and CO_2 during CO_2 hydrogenation are rationalized on catalyst formulations with and without ZnO based on experimental and computational results. We show herein that reaction occurs on Cu surfaces saturated by H* and HCOOH** with methanol synthesis and RWGS involving distinct intermediates and rate-determining steps.

ELECTRO PHOTO - ELECTROCATALYSIS AND PHOTOCATALYSIS

ELECTRO PHOTO - WATER ELECTROLYSIS

Tuesday, June 10, 2025 3:40 PM - 5:40 PM
Centennial Ballroom I

Chair: Joaquin Resasco, The University of Texas at Austin

Co-Chair: Kasun Gunasooriya, University of Oklahoma

Intermittency Accelerates Catalyst Transformations and Degradation during Water Electrolysis.

Raul Marquez[1]*, Jay Bender*[2]*, Ashton Aleman*[3,4]*, Emma Kalokowski*[1]*, Thuy Vy Le*[1]*, Morten Linding Frederiksen*[5]*, Kenta Kawashima*[1]*, Chikaodili Chukwuneke*[1]*, Andrei Dolocan*[6]*, Michaela Burke Stevens*[4]*, Delia Milliron*[1,7,8,9]*, Joaquin Resasco*[2,9]*, Thomas Jaramillo*[3,4]*, and C. Buddie Mullins*[1,2,6,8,9]

(1)Department of Chemistry, The University of Texas at Austin, Austin, TX, (2)McKetta Department of Chemical Engineering, The University of Texas at Austin, Austin, TX, (3)Department of Chemical Engineering, Stanford University, Stanford, CA, (4)SUNCAT Center for Interface Science and Catalysis, SLAC National Accelerator Laboratory, Menlo Park, CA, (5)Department of Biological & Chemical Engineering, Aarhus University, Aarhus, Denmark, (6)Texas Materials Institute, The University of Texas at Austin, Austin, TX, (7)Chemical Engineering, The University of Texas at Austin, Austin, TX, (8)Center for Electrochemistry, The University of Texas at Austin, Austin, TX, (9)H2@UT, The University of Texas at Austin, Austin, TX

This work reveals the impact of intermittency and reverse currents on catalyst durability in liquid alkaline water electrolyzers. Through systematic *in situ/operando* characterization, we demonstrate that intermittent operation affects electrode discharge, alters the surface composition, degrades catalytic films, accelerates corrosion, and induces local pH swings.

Understanding the Factors That Govern Stability of Ru-Based Pyrochlores for Acidic Oxygen Evolution Reaction.

***Kunal Velinkar**, Michael Allan, and Eranda Nikolla*
Department of Chemical Engineering, University of Michigan, Ann Arbor, MI

This work investigates the stability of Ru-based pyrochlores for acidic OER, showing that smaller A-site cations enhance stability by reducing Ru dissolution. Stability trends correlate with A-site cation radius, oxide reducibility, and Ru–O bond strength, offering insights into structure-stability relationships and design strategies for durable electrocatalysts.

Porous Tantalum Oxide-Supported Ir Catalyst for Reducing Ir Loading in the Anode of Membrane Electrode Assembly for Proton Exchange Membrane Water Electrolyzer.

*Je Yeon Choi[1], Song Gyun Kim[2], Hoseong Yang[2], Yong Won Kim[2], and **Chanho Pak**[1]*
(1)Graduate School of Energy Convergence, Institute of Integrated Technology, Gwangju Institute of Science and Technology, Gwangju, Korea, Republic of (South), (2)Graduate School of Energy Convergence, Gwangju Institute of Science and Technology, Gwangju, Korea, Republic of (South)

This study highlights the benefits of using iridium catalysts supported on hierarchical porous Ta_2O_5 with both mesopores and macropores. The MEA with 0.2 mg_{Ir}/cm^2 presented superior performance and durability at 1 A/cm^2 under PEMWE conditions.

Seawater Electrolysis Using Oxide Encapsulated Ruthenium Oxide Catalysts in Unbuffered pH-Neutral Seawater.

***Daniela Bushiri**[1], Amanda Baxter[1], Onaolapo Odunjo[1], Daniela Fraga Alvarez[2], Yong Yuan[3], Daniel Esposito[1], and Jingguang G. Chen[4]*
(1)Department of Chemical Engineering, Columbia Electrochemical Energy Center, Lenfest Center for Sustainable Energy, Columbia University, New York, NY, (2)Chemical Engineering,

Columbia University, New York, NY, (3)Department of Chemical and Biomolecular Engineering, University of Delaware, Newark, DE, (4)Chemistry Division, Brookhaven National Laboratory, Upton, NY

Direct seawater electrolysis offers a pathway to green hydrogen but faces challenges from chlorine evolution competing with oxygen evolution in unbuffered pH-neutral solutions. This study demonstrates SiO_x and TiO_x overlayers on Ru and RuO_x thin films suppress chloride transport, enhancing OER selectivity and efficiency while balancing the activity and stability.

Identifying Role of Hydronium Cation in Acidic Oxygen Evolution Reaction over IrO_2.

***Tianyou Mou**[1], Daniela Bushiri[2], Daniel Esposito[3], Jingguang G. Chen[1,2], and Ping Liu[1]*
(1)Chemistry Division, Brookhaven National Laboratory, Upton, NY, (2)Chemical Engineering, Columbia University, New York, NY, (3)Department of Chemical Engineering, Columbia Electrochemical Energy Center, Lenfest Center for Sustainable Energy, Columbia University, New York, NY

This study highlights the importance of an explicit description of the acidic environment of OER in theoretical modeling, being able to enhance modeling accuracy, gaining better mechanistic insights, and opening new opportunities for optimization of IrO_2-based catalysts.

Theoretical Prediction and Experimental Verification of IrO_x Supported on Titanium Nitride for Acidic Oxygen Evolution Reaction.

***Xue Han**[1], Tianyou Mou[2], Ping Liu[2], and Jingguang G. Chen[2]*
(1)Chemistry Division, Brookhaven National Lab, Upton, NY, (2)Chemistry Division, Brookhaven National Laboratory, Upton, NY

This study highlights the importance of combining theoretical prediction and experimental studies of model catalysts and commercially viable powder catalysts in the discovery of OER catalysts with enhanced activity and stability.

FUNDAMENTALS - FUNDAMENTALS OF CATALYSIS AND SURFACE SCIENCE

FUNDAMENTALS - CATALYST DESIGN AND SURFACE SCIENCE

Tuesday, June 10, 2025 3:40 PM - 5:40 PM
Centennial Ballroom II

Chair: Elizabeth Bickel Rogers, University of Minnesota

Co-Chair: Konstantin Khivantsev, Pacific Northwest National Laboratory

Surface Roughening in Nanoparticle Catalysts.

*Cameron Owen[1], Nicholas Marcella[2], **Christopher O'Connor**[1], Taek-Seung Kim[3,4], Ryuichi Shimogawa[5,6], Clare Yijia Xie[7], Ralph G. Nuzzo[2], Anatoly I. Frenkel[5,8], Christian Reece[1], and Boris Kozinsky[1,9]*

(1)Harvard University, Cambridge, MA, (2)University of Illinois Urbana-Champaign, Urbana, IL, (3)Korea Institute of Energy Research, Daejeon, Korea, Republic of (South), (4)Rowland Institute at Harvard, Harvard University, Cambridge, MA, (5)Stony Brook University, Stony Brook, NY, (6)Mitsubishi Chemical Corporation, Science and Innovation Center, Yokohoma, Japan, (7)Harvard John A. Paulson School of Engineering and Applied Sciences, Harvard University, Cambridge, MA, (8)Brookhaven National Laboratory, Upton, NY, (9)Robert Bosch LLC Research and Technology Center, Watertown, MA

We demonstrate that reactive MD simulations, powered by machine learned force fields, coupled with in situ infrared and X-ray absorption spectroscopy measurements makes it feasible to gain full atomistic understanding into dynamic structural responses of catalytically relevant metal nanoparticle systems.

The Counterintuitive Influences of Surface Entropy and Surface Hydroxyl Density on Hydrogen Spillover.

Kelle Hart[1] *and Bert Chandler*[2]
(1)Chemistry, Pennsylvania State University, State College, PA, (2)Chemical Engineering, Pennsylvania State Univerisity, State College, PA

Our data show hydrogen spillover coverage increases as surface hydroxyl density decreases. This counterintuitive result provides the first method for invoking spillover in a catalytic reaction. We also find the stabilization of spillover on a metal oxide support likely stems from a surface entropy effect rather than conventional enthalpic stabilization.

Predicting Adhesion Energies of Metal Nanoparticles to Many Oxide Support Surfaces, Metal Chemical Potential Versus Particle Size and Support, and Catalyst Performance.

Charles Campbell[1] *and Nida Janulaitis*[2]
(1)Chemistry and Chemical Engineering Departments, University of Washington, Seattle, WA, (2)Department of Chemical Engineering, University of Washington, Seattle, WA

A simple way to estimate adhesion energies between metal nanoparticles and oxide supports is discovered, which in turn predicts metal atom chemical potential as a function of the particle size and support. This chemical potential allows quantitative prediction of sintering rates and qualitatively corelates with the metal nanoparticle’s reactivity.

Bottom-up Design of Microporous SiO_2 Layers on TiO_2 for Alcohol Dehydration Catalysis.

Stephanie Kwon
Chemical and Biological Engineering, Colorado School of Mines, Golden, CO

This work develops bottom-up synthesis procedures to create SiO_2 micropores around Lewis acid-base sites in bulk oxides to enhance their reactivity for alcohol dehydration catalysis.

Engineering Active Sites of Metal/Metal Oxide Catalysts By Oxide Ligand Overlayers.

Jiahua Zhou[1], *Piaoping Yang*[1], *Stavros Caratzoulas*[2], *Weiqing Zheng*[3], *and Dionisios Vlachos*[2]
(1)University of Delaware, Newark, DE, (2)Delaware Energy Institute, University of Delaware, Newark, DE, (3)Delaware Energy Institute, University of Delaware, Newark, DE, University of Delaware, Newark, DE

This work presents strategy to engineer active sites of Pt catalysts using WOx as oxide ligands, which selectively block Pt terraces. Adjusting WOx coverage tunes site composition, alters reactant adsorption, and shifts selectivity from terrace- to step-dominated pathways. The insights open avenues for improving metal/metal oxide catalysts beyond specific system.

Non-Innocent Supports Enable Single-Site First-Row Metals for Carbon-Oxygen Bond Activation.

Long Qi[1], *Wenyu Huang*[2], *Bin Wang*[3], *and Susannah Scott*[4]
(1)Division of Chemical & Biological Sciences, Ames Laboratory, Ames, IA, (2)Chemistry, Iowa State University, Ames, IA, (3)School of Sustainable Chemical, Biological and Materials Engineering, University of Oklahoma, Norman, OK, (4)Department of Chemical Engineering, University of California, Santa Barbara, Santa Barbara, CA

We demonstrated redox and chemical processes mediated with non-innocent supports for a chemical transformation using single-site first-row transition metals involving reactant binding and multiple bond activations in a single catalytic turnover. Such processes are common in upgrading renewable feedstocks such as biomass and CO_2.

HYDRO ECON - CATALYSIS FOR THE HYDROGEN ECONOMY

HYDRO ECON - LIQUID ORGANIC HYDROGEN CARRIERS

Tuesday, June 10, 2025 3:40 PM - 5:40 PM
Centennial Ballroom III

Chair: Siwen Wang, Toyota Research Institute of North America

Co-Chair: Yizhen Chen, University of Virginia

Design of Pd Catalysts for Liquid Organic Hydrogen Carriers.

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

Liquid organic hydrogen carriers (LOHCs) are considered as an attractive approach for transporting and storing hydrogen. In this study, we present a catalyst design strategy to enhance the efficiency of LOHC reactivity by using N-heterocyclic compounds as substrates.

The Role of Support on the Performance of Platinum Catalysts for Methylcyclohexane Dehydrogenation.

Patrick Holcombe, *Kaveh Shariati, Thossaporn Onsree, and Jochen Lauterbach*
Department of Chemical Engineering, University of South Carolina, Columbia, SC

This work analyzes metal oxides and platinum supported on metal oxides to characterize the acidity of supports and gain an understanding of the effect support has on catalyst performance in methylcyclohexane dehydrogenation. Relative amounts and strengths of Lewis and Brønsted acid sites are determined.

Dehydrogenation of Liquid Organic Hydrogen Carriers Catalyzed By Defect-Rich Boron Nitride Catalyst.

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

Our study demonstrates a novel flux reconstruction strategy to create highly crystalline metal-free BN catalysts with high surface area and abundant exposed B/N defects, enhancing their dehydrogenation activity towards nitrogen-substituted heterocycles LOHCs for hydrogen economy.

A Computational Study on the Dehydrogenation of Methylcyclohexane to Toluene on Platinum Catalyst.

Andreas Heyden[1], ***Bhawana Rayamajhi***[2], *Wenqiang Yang*[2], *Mubarak Bello*[2], *and Olajide Bamidele*[2]
(1)Department of Chemical Engineering, University of South Carolina, Columbia, SC, (2)Chemical Engineering, University of South Carolina, Columbia, SC

The systematic investigation of stepwise dehydrogenation of MCH to Toluene from the first principle using Density Functional Theory was done to identify the role of the various active sites on three Platinum surface facets and the reaction mechanism and determine the rate and selectivity controlling steps over the active sites.

Mechanistic Insights and Trends of Selectivity for Methylcyclohexane Dehydrogenation on Oxide-Supported Pt, Pd, and Ni Nanoparticles.

Karoline Kvande[1], *Fang Wan*[1], *Zhongyao Zhang*[1], *Sai Chen*[1], *Trenton Otto*[2], *and Enrique Iglesia*[1,3]
(1)Chemical and Biomolecular Engineering, University of California, Berkeley, Berkeley, CA, (2)Chevron Technical Center, Richmond, CA, (3)Chemical Engineering, Purdue University, West Lafayette, IN

This study report similarities among kinetic trends, identity and kinetic relevance of methylcyclohexane dehydrogenation elementary steps on Pt, Pd, and Cu/Ni nanoparticles dispersed on oxides, as well as consequences of metal and support identity on rates and

dehydrogenation selectivity. These findings are relevant for the design of catalytic dehydrogenation-hydrogenation cycles.

Surface Structure Effects on Methylcyclohexane Dehydrogenation over Ni Catalysts: A DFT Investigation.

Wenqiang Yang[1]*, Mubarak Bello*[1]*, Bhawana Rayamajhi*[1]*, and Andreas Heyden*[2]
(1)Chemical Engineering, University of South Carolina, Columbia, SC, (2)Department of Chemical Engineering, University of South Carolina, Columbia, SC

Ni(211) is the most active site for MCH dehydrogenation to toluene and also the site prone to excessive dehydrogenation and coking. The findings will contribute to the rational design of improved Ni-based catalysts with high activity, reduced coke formation, and overall enhanced stability.

MICRO MESO - MICROPOROUS AND MESOPOROUS MATERIALS

MICRO MESO - MICROPOROUS AND MESOPOROUS MATERIALS FOR OXIDATION CATALYSIS

Tuesday, June 10, 2025 3:40 PM - 5:40 PM
Hanover Hall CDE

Chair: Pearl Kim, Micromeritics

Co-Chair: Charles Kanyi, Johnson Matthey

Binuclear Ti-Fe Sites in MFI Framework for Synergistically Catalysing Alkene Epoxidation.

Dong Lin[1] *and Richard J. Lewis*[2]
(1)Cardiff University, Cardiff, United Kingdom, (2)School of Chemistry, Cardiff University, Cardiff, United Kingdom

Binuclear Ti-Fe metal sites in MFI framework exhibit a marked improvement in alkene epoxidation compared to analogous materials containing only mononuclear Ti sites. This enhanced performance is attributed to a lower-energy reaction pathway, facilitated by the key oxygen transfer process involving more electrophilic bridging intermediates on binuclear Ti-Fe metal sites.

Investigating the Interplay of Fe Coordination Environment and Reaction Dynamics during MOF-Catalyzed Oxidations.

Joshua Miller[1]*, Rachel A. Yang*[2]*, and Michele Sarazen*[1]
(1)Department of Chemical and Biological Engineering, Princeton University, Princeton, NJ, (2)Department of Chemical Engineering, University of Michigan, Ann Arbor, MI

This work investigates the dynamics of MIL-100(Fe) to construct structure-property relationships for oxidation reactions. Oxidant identity (*tert*-butyl hydroperoxide vs. hydrogen peroxide) and local coordination effects had significant influence on reactivity, selectivity, and deactivation trends. Insights here can be extended to other MOF-catalyzed systems with similar active site requirements.

Oxidation Chemistries over Catalysts Containing M-N_4 Active Sites.

Ethan Iaia[1], *Ademola Soyemi*[1], *Ganesh Rana*[2], *Tibor Szilvasi*[1], *Martin G. Bakker*[2], *and James W. Harris*[1]
(1)Department of Chemical and Biological Engineering, The University of Alabama, Tuscaloosa, AL, (2)Department of Chemistry & Biochemistry, University of Alabama, Tuscaloosa, AL

We compare rates of three different oxidation reactions over metal phthalocyanine and metal nitrogen doped carbon catalysts, which have similar M-N_4 binding sites. M-N_4 sites can accommodate two reactive adsorbates and perform oxidation chemistries through an LH pathway. Insights gained over well-defined phthalocyanine will be applied to less-uniform doped carbons.

Oxidation of Linear Alkanes Using TS-1 and H_2O_2 Toward Chemical Upcycling of Polyolefins.

Seyeon Park, *Daeyeon Lee, Raymond Gorte, and John Vohs*
Department of Chemical and Biomolecular Engineering, University of Pennsylvania, Philadelphia, PA

Mild oxidation of alkanes from n-C_8H_{18} to n-$C_{36}H_{74}$ using TS-1 catalysts and H_2O_2 demonstrates that alkane concentrations in the aqueous phase significantly impact the oxidation rates. ^{1}H-NMR spectra indicate the 2 position of alkane chains as a preferential reaction site, with notable reactivity at central carbons.

Screening of Indirect Second Sphere Coordination Effects in the MIL-100 Metal-Organic Framework for Methane Partial Oxidation.

Stephen Vicchio
Savannah River National Lab, Aiken, SC

Residual H_2O ligands anchored to the inactive Fe sites within MIL-100(Fe) indirectly alter the chemical reactivity of the Fe active site. Herein, these indirect second sphere coordination effects are further investigated using DFT to identify potential descriptors linking reactivity and the coordinating ligands at the inactive metal centers in MIL-100.

Pairing Hetero-Substituted Zeolites with Tailored Acidity As Tandem Catalysts for Enhanced Light Olefins Production.

Amir Abutalib[1,2], *Deependra Parmar*[2], *Jaeyul Kim*[2], *MD Shahriar Hossain*[3], *Sangho Chung*[4], *Lars Grabow*[2], *Javier Ruiz-Martinez*[4], *and Jeffrey Rimer*[1,2]

(1)Department of Chemistry, University of Houston, Houston, TX, (2)William A. Brookshire Department of Chemical and Biomolecular Engineering, University of Houston, Houston, TX, (3)William A. Brookshire Department of Chemical and Biomolecular Engineering & Texas Center for Superconductivity (TcSUH), University of Houston, Houston, TX, (4)KAUST Catalysis Center, KAUST, Thuwal, Thuwal, Saudi Arabia

Tandem catalysts with tunable acidity for the enhanced production of olefins were assessed through two reactions: methanol to hydrocarbons (MTH) and oxidative dehydrogenation (ODH). A dual fixed bed reactor configuration was utilized combining gallosilicates and aluminosilicates, which were both synthesized with distinct zeolite pore topologies (MWW, CHA, and MFI).

POLYMER - CATALYSIS FOR POLYMER SYNTHESIS, UPCYCLING, AND RECYCLING

POLYMER - POLYOLEFIN SYNTHESIS AND HYDROGENOLYSIS

Tuesday, June 10, 2025 3:40 PM - 5:40 PM
Regency Ballroom VI

Chair: Kunlun Ding, Louisiana State University

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

KEYNOTE: Reactive Separations and Processivity in Polyolefin Hydrogenolysis.

Aaron Sadow
Division of Chemical & Biological Sciences, Ames Laboratory, Ames, IA

Our team has been investigating heterogeneous catalytic materials and reaction conditions to bypass statistically-controlled scission processes and establish selective conversions of polyolefins into smaller alkanes via hydrogenolysis. Chemical properties of the alkane products and the polyolefin reactants are similar, we have developed methods to create selectivity by leveraging physical differences.

Mechanocatalytic Depolymerization of Polyethylene By Hydrogenolysis Using Metal Hydride Catalysts.

***Jouke van Westrenen**[1] and Carsten Sievers[2]*
(1)Chemical and Biomolecular Engineering, Georgia Tech, Atlanta, GA, (2)School of Chemical and Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA

Mechanocatalytic hydrogenolysis provides an option for converting polyolefins to smaller hydrocarbons under controlled conditions in a solvent-free process. Thus, it avoids many of the drawbacks of other strategies in literature and could be an economically viable path to the reintegration of plastic waste.

Predicting a Generalized Branched Hydrogenolysis Mechanism on Ru, Ir, and Pt Surfaces for Polymer Upcycling Applications.

***Andy Simonson**, Lydia Thies, and David Hibbitts*
Department of Chemical Engineering, University of Florida, Gainesville, FL

Hydrogenolysis chemistry can upcycle polymers to generate value from plastic waste. We present a fundamental study investigating C–C hydrogenolysis mechanisms at branch points of alkanes on Ir, Pt, and Ru surfaces using density functional theory investigations of model compounds to predict macromolecular reactions during polymer upcycling.

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

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

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

Polyolefin Melt-Phase Effects on Alkane Hydrogenolysis over Pt Catalysts.

*Andreas Heyden[1] and **Mehdi Zare**[2]*
(1)Department of Chemical Engineering, University of South Carolina, Columbia, SC, (2)Chemical Engineering, University of South Carolina, Columbia, SC

Using a hybrid quantum mechanical/molecular mechanical (QM/MM) approach, we systematically study polyolefin melt phase effects on small alkanes hydrogenolysis over Pt(111) catalyst surface in a polymer melt.

OTHER EVENTS

TUESDAY POSTER SESSION

Tuesday, June 10, 2025 6:00 PM - 8:00 PM
Grand Hall

A New Method for the Simulation of Catalyst Deactivation in Fluidized Bed Reactors.

*Andrea Pappagallo[1], Hugo Pétremand[1], Tilman Schildhauer[2], and **Emanuele Moioli**[3]*
(1)Paul Scherrer Institute, Villigen, None, Switzerland, (2)Paul Scherrer Institut, Villigen PSI, Switzerland, (3)Politecnico di Milano, Milano, None, Italy

This work describes a new methodology for the description of catalyst deactivation in fluidized bed reactors. The methodology includes the description of particle motion in the reactor and the estimation of the time-on-stream evolution in a CO/CO2 methanation reactor.

Selective Conversion of 2,3-Butanediol to Aviation Fuel and Chemical Precursors Via Dioxolane Intermediates.

Michael Cordon[1], *Peter Neate*[2], *Xiaokun Yang*[2], *Chenjiao Bu*[3], *Liangliang Huang*[3], *Meijun Li*[1], *and Andrew D. Sutton*[1]
(1)Manufacturing Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN, (2)Chemistry Division, Los Alamos National Laboratory, Los Alamos, NM, (3)School of Sustainable Chemical, Biological and Materials Engineering, University of Oklahoma, Norman, OK

This work addresses a bottleneck in 2,3-butanediol conversion processes for sustainable fuels and chemicals production. Using coupled catalyst and process design principles, catalysts were tailored to form the isobutanal intermediate critical for dioxolane formation which enables the sustainable and commercial viability of biomass-derived 2,3-butanediol separation and valorization processes.

Understanding Glycine Oxidation Mechanism: Pathway Towards Nutrient Recovery from Waste Sludge.

Samuel Olusegun[1], *Haldrian Iriawan*[2], *Nianhan Tian*[3], *Andrew Medford*[3], *Yang Shao-Horn*[2], *and Joseph Gauthier*[1]
(1)Chemical Engineering, Texas Tech University, Lubbock, TX, (2)Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, MA, (3)School of Chemical & Biomolecular Engineering, Georgia Institute of Technology, Atlanta, GA

Understanding the glycine oxidation mechanism provides fundamental insights into electrochemical waste sludge oxidation into value-added products and could inform methods to improve the reaction rate and selectivity towards desired value-added products. This work combines theoretical and experimental approaches to develop a deeper mechanistic understanding of the glycine oxidation reaction

Evaluation of the Potential of Producing SAF and Renewable Diesel Fractions from Upgrading Bio-Oils Using Dispersed Catalyst.

Yi Zhang *and Jacques Monnier*
Natural Resources Canada, CanmetENERGY-Ottawa, Ottawa, ON, Canada

This study evaluated the potential of producing biojet and renewable diesel fractions by upgrading biomass fast pyrolysis oil and catalytic pyrolysis oil using dispersed unsupported MoS_2 catalyst, and assessed how close the final products are to meet jet and diesel fuels standards (ASTM D7566 and D975, respectively).

Harnessing Ultrasound Irradiation for Selective Radical-Driven Aldehyde Oxidation to Carboxylic Acids.

Ari Fischer[1], *Teseer Bahry*[2], *Zhangyue Xie*[1], *Kaicheng Qian*[3], *Renhong Li*[4], *James Kwan*[5],

Francois Jerome[2], Sabine Valange[2], Wen Liu[1], Prince N. Amaniampong[2], and Tej Choksi[1]
(1)School of Chemistry, Chemical Engineering and Biotechnology, Nanyang Technological University, Singapore, Singapore, (2)Institut de Chimie des Milieux et Matériaux de Poitiers, CNRS, Poitiers, France, (3)Zhejiang Sci-Tech University, Hangzhou, Zhejiang, China, (4)National Engineering Lab for Textile Fiber Materials and Processing Technology, Zhejiang Sci-Tech University, Hangzhou, China, (5)Engineering Science, University of Oxford, Oxford, United Kingdom

Ultrasound irradiation generates free radicals enabling aqueous radical oxidation chemistry. The kinetics of one such process, glyoxal oxidation, are described robustly by combining density functional theory calculations with experiments. These descriptions inform experimental conditions that afford selective aldehyde oxidation in favor of deleterious C-C cleavage.

Biocrude Upgradation Via Hydrodeoxygenation Using Ni-Mo Doped Hydrochar Catalysts Derived from Sawdust.

***Priyanka Tirumareddy**, Ajay Dalai, and Philip Boahene*
Chemical and Biological Engineering, University of Saskatchewan, Saskatoon, SK, Canada

Biocrude was produced via hydrothermal liquefaction of canola and mustard meal, achieving 42 wt.% yield at optimized conditions. Catalytic upgrading with Ni-Mo doped hydrochar derived from sawdust reduced oxygen content from 9-10 wt.% to 2-4 wt.%, significantly enhancing biocrude quality for sustainable renewable fuel production.

Synergistic Effect of Metal and Acid Sites in Chemical Recycling of Plastic Wastes.

***Junho Suh** and Do Heui Kim*
Seoul National University, Seoul, Korea, Republic of (South)

It was found that through the bifunctional mechanism over Ru/BEA, high conversion of PE, low production of methane, and improved product distribution toward naphtha range could be achieved.

One Pot Synthesis of Fully Formulated Sustainable Aviation Fuel from Brown Grease Via Multifunctional Catalysts.

*Clara Mongelli[1], Great Umenweke[2,3], **Robert Pace III**[3], and Eduardo Santillan-Jimenez[2,3]*
(1)Université de Bourgogne Franche-Comté, Dijon, France, (2)Department of Chemistry, University of Kentucky, Lexington, KY, (3)Center for Applied Energy Research, University of Kentucky, Lexington, KY

Multifunctional nickel copper catalysts supported on zeolites and zeotypes were employed in the upgrading of brown grease to fully formulated sustainable aviation fuel. 10% Ni-2.5% Cu supported on ZSM-5 was found to have quantitative conversion and good selectivity to all four hydrocarbon types found in aviation fuel.

Carbon Dioxide to Ethylene Conversions on Iron-Based Catalysts.

Bin Liu
Chemical Engineering, Kansas State University, Manhattan, KS

This study helps provide molecular insights into the active sites, reaction mechanisms and CO_2 conversion product selectivities for the important Fe-based catalysts.

CuO-ZnO Oxides Derived from Lamellar Structures As Catalysts for the Hydrogenation of CO_2 to Methanol.

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

The conversion of CO_2 into methanol is typically carried out using copper-based mixed oxides. Although these oxides have high reactivity, they also exhibit low catalytic stability. In this context, this work proposes modifications to classical methods for obtaining Cu-Zn-based metal precursors, investigating the impact of urea and cetyltrimethylammonium bromide.

通过优化活性位点接近度和 CO 中间体促进反铁基催化剂上co 2加氢制烯烃.

Wei Wang[1]*, Bowen Li*[2]*, Caiqi Wang*[1]*, Norbert Kruse*[1]*, and Hongfei Lin*[1]
(1)The Gene and Linda Voiland School of Chemical Engineering and Bioengineering, Washington State University, Pullman, WA, (2)Department of Chemical Engineering, Northeastern University, Boston, MA

This work develops inverse Fe-based catalysts for CO_2 hydrogenation to olefins, optimizing active site proximity and CO intermediate transport. The inverse catalysts achieve 53.9% olefin selectivity at 48.7% CO_2 conversion, outperforming traditional catalysts. In situ DRIFTS shows a combined RWGS and CO hydrogenation pathway, enhancing CO_2 conversion and olefin selectivity.

Understanding Sulfur-Induced Deactivation in Ru/Al_2O_3 Catalysts for CO_2 Hydrogenation Via Combined *in-Situ* and *Ex-Situ* Methods.

Clara Larghi[1]*, Alessandro Porta*[1]*, Carlo Giorgio Visconti*[1]*, Janos Szanyi*[2]*, and Luca Lietti*[1]
(1)Dipartimento di Energia, Politecnico di Milano, Milan, Italy, (2)Pacific Northwest National Laboratory, Richland, WA

Sulfur contaminants in CO_2 flows strongly hinder the methanation process. This study used *ex-situ* and *in-situ* poisoning to analyze sulfur's impact on the morphology and activity of a 4% Ru/Al_2O_3 catalyst. Additionally, a kinetic model developed was able to effectively describe the catalyst's deactivation.

Sustainable CO_2 Electrolysis to Concentrated Formate in the CEM-Based Electrolyzer..

Haocheng Xiong[1]*, Bingjun Xu*[2]*, and Qi Lu*[3]
(1)Department of Chemical Engineering, Tsinghua University, Beijing, China, (2)Catalysis Center for Energy Innovation, Department of Chemical and Biomolecular Engineering, University of Delaware, Newark, DE, (3)Chemical Engineering, Tsinghua University, Beijing, China

I will present various CO_2 electrolysis strategies to produce concentrated formate products up to 5.3 M using a cation exchange membrane-based flow-type electrolyzer. This approach demonstrated substantial profitability for valuable chemical production from CO_2 in the TEA analysis, even without considering potential subsidies and carbon taxes.

Catalytic Roles of Reactive Hydrogen in CO_2 activation Via Reverse Water Gas Shift on Rh and Pt Surfaces.

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Despite extensive investigations, Reverse Water Gas Shift mechanism over supported metal nanoparticles remains unclear. To address these uncertainties, we performed a rigorous kinetic investigation on Pt and Rh nanoparticles supported on alumina, deriving apparent reaction orders, activation energies and two rate equations based on different CO_2 activation pathways.

Material and Process Optimization of Reactive Carbon Capture to Methanol Using Cu-ZnO-Al_2O_3 Dual Function Materials.

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

We report the development and evaluation of Cu-Zn-Al based dual function materials for combined capture and conversion of CO_2 to methanol. Through a rigorous design of experiments, the DFM composition (alkali identity and loading) and process conditions (hydrogenation parameters) were optimized, resulting in increased MeOH selectivity from 53% to 97%.

Computational Investigation into Supported and Inverted Cu-ZrO_2 Catalysts for Selective CO_2 Hydrogenation to Methanol.

Anshuman Goswami[1,2]*, Junjie Chen*[1,2]*, Alessandro Gallo*[1,2]*, Thomas Jaramillo*[1,2]*, and Frank Abild-Pedersen*[1,2]
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We utilize Density Functional Theory (DFT) calculations for atomistic models of supported and inverted Cu-ZrO_2 systems. We evaluate reaction pathways and energetics for energetically favorable configurations in both systems. Through this, we finally elucidate the role of supported and inverted catalyst systems in assisting selective CO_2 hydrogenation to methanol.

Integrated CO_2 Capture and Utilization over Cu-K_2CO_3/MgO Dual Functional Catalyst.

Saiyed Tasnim Md Fahim[1]*, Bruno Henrique Arpini*[2]*, and Kandis Leslie Gilliard-Abdulaziz*[3]
(1)Sonny Astani Department of Civil and Environmental Engineering, University of Southern California, Los Angeles, CA, (2)Chemical Engineering, University of Southern California, Los Angeles, CA, (3)Sonny Astani Civil and Environmental Engineering Department, University of Southern California, Los Angeles, CA

This work showed the preparation and application of a dual functional Cu-K_2CO_3/MgO catalyst for CO_2 capture and selective conversion to CO, an important step towards methanol synthesis.

设计CO2加氢制备C2 +烃和含氧化合物的反应路径和产物效率.

Hongfei Lin[1]*, Caiqi Wang*[1]*, Wei Wang*[1]*, Bowen Li*[2]*, and Norbert Kruse*[1]
(1)The Gene and Linda Voiland School of Chemical Engineering and Bioengineering, Washington State University, Pullman, WA, (2)Department of Chemical Engineering, Northeastern University, Boston, MA

This study investigates CO2 hydrogenation to C2+ hydrocarbons and oxygenates using CoM-based catalysts (M = Cu, Mn, Fe) with a potassium promoter. It highlights the synergistic effect of CO_2 activation and C-C coupling in product selectivity. In situ DRIFTS shows that formate intermediates enhance C-C coupling for selective product formation.

Catalytic Functionalities of Ni-Based Catalysts for CO_2 hydrogenation By Hydrogen Transfer from Isopropanol.

Julieth García Sánchez[1]*, Josefine Schnee*[2]*, Alejandro Karelovic*[3]*, Luz Marina Ballesteros Rueda*[4]*, Daviel Gómez*[5]*, Patricia Concepción*[5]*, and* ***Victor Gabriel Baldovino Medrano***[6]
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From a thermodynamic point of view, the hydrogenation of CO_2 by hydrogen transfer from isopropanol would be possible and the ability to carry out these reactions depends on catalytic functionalities such as acid-base properties and Ni loading; but it is limited by the competition between reactants on the catalyst surface.

Pathway of CO_2 Conversion over a Ru-K_2CO_3/CNF Dual Functional Material for Direct Air Capture.

Freek Karaçoban, *Tomas Haasterecht, van, and Johannes Hendrik Bitter*
Wageningen University, Wageningen, Netherlands

In Ru/K_2CO_3 on carbon, a dual functional material for CO_2 capture (from air) and conversion special sites are present which can retain captured CO_2 until a temperature relevant for the methanation is reached.

Novel Thermal Catalytic CO_2 Conversion without External Hydrogen: A Tandem Process for Methane, Bio-Lubricant, and Hydrogen Production Via Methyl Palmitate Ketonization.

Piyasan Praserthdam[1] *and Supareak Praserthdam*[2]
(1)Chemical Engineering, Chulalongkorn University, Bangkok, -, Thailand, (2)Chemical Engineering, Chulalongkorn University, Bangkok, Thailand

This study introduced a tandem thermal approach to converting CO_2 into methane without external hydrogen and methyl palmitate ketonization. TiO_x catalysts with varying oxygen vacancy levels were investigated. Co-feeding CO_2 improves not only methane production but also hydrogen production.

One-Step CO_2 Hydrogenation to Hydrocarbons on K Promoted Fe Catalyst on an Alginate-Based Carbon Support..

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(1)Department of Chemical Engineering, Norwegian University of Science and Technology, Trondheim, Norway, (2)College of Smart Energy, Shanghai Jiao Tong University, Shangai, China, (3)SINTEF Industry, Kinetics and Catalysis Research Group, Trondheim, Norway

This work provides an interesting way of valorizing CO_2 streams into high added-value liquid fuels. An innovative synthesis, based on alginate, was employed to produce K, Fe carbon-supported catalysts. The catalyst was able to hydrogenate CO_2, with a conversion up to 40%, and a selectivity towards Fischer-Tropsch products of 80%.

Dynamic Reconstruction Behavior of Complex Oxides in Dry Reforming of Methane: In Situ Generation of Stable Nicu Alloy Active Sites.

Junyan Zhang[1], *Meijia Li*[1], *Yuanyuan Li*[1], *Kevin Siniard*[2], *Alexander Ivanov*[1], *Harry M. Meyer III*[1], *Shize Yang*[3], *Zili Wu*[1], *Zhenzhen Yang*[1], ***Felipe Polo-Garzon***[1], *and Sheng Dai*[1]
(1)Chemical Sciences Division, Oak Ridge National Laboratory (ORNL), Oak Ridge, TN, (2)Chemistry, University of Tennessee, Knoxville, TN, (3)Yale University, New Haven, CT

Dry reforming of methane operates at high reaction temperatures, leading to catalyst deactivation. Tightly anchored Ni-Cu bimetallic nanoparticles were in situ exsoluted from a solid oxide solution ($NiMgCuZnO_x$) to catalyze DRM and repel coke.

High Performance M (Ga, Ce, Mn, Mg, La)-Promoted Cu-ZnO-ZrO_2 Catalysts for CO/CO_2 Hydrogenation to CH_3oh.

Shihang Meng[1], ***Yujing Weng***[1], *Qi Sun*[1], *and* ***Yulong Zhang***[2]
(1)Chemical Engineering, Henan Polytechnical University, Jiaozuo, China, (2)Chemical Engineering, Henan Polytechnical University, Jiaozuo, Henan, China

The Ga promoted $CuZnOZrO_2$ catalyst were prepared by coprecipitation with Na_2CO_3. CO/CO2 co-hydrogenation to methanol were carried out to study the catalyst performance CO and CO2 conversion collectively. The Ga promoted CZZ catalyst showed notable enhancement of CO_2 adsorption and exhibited excellent performance for CO/CO_2 co-conversion with high methanol yield.

Deciphering Transition-Metal B-Site Reactivity, Selectivity, and Stability for Oxidative C_1 Hydrocarbon Upgrading on Perovskite Oxides.

Rachel A. Yang *and Eranda Nikolla*
Department of Chemical Engineering, University of Michigan, Ann Arbor, MI

Perovskite oxides with systematically varied transition metal cation identities demonstrate distinct reactivities, C_2 selectivities, and stabilities for the oxidative coupling of methane. Reaction pathways are a function of intrinsic metal properties and cation compositions that can be tuned and leveraged for more atom-efficient C_1 conversion to chemicals and fuels.

Unraveling the Silver-Catalyzed Methanol to Formaldehyde Reaction: Understanding the Sub-Reactions, Kinetics and Restructuring.

Tina Bergh[1], *Youri van Valen*[1], *Ole Håvik Bjørkedal*[2], *Ann Kristin Lagmannsveen*[3], *and Hilde Johnsen Venvik*[1]
(1)Department of Chemical Engineering, Norwegian University of Science and Technology (NTNU), Trondheim, Norway, (2)Dynea AS, Lillestrøm, Norway, (3)K.A. Rasmussen, Hamar, Norway

We study the silver-catalyzed methanol to formaldehyde (MTF) reaction and its sub-reactions. The reaction data obtained from our annular reactor setup using a cylindrical silver catalyst provides mechanistic insights relevant to industrial conditions, while thorough nanoscale characterization (SEM, FIB, 4D-STEM) highlights the effects of various reactants on catalyst restructuring.

Light Alkane Conversion through Ammonia Assisted Reforming and Dehydrogenation.

Yizhi Xiang

Department of Chemical and Biomedical Engineering, University of Missouri Columbia, Columbia, MO

We proposed to convert light alkane through ammonia assisted reforming and dehydrogenation, for energy and chemical production. From a fundamental point of view, we will discuss the catalytic active sites and mechanism of these new catalytic reactions based on extensive catalyst characterization and kinetic analyses.

Mechanochemical Synthesis of Multicomponent Bismuth-Based Molybdate Catalysts for Propylene Ammoxidation to Produce Acrylonitrile.

ChangJin Han *and Do Heui Kim*
Seoul National University, Seoul, Korea, Republic of (South)

The bismuth molybdenum-based multi-metal oxide catalysts were mechanochemically synthesized using the ball milling method without the use of nitric acid and exhibited excellent performance in propylene ammoxidation. The physicochemical properties and catalytic activities of the iron or cobalt phase added to the bismuth molybdenum phase were investigated.

Catalytic Activity of MoO_x@SiO_2 Yolk-Shell Structures in Propane Dehydrogenation and Subsequent Propylene Metathesis.

Anna Rokicinska[1]*, Mariya Myradova*[2]*, Mateusz Mandrela*[1]*, Dominika Waśniowska*[1]*, Marek Debosz*[1]*, Piotr Michorczyk*[2]*, and* ***Piotr Kustrowski***[1]
(1)Faculty of Chemistry, Jagiellonian University, Krakow, Poland, (2)Department of Organic Chemistry and Technology, Cracow University of Technology, Krakow, Poland

MoO_x@SiO_2 nanoreactors with a yolk-shell structure were developed for efficient propane dehydrogenation combined with subsequent metathesis of produced propylene. The key role in achieving high activity in both industrially important processes was played by controlled dispersion of the active phase within the composite.

High-Yield Ethanol to Acetone Reaction Using Induction Heating.

Ryan Thompson[1]*, Ben Ko*[1]*, Han Wang*[1]*, Carlos L. Pueyo*[2]*, Jianping Chen*[3]*, Roel Sanchez-Carrera*[4]*, and Erdem Sasmaz*[1]
(1)Chemical and Biomolecular Engineering, University of California, Irvine, Irvine, CA, (2)BASF, Ludwigshafen am Rhein, Germany, (3)BASF, Beachwood, OH, (4)BASF, Iselin, NY

Induction heating has been shown to be an effective method for electrifying heating. The production of acetone from ethanol using Fe_2O_3-ZnO was studied in a packed-bed reactor with steel receptors. Improvements in temperature gradients in the catalyst bed were shown. Magnetic effects were also hypothesized and analyzed in adsorbed intermediates.

Unifying Dehydrogenation and Coupling of Isoalkane Feedstocks to SAF-Range Precursors in a Single Reactor..

Alexander J. Hill[1], *Anh To*[2], *Claire Nimlos*[2], *Susan E. Habas*[2], *and Daniel Ruddy*[2]
(1)National Renewable Energy Laboratory, Golden, CO, (2)Catalytic Carbon Transformation and Scale-Up Center, National Renewable Energy Laboratory, Golden, CO

This work explores mixed beds of dehydrogenation and olefin coupling catalysts to conduct dehydrogenative coupling of isoalkanes to SAF-range olefins in a single reactor. Tuning acid properties of the olefin coupling catalysts catalysts improves compatibility with dehydrogenation conditions. Combining these two reactions enables equilibrium conversion of isoalkanes to be surpassed.

Conversion of Ethanol to 1,3-Butadiene over Supported Cobalt Catalyst with Induction Heating.

John Pham[1], *Han Wang*[1], *Ben Ko*[1], *Carlos L. Pueyo*[2], *Jianping Chen*[3], *Roel Sanchez-Carrera*[4], *and Erdem Sasmaz*[1]
(1)Chemical and Biomolecular Engineering, University of California, Irvine, Irvine, CA, (2)BASF, Ludwigshafen am Rhein, Germany, (3)BASF, Beachwood, OH, (4)BASF, Iselin, NY

Induction heating, showing great potential in decarbonization efforts, is utilized to investigate the promising enhancement of the selectivity of the (bio)ethanol-to-1,3-butadiene reaction over a bifunctional $Co/ZrO_2/SiO_2$ catalyst. The results suggest that the magnetic field and SiO_2 (SBA-16)-ZrO_2 interactions contribute to the catalyst activity improvement.

DFT and Microkinetic Study of the Mechanism of Propene Metathesis on MoO_x/SiO_2 and $MoO_x/(AlO_y\text{-}SiO_2)$ Catalysts.

Joseph Thompson[1], *Eli Ream*[2], *Israel Wachs*[3], *and Srinivas Rangarajan*[2]
(1)Lehigh University, Bethlehem, PA, (2)Chemical and Biomolecular Engineering, Lehigh University, Bethlehem, PA, (3)Department of Chemical and Biomolecular Engineering, Lehigh University, Bethlehem, PA

Density functional theory study of the mechanisms of propene metathesis on activated MoO_4/SiO_2 and $MoO_4/AlO_4/SiO_2$ showed that transition and intermediate states are significantly stabilized for $MoO_4/AlO_4/SiO_2$ compared to MoO_4/SiO_2 indicating higher activity. This work will address key atomic-scale details of how catalyst structure influences catalytic activity on supported MoO_x/SiO_2 catalysts.

Iso-Butanol Production from Methanol/Ethanol Mixtures Via the Guerbet Reaction Using Hydrotalcite Ni/Cu-Al Catalysts.

Quoc Khanh Tran[1], *Joachim Pasel*[2], *and Ralf Peters*[3]
(1)Julich Research Center, Julich, Germany, (2)Electrochemical Process Engineering (IEK-14), Jülich Research Center, Jülich, Germany, (3)Forschungszentrum Jülich GmbH, Jülich, Germany

In this study, a sustainable method of producing iso-butanol was introduced via Guerbet using Ni/Cu-Al catalyst. The mixture of methanol/ethanol was mainly converted into iso-butanol. 5 wt% of 10Ni/2Cu-Al showed the best performance with 124 mmol/L of iso-butanol and 7.7 % of ethanol conversion at 185 °C, and 4h.

Single Nickel Site Catalyst on Mesoporous Silica for Light Olefin Oligomerization.

Alba Scotto d'Apollonia[1], *Michael Appoh*[2], *William Schneider*[1], *and Jason Hicks*[1]
(1)Chemical and Biomolecular Engineering, University of Notre Dame, Notre Dame, IN,
(2)Chemistry and Biochemistry, University of Notre Dame, Notre Dame, IN

Nickel-substituted polyoxometalates on mesoporous silica exhibit excellent stability and promising performance in light olefin oligomerization. Our work offers valuable mechanistic insights into the impact of pore size on catalyst deactivation, which can be applied to other porous materials. Rates and selectivity for pure and mixed feeds are also showcased.

Active and Selective Nature of Cezn and Cucezn for the Oxidative Dehydrogenation of Propane with Carbon Dioxide.

Cedric Karel Fonzeu Monguen[1,2], *Samuel Daniel*[2,3], *Hannington Nevin Otieno*[2,3], ***Patrick Lott***[1], *Olaf Deutschmann*[1], *and Zhen-Yu Tian*[2,3]
(1)Institute for Chemical Technology and Polymer Chemistry, Karlsruhe Institute of Technology, Karlsruhe, Germany, (2)Institute of Engineering Thermophysics, Chinese Academy of Sciences, Beijing, China, (3)University of Chinese Academy of Sciences, Beijing, China

The CeZn binary oxide catalyst exhibited attractive performance for CO_2-ODHP. Loading Cu into the (Ce/Zn) structure was found to promote propane conversion and propene yield with CO_2. Thus, the novel catalyst exhibits high potential for application in the petrochemical industry.

Ethane Dehydrogenation with CO_2 Using LDH-Derived Mixed Oxides of V, Mn, and Ga.

Gabriel Liscia Catuzo, *Rosembergue G. L. Gonçalves, and Elisabete Assaf*
Instituto de Química de São Carlos/Universidade de São Paulo, São Carlos, Brazil

Layered double hydroxide-derived catalysts doped with V, Mn, and Ga were evaluated for ethane dehydrogenation with CO_2. The MgZnGa catalyst showed the highest ethylene yield of 479 µmol $min^{-1}.g^{-1}$ even after 5 h of reaction, owing to its resistance to deactivation and the retention of active sites.

Copper-Based Catalysts for DME Steam Reforming: Investigating Reaction Mechanisms for Hydrogen Production.

Yulu Ge[1], *Ricardo Navar*[2], *Jie Liu*[2,3], ***Xiaokun Yang***[1], *and Qi An*[3]
(1)Chemistry Division, Los Alamos National Laboratory, Los Alamos, NM, (2)Los Alamos National Laboratory, Los Alamos, NM, (3)Illinois State University, Normal, IL

We synthesized copper-based catalysts with a CeO_2 core and zeolite shell for DME steam reforming. The catalysts exhibit different reaction mechanisms depending on copper loading, with formate and methyl formate intermediates observed. DFT calculations confirm the feasibility of these pathways, offering insights for enhancing hydrogen production in the hydrogen economy.

Catalytic Pyrolysis of Plastic Waste for the Synthesis of Hydrogen and Nanocarbons.

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(1)Department of Chemical Engineering, Indian Institute of Technology Delhi, New Delhi, India,
(2)Chemical Engineering Department, Indian Institute of Technology Delhi, New Delhi, India,
(3)Chemical Engineering, Indian Institute of Technology Delhi, New Delhi, India

The alarming rise in plastic waste necessitates innovative solutions. Thermo-catalytic conversion transforms plastics into hydrogen and CNTs, addressing pollution and energy needs. Conventional Fe/Al2O3 and Ni/Al2O3 and novel flyash acts as catalyst. This sustainable approach supports clean energy production and a circular economy, reducing environmental impact.

Ammonia Production from the Catalytic Decomposition of Hydroxylammonium Nitrate As Green Energetic Source for Clean Space.

Rachid Amrousse
University of Chouaib Doukkali, Faculty of Sciences, El Jadida, Morocco

This study explores ammonia (NH3) production via the thermal decomposition of hydroxylammonium nitrate (HAN), a green propellant, using an iridium-based catalyst. The research combines experimental and theoretical methods to confirm NH3 generation, suggesting HAN as a sustainable energy source for space propulsion systems.

Defect-Induced Nanocrystalline Colored Titania - Inspiring Next Generation Photocatalyst: Application in Cellulose Reforming for Hydrogen Production.

Parasuraman Selvam
Department of Chemistry & NCCR, IIT-Madras, CHENNAI, India

Defect-induced colored titania photocatalysts were evaluated for photoreforming of cellulose which gave remarkable activity as compared to the white TiO_2. Importantly, the CO_2 evolution was much lower for the colored samples than that of the corresponding white titania which suggests the importance of intrinsic defects for the photocatalytic reaction.

Multifunctional Graphene-Nickel Single-Atom Catalyst for AEM Water Electrolysis and UV/Chlorine Treatment.

Lee Jihoon, *Yang Eunju, and Yoon Yeojoon*

Department of environmental and energy engineering, Yonsei university, Wonji-si, Gangwon-do, Korea, Republic of (South)

We developed a low-cost graphene-nickel single-atom catalyst for AEM water electrolysis using an impregnation method. The catalyst's effectiveness was demonstrated in both AEM water electrolysis and a UV/chlorine reactor for water treatment. This integrated approach demonstrates the catalyst's multifunctional potential in hydrogen production and water treatment applications.

Mechanistic Understanding of Iron-Aluminum Composites in Methane Cracking for Turquoise Hydrogen and Fibrous Carbon Production.

Shih-Yuan Chen
Department of Energy and Environment, National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Ibaraki, Japan, Japan

From an industrial perspective, CH_4 conversion over FeAl mixed oxides was studied and modeled to predict Fe-based catalyst performance for turquoise hydrogen and valuable carbon production. A strategy to improve catalyst longevity was proposed, enhancing the commercial feasibility of CH_4 cracking and increasing the industrial value of nanostructured carbon materials.

Development of Nickel Catalysts with Core-Shell Structure for Ethanol Steam Reforming.

***Andrelaine de Souza Bernardes**[1], Leticia Forrer Sosa[2], and Pedro Romano[3]*
(1)Chemistry School, Federal University of Rio de Janeiro (UFRJ), Rio de Janeiro, Brazil, (2)Universidade Federal do Rio de Janeiro, Rio de Janeiro, Brazil, (3)Campus D. de Caxias, Federal University of Rio de Janeiro, Rio de Janeiro, Brazil

This study focuses on synthesizing and evaluating nickel-based core-shell catalysts ($Ni\text{-}SiO_2@CeO_2$) for steam ethanol reforming to produce hydrogen. Cerium oxide (CeO_2) is employed as a shell to enhance stability, prevent coke deposition, and reduce nickel deactivation, promoting an economically viable and sustainable hydrogen production process from renewable ethanol sources.

A First-Principles Based Microkinetic Investigation of the Dehydrogenation of C_7H_{14} to C_7H_8 on Pt(111).

***Alvaro Posada-Borbon**[1], Tobias Möslinger[2], and Henrik Grönbeck[1]*
(1)Department of Physics and Competence Centre for Catalysis, Chalmers University of Technology, Göteborg, Sweden, (2)Department of Physics, Chalmers University of Technology, Göteborg, Sweden

We interrogate the dehydrogenation of methylcyclohexane (MCH) to toluene and a competing demethylation to benzene on Pt(111) through DFT calculations and microkinetic modelling. Kinetic analysis shows the dehydrogenation reaction is controlled by the adsorption/desorption of MCH and toluene. The work provides handles for the rational design of LOHC dehydrogenation catalysts.

Niobia Supported Cu-Zn Catalysts for Sour Water Gas Shift Reaction.

Ludmila P. C. Silva[1]*, Ana Carla Coutinho*[1]*, Luis E Terra*[1]*, and* ***Fabio B. Passos***[2]
(1)Department of Chemical and Petroleum Engineering, Fluminense Federal University, Niteroi, Brazil, (2)Department of Chemical and Petroleum Engineering, Universidade Federal Fluminense, Niteroi, Brazil

Sulfur compounds poison typical water-gas shift reaction (WGSR) catalysts required to increase H_2 production. Here we present an investigation on the use of niobia as support for CuZn catalysts, addressing how active sites interact with sulfur poison and WGSR reactants.

Hydrogen Production from Water on Molybdenum Carbide: A Mechanistic Study.

Milad Ahmadi Khoshooei
Northwestern University, Evanston, IL

This work focused on elaborating mechanisms of activating water in the presence of a carbonaceous source for hydrogen production over a molybdenum carbide catalyst. Isotopic labeling, spectroscopic analysis, and kinetic experiments revealed that the catalyst is prone to oxidation in the presence of water.

Improving Quality and Increasing Throughput in Catalyst Manufacturing Unit Operations.

Benjamin Glasser *and William Borghard*
Chemical and Biochemical Engineering, Rutgers University, Piscataway, NJ

By combining our expertise in particle technology and optimization we are developing and promoting science-based methods for designing, scaling up and optimizing catalyst manufacturing processes. A combination of experiments and computer models has been used to improve the understanding and performance of unit operations used to make catalysts.

Highly Dispersed Bimetallic Catalysts for Semi Hydrogenation of Acetylene with Galvanic Displacement.

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

This study offers a general synthesis strategy for Pd-Cu bimetallic system with controlled surface composition and structure. It has the potential to be applied to other bimetallic catalysts with suitable metal precursors and reaction conditions. GD is a promising method for immobilizing secondary active components onto the supported metallic catalysts.

Synthesis of MFI Zeolites with Small Crystallite Sizes to Generate Stable Product Selectivity from Alkene Oligomerization.

Sanghyun Ahn, *Elizabeth Bickel Rogers, Songhyun Lee, Evan E. Sowinski, and Rajamani Gounder*
Charles D. Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN

Synthesis recipes were developed to prepare small crystallite-size (<50 nm) MFI zeolites that meet commercial manufacturing targets to enable future catalyst scale-up efforts, and evaluated against conventionally prepared larger-crystallite zeolites, to demonstrate improved olefin oligomerization rate and product stability with time-on-stream.

Aqueous-Based Granulation Method Towards Clean Energy Applications.

Divakar Reddy Aireddy[1], *Christopher Marin*[2], *Biswanath Dutta*[3], *Eric Popczun*[2], *Christina Wildfire*[4], *and Douglas Kauffman*[2]
(1)Reaction Engineering Team, National Energy Technology Laboratory (/Leidos), Morgantown, WV, (2)National Energy Technology Laboratory, Pittsburgh, PA, (3)NETL Support Contractor, Morgantown, WV, (4)National Energy Technology Laboratory, Morgantown, WV

An aqueous-based granulation method is developed to combat the structural changes associated with binder-based granulation techniques. Microwave-assisted methane reforming studies showed an improved catalyst efficiency for these aqueous-based granules compared to the powder catalysts. This granulation method has been extended to other practical applications (chemical looping gasification and air separations).

Evaluation of Fumed and Precipitated Silica Extrudates: Balancing Surface Area, Crush Strength, and Pore Volume.

Chris Bauer
Smart Effects, Evonik Corporation, Piscataway, NJ

This study evaluates fumed and precipitated silica extrudates, highlighting their impact on catalyst support properties. By optimizing formulations and processing conditions, the research aims to achieve high mechanical strength, surface area, and porosity, offering potential improvements in industrial catalyst applications.

The Growth of Titanium-doped Ceria Thin Films by Pulsed Laser Deposition for CO_2 Splitting with H_2O.

Rosa Virginia Melinda[1], *David King*[2], *Nishan Paudyal*[1], *Jinke Tang*[2], *and Jing Zhou*[1]
(1)Chemistry, University of Wyoming, Laramie, WY, (2)Physics and Astronomy, University of Wyoming, Laramie, WY

This study utilized pulsed laser deposition method coupled with glancing angle deposition technique to synthesize titanium-doped ceria thin films with controlled nanostructures, morphologies, and compositions. This allows for a fundamental investigation of the interaction with CO_2 and H_2O for thermochemical cycles of CO_2 conversion to chemicals and fuels.

Catalytic Consequences of Catalyst Pellet Architecture on the Direct Production of Dimethoxymethane from Methanol..

Sebastian Cook[1], ***William Broomhead***[2], *Adam Johnston*[3], *Ya-Huei (Cathy) Chin*[1], *and Jose Herrera*[3]
(1)Department of Chemical Engineering and Applied Chemistry, University of Toronto, Toronto, ON, Canada, (2)Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA, (3)Department of Chemical and Biochemical Engineering, Western University, London, ON, Canada

The considerations required to scale up a lab-scale catalyst formulation to industrial-scale pellets requires are presented. Active phase dispersion and distribution need to be carefully controlled to minimize temperature gradients and optimize catalyst performance.

Design and Assessment of Pt-Fe/SiO2 Catalysts for Stoichiometric Methane Combustion: Does Fe Really Contribute?.

Carol Bibiana Espinosa Lobo[1], *Julieth García Sánchez*[1], *Edwing Velasco Rozo*[2], *and* ***Victor Gabriel Baldovino Medrano***[3,4]
(1)Chemical Engineering, Centro de Investigaciones en Catálisis, Universidad Industrial de Santander, Bucaramanga, Santander, Colombia, (2)Grupo de Investigación GREIP, Instituto Universitario de la Paz-UNIPAZ, Barrancabermeja, Santander, Colombia, (3)Chemical Engineering, Centro de Investigaciones en Catálisis (CICAT), Universidad Industrial de Santander, Bucaramanga, Santander, Colombia, (4)Laboratorio Central de Ciencia de Superficies (SurfLab), Universidad Industrial de Santander, Piedecuesta, Santander, Colombia

We probed Pt-Fe phases in the stoichiometric combustion of methane doing as follows: (1) synthesizing Pt-Fe/SiO_2 catalysts of uniform particle sizes; (2) testing without transport artifacts. Thus, iron and platinum establish a synergistic and constant effect only around 390°C. Otherwise, iron has a null role in these catalysts.

Improved Catalytic NO Oxidation over Pt Supported on Sulfuric Acid Treated TiO_2.

Wo Bin Bae[1], *Jiseok Park*[2], *Sung Bong Kang*[3], *and Jun Hee Jang*[1]
(1)Department of Chemical Engineering, Rowan University, Glassboro, NJ, (2)School of Environment and Energy Engineering, Gwangju Institute of Science and Technology, Gwangju, Korea, Republic of (South), (3)Department of Environment and Energy Engineering, Gwangju Institute of Science and Technology, Gwangju, Korea, Republic of (South)

In this study, we demonstrate that the increase of acidic sites on the TiO_2 surface during the catalyst synthesis promotes the dispersion and formation of the metallic phase of Pt with the beneficial effects of sulfur species introduced on the surface of catalyst supports.

Opportunities and Challenges of Thin-Film Technology for Thermocatalytic Applications.

Daniel Amkreutz
PVcomB, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany

The application of thin-film technology in thermocatalysis is mostly applied for model systems today. However, it was demonstrated that for specific reactions, thin film catalysts can outperform power catalysts. We present an overview on the concept of thin-film catalysis with a focus on deposition, characterisation and potential.

Effect of Binder Selection in Cu-Zn-Y/Beta Extruded Catalysts for Ethanol Upgrading to Olefins.

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

Metal-loaded dealuminated beta zeolites have previously been identified as promising catalysts in direct ethanol upgrading to olefins. In order for these materials to be viable for scale-up efforts, extruded forms must be also developed. This work shows that extrudate binder selection can have drastic effects on catalyst structure and performance.

Dual-Templated Syntheses, Characterization, and Application of MFI/Ton-Type Zeolite Intergrowth.

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

An MFI/TON intergrown zeolite was synthesized via a dual co-templating approach, combining MFI's three-dimensional channels with TON's one-dimensional channels. Characterization confirmed the intergrowth, and catalytic testing showed high p-xylene selectivity similar to TON, indicating the zeolite retains TON-like selectivity within a single crystalline material.

Harnessing Drying Dynamics to Control Nanoparticle Size in Silica Supported Pt Catalysts.

Ismail Paykar[1]*, Simon Friedrich*[2]*, Chigozie Ezeorah*[3]*, Frank Gupton*[4]*, John Regalbuto*[5]*, and Christopher Williams*[5]
(1)Chemical Engineering Department, University of South Carolina, Columbia, SC, (2)Virginia Commonwealth University, Richmond, VA, (3)Chemistry and Biochemistry, University of South

Carolina, Columbia, SC, (4)Chemical and Life Science Engineering, Virginia Commonwealth University, Richmond, VA, (5)Chemical Engineering, University of South Carolina, Columbia, SC

Drying dynamics control nanoparticle size and active sites in silica-supported Pt catalysts. Balancing convective flow and molecular back-diffusion during drying reduces particle size from 11.2 nm to 2.8 nm, significantly enhancing the active surface area. These findings integrate crystallization and transport principles to optimize catalyst synthesis and performance.

Synthesis of Supported Metal Nanoparticles Using a Surface Support As a Reducing Agent: Characterization and Catalytic Performance in HMF Electrooxidation to Fdca.

Nataliya Shcherban[1,2]*, Moritz Krebs*[2]*, Ivan Kopa*[1]*, Eko Budiyanto*[2]*, Dmitry Murzin*[3]*, and Ferdi Schüth*[2]
(1)Department of porous substances and materials, L.V. Pisarzhevsky Institute of Physical Chemistry, National Academy of Sciences of Ukraine, Kyiv, Ukraine, (2)Department of Heterogeneous Catalysis, Max-Planck-Institut für Kohlenforschung, Mülheim an der Ruhr, Germany, (3)Laboratory of Industrial Chemistry and Reaction Engineering (TKR), Johan Gadolin Process Chemistry Centre (PCC), Åbo Akademi University, Turku, Finland

Application of the support (g-C_3N_4) surface as a reducing agent resulted in the formation of smaller and more uniform metal nanoparticles in comparison with a traditional reduction of metal precursors with hydrazine. Supported metal nanoparticles demonstrated higher catalytic performance in the electrochemical oxidation of HMF.

Controlling Metal Nanoparticle Size on Carbon Supports with Surface Tension.

Nathan Thornburg and ***John Regalbuto***
Chemical Engineering, University of South Carolina, Columbia, SC

By oxidizing carbon supports, the surface hydrophilicity increases with a decrease in the point of zero charge. With powder X-ray diffraction and scanning transmission electron microscopy (STEM), there is a scientifically significant effect on nanoparticle size and the percentage of atomic isolation from increased support hydrophilicity.

Synthesis Strategies for Porous High-Entropy Oxides and Their Activity in Thermocatalytic CO2 Hydrogenation.

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

As the field of high-entropy oxides (HEOs) is expanding into applications like catalysis, synthesis strategies control physical properties are needed Here we utilize different synthesis strategies (hydrothermal, precipitation, and solvothermal) to produce porous high-entropy precursors. Selected calcined HEOs were then tested for activity in the thermocatalytic CO2 hydrogenation reaction.

The Importance of Full Reduction and the Choice of Precursor on the Site Distribution of Rh on TiO_2 and Activity for CO Oxidation.

Vishwas Reddy Akavaram[1], *Zhanyuan Liu*[2], *Dionisios Vlachos*[3], *John Vohs*[4], *and Ayman M. Karim*[5]
(1)Chemical Engineering, Virginia Tech, Blacksburg, VA, (2)Chemical and Biomolecular Engineering, University of Pennsylvania, Philadelphia, PA, (3)Delaware Energy Institute, University of Delaware, Newark, DE, (4)Department of Chemical and Biomolecular Engineering, University of Pennsylvania, Philadelphia, PA, (5)Department of Chemical Engineering, Virginia Polytechnic Institute and State University, Blacksburg, VA

This study identifies optimal pretreatment conditions for complete Rh reduction and precursors favoring single atoms, enabling investigation of CO oxidation kinetics on single atoms, nanoparticles, and their mixtures. It also examines how precursor environments influence the size and uniformity of Rh species on Rh/TiO_2.

Nenu-5 a New Route to Prepare Mo_2c with High Specific Surface Area for Use in Catalysis.

Adrian Ortega[1], *Mario Caccia*[2], *and* ***Javier Narciso***[1]
(1)University of Alicante, Alicante, Spain, (2)Alfred University, Alfred, Spain

In this work, a new synthetic route of Mo_2C from MOF is presented, where Mo_2C has been obtained with catalytic activity superior to Pt, even an order of magnitude higher than conventional carbide. The hydrogenation reaction of nitroarenes is presented as an example.

Enhancing Hydrothermal Stability of Alumina-Based Carrier and Its Characterization.

Xueqin Wang[1], *Jing Su*[2], *Seth Riehemann*[1], *and Yeping Cai*[1]
(1)R&D Center-Louisville, Clariant Co., Louisville, KY, (2)R&D Center-Shanghai, Clariant Co., Shanghai, China

Catalysts made over alumina-based carriers are widely used for water-forming reactions or reactions containing water feed. Alumina phase transition to Boehmite at steam environment is hydrodynamically favored. Promoters prevent water attack. SEM is a good tool to identify Boehmite precursor formed on the alumina surface.

Hybrid Kinetic Modeling for Dynamic Catalytic Systems.

Kenneth Kusima[1] *and Lars Grabow*[2,3]
(1)William A. Brookshire Department of Chemical and Biomolecular Engineering, University of Houston, Houston, TX, (2)Center for Programmable Energy Catalysis (CPEC), Minneapolis, MN, (3)William A. Brookshire Department of Chemical and Biomolecular Engineering & Texas Center for Superconductivity (TcSUH), University of Houston, Houston, TX

Traditional kinetic models such as microkinetic and lumped/global models face limitations in dynamic conditions. Kinetic Monte Carlo simulations may overcome some limitations but are computationally intensive. Hybrid kinetic models, integrating machine learning and mechanistic methods, enhance adaptability, accuracy, and robustness for applications in dynamic or programmable catalysis.

Enhanced CO_2 Hydrogenation to Methane: The Role of Feed Modulation and Electric Field.

Debasish Sarkar, Rajagopalan V. Ranganathan, Jeremy Hartvigsen, ***Debtanu Maiti****, and Rebecca Fushimi*
Catalysis and Transient Kinetics Group, Idaho National Laboratory, Idaho Falls, ID

The synergistic role of feed modulation and electric field effects has been explored towards enhanced CO_2 hydrogenation to methane on Ru/CeO_2 catalysts. The improvement of reaction performance is attributed to a combination of accelerated surface protonics, and dynamic distribution of surface coverages, leading to changes in reaction pathways.

Coverage Effects for Dynamic Modulation of Formic Acid Oxidation.

Atharva Burte *and Omar Abdelrahman*
William A. Brookshire Department of Chemical and Biomolecular Engineering, University of Houston, Houston, TX

Comprehending the pseudo-steady state coverages or rather the time-averaged coverages under oscillatory conditions deeply enhances the scope of understanding the fundamentals of dynamic catalysis. Researchers would better tune and modulate catalytic turnovers beyond formic acid oxidation with this deeper understanding.

Investigating Dynamic Redox Properties of Bismuth Molybdates in Selective Propylene Oxidation.

Tanmayi Bathena[1]*, Kenneth Kusima*[2]*, Bhuvaneswari M Shivakumaran*[3]*, Venkateshkumar Prabhakaran*[3]*, Shutthanandan Vaithiyalingam*[3]*, Konstantinos Goulas*[4]*, Ajay S. Karakoti*[3]*, and Lars Grabow*[2]
(1)CHEMICAL ENGINEERING, OREGON STATE UNIVERISITY, CORVALLIS, OR, (2)William A. Brookshire Department of Chemical and Biomolecular Engineering, University of Houston, Houston, TX, (3)pacific northwest national lab, Richland, WA, (4)Oregon State University, Corvallis, OR

This study examines catalytic effects of crystal restructuring in bismuth molybdates during propylene oxidation to acrolein. The dynamic redox properties of supported vs unsupported samples show irreversible repositioning of active sites and active phases that effect the overall activity

Exploring Adsorbate-Induced Dynamic Structuring and Transport Properties of Supported Liquid Metal Catalysts Using DFT & Reaxff.

Gunnar Sly[1], *Kathryn MacIntosh*[1], *Adri van Duin*[2], *Robert Rioux*[3], *and Michael Janik*[4]
(1)Chemical and Biomedical Engineering, The Pennsylvania State University, University Park, PA, (2)Mechanical Engineering, The Pennsylvania State University, University Park, PA, (3)Department of Chemical Engineering, The Pennsylvania State University, University Park, PA, (4)Chemical Engineering, The Pennsylvania State University, University Park, PA

The structures of PdGa low-melting temperature alloys used in catalytic propane dehydrogenation are explored with a combination of DFT and ReaxFF. Surface interactions with H and C_x intermediates are examined through adsorption isotherms, induced Pd surface segregation, and reactive simulations in experimentally relevant gaseous environments.

A Bulk Phase Transformation Drives Ammonia Synthesis on Barium Hydride.

Axel tosello Gardini[1,2], *Umberto Raucci*[3], *and Michele Parrinello*[1]
(1)Atomistic Simulations, Italian Institute of Technology, Genova, Italy, (2)Department of Materials Science, University of Milano-Bicocca, Milan, Italy, (3)Italian Institute of Technology, Genova, Italy

A successful heterogeneous catalyst relies on dynamic behavior under operating conditions. Machine learning simulations confirm this for BaH_2 in ammonia synthesis via chemical looping. BaH_2 transforms into a superionic compound under N_2, enabling high ionic mobility and efficient ammonia formation after H_2 exposure, showcasing its dynamic catalytic nature.

Unveiling the Dynamics of Cu/ZIF-8 Catalysts during CO_2 Hydrogenation Using Forced Dynamic (Operando) Conditions.

Pia Dally[1] *and Pedro Castano*[2]
(1)Imaging and Characterization Core Lab, KAUST, Thuwal, -, Saudi Arabia, (2)King Abdullah University of Science and Technology (KAUST), Thuwal, Saudi Arabia

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

Investigating the Effect of a Back-Gate on the Filling of Trap Density of States in Ultrathin TiO_2 Films.

Shreya Singh *and C. Daniel Frisbie*
Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN

We discuss a back-gated electrode structure with TiO_2 simultaneously acting as the semiconductor in the metal-insulator-semiconductor stack and as the working electrode in the

electrochemical cell. We perform chronoamperometry measurements to show that back-gate potential affects filling of trap states in the TiO_2 film, independent of the working electrode potential.

Generalizing Reactive Surfaces of Ir Complex Metal Oxide Catalysts for the Oxygen Evolution Reaction in Acidic Electrolytes.

Harrison Lippie *and Joaquin Resasco*
McKetta Department of Chemical Engineering, The University of Texas at Austin, Austin, TX

Ir-based double perovskites for the OER in acidic media converge to similar surface activities and structures at steady-state. Non-Ir elements leach, forming a disordered IrO_x surface with higher specific area and activity than rutile IrO_2. Differences in short-term activity relate to stability, but long-term performance equalizes across perovskites.

Thermodynamic Insights of CO_2 Reduction in Solid Oxide Electrolysis Cells with Sulfur Containing Feed Flows.

Johari Dramiga
Lehigh University, Bethlehem, PA

Understanding the kinetic consequences of S poisoning on SOEC cathode electrocatalysts to improve efficiency and mitigate contaminate induced degradation. Competitive adsorption between CO_2 and SO_2 coupled with thermodynamics of respective dissociation reactions, can result in surface converge effects which reduce catalytic performance.

Visible Light As a Leverage to Accelerate the Reverse Water Gas Shift Reaction over Cu-$Ce_x(Ti_{1-x})O_2$ Catalysts.

Miha Okorn[1,2]*, Petar Djinović*[1,2]*, Nataša Novak Tušar*[1,2]*, and Kristijan Lorber*[1]
(1)Department of Inorganic Chemistry and Technology, National Institute of Chemistry, Ljubljana, Slovenia, (2)University of Nova Gorica, Nova Gorica, Slovenia

The $Cu/Ce(Ti)O_2$ nanorod catalysts demonstrate significant potential for the light-assisted RWGS reaction, yielding significantly higher R_{CO} compared to thermal catalysis at moderate temperatures. This work is focused in the areas of structural and in-situ spectroscopic characterization for better understanding of the mechanistic origins of visible light on the catalytic process

Enhancing Electrocatalytic Conversion of CO_2 Via Bicarbonate Reduction to Formate Via Indium-Bismuth Alloys.

Yukun Hu[1]*, Yuke Li*[2]*, Jia Zhang*[2]*, and Andrew Wong*[3]
(1)Chemical & Biomolecular Engineering, National University of Singapore, Singapore, --- None ---, Singapore, (2)Institute of High Performance Computing (IHPC), Agency for Science,

*Technology, and Research (A*STAR), Singapore, --- None ---, Singapore, (3)Materials Science and Engineering, National University of Singapore, Singapore, Singapore*

For the first time, we have designed, synthesized, and characterized novel indium-bismuth alloy phases, achieving exceptional electrochemical bicarbonate reduction reaction (BRR) performance with formate Faradaic efficiencies ranging from 83.67% at 100 mA·cm^{-2} to 60.24% at 400 mA·cm^{-2} with mechanistic insights into improving BRR selectivity by theory and experiments.

The Microenvironment Frontier for Electrochemical CO_2 Conversion.

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

For electrochemical CO2 reduction, focusing on the microenvironment offers many new possibilities to towards developing selective CO2 conversion. This overview talk shares perspectives for tuning electrochemical CO2 reduction in terms of activity of critical species (CO2, CO, and H2O). Strategies inspired by these perspectives will be discussed.

A New Member to Electrocatalyst Family.

Xianqin Wang
Chemical and Materials Engineering, New Jersey Institute of Technology, Newark, NJ

A new member, polynitrogen, was synthesized by accelerating the rate-limiting step with the UV irradiation. N8 is found to be more stable and more active than the Pt/C commercial catalyst in DMFCs. A four-electron process at N8 is confirmed with the SHINERS experiments and DFT calculations.

Atomic-Level Insights on Electrocatalytic Decarboxylation of Acetic Acid over Anatase-Supported Pt Clusters.

Alexander von Rueden*, Juan A. Lopez-Ruiz, and Mal Soon Lee*
Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA

Our work reveals the atomic structures that metallic/oxidized Pt clusters and adsorbates adopt on anatase supports. By correlating these structures with our density functional theory-calculated electrocatalytic decarboxylation/oxygen evolution energetics and experimental activities, we provide a fundamental understanding that will help guide the electrocatalytic valorization of biomass-derived molecules.

Effects of Mixed Solvents on CO_2 Electrocatalytic Reduction.

Huy Nguyen *and Matthew Neurock*

Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN

We examine the effects of mixed solvents between water and polar aprotic solvents for CO2 electrochemical reduction over gold electrodes and show reactivity can be tuned using different solvents. This work highlights the importance of solvent effects in controlling the electrochemical reactions, facilitating the design of electrolytes for electrocatalysis.

Electrochemical Stability of Iridium Metal - Effect of Surface Structure.

Maira Amjad[1] *and Ian McCrum*[2]
(1)Material Science and Engineering, Clarkson University, Potsdam, NY, (2)Chemical & Biomolecular Engineering, Clarkson University, Potsdam, NY

The stability of iridium and iridium oxide in the electrochemical environment is influenced by the adsorption of electrolyte species including hydrogen, hydroxide, and oxygen on the surface. Our work builds on prior work quantifying the thermodynamic stability of defect-free iridium for OER electrocatalysis.

Detection of Hydroxylamine Intermediate Opens a New Perspective on Ammonia Selectivity in Metal-Catalyzed Nitrate Reduction.

Janek Betting[1]*, Leon Lefferts*[1]*, and Jimmy A. Faria*[2]
(1)Catalytic Processes and Materials (CPM) - TNW Faculty, University of Twente, Enschede, Netherlands, (2)Catalytic Processes and Materials, MESA+ Institute for Nanotechnology, Faculty of Science and Technology, University of Twente, Enschede, Overijssel, Netherlands

In the catalytic reduction of nitrates and nitrites in drinking water, undesired ammonia formation is the main drawback yet hindering industrial application. Despite that most studies claim nitrites, ammonia, and nitrogen as exclusive products, we additionally found hydroxylamine under typical reaction conditions, which questions the ammonia selectivities reported in literature.

Enhancing Activity and Stability of Pd-on-TiO_2 Single-Atom Catalyst for Low-Temperature CO Oxidation through *in Situ* Local Environment Tailoring.

Yubing Lu[1]*, Fan Lin*[1]*, Coogan Thompson*[2]*, Libor Kovarik*[1]*, John L. Fulton*[1]*, Zdenek Dohnalek*[1]*, Ayman M. Karim*[2]*,* ***Huamin Wang***[1]*, and Yong Wang*[1]
(1)Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA, (2)Department of Chemical Engineering, Virginia Polytechnic Institute and State University, Blacksburg, VA

The development of efficient Pd single-atom catalysts for CO oxidation is hindered by limited reactivity and thermal stability. Here, we report a TiO_2-supported Pd catalyst with enhanced CO oxidation activity and thermal stability, achieved by adjusting the local coordination of Pd atoms through H_2 treatment.

Site-Specific Monomeric Fe Sites Catalyze the N2o Decomposition Reaction.

Daniel Camilo Cano Blanco[1,2]*, Jörg W.A. Fischer*[3]*, Gunnar Jeschke*[3]*, Oliver Kröcher*[1,2]*, and Davide Ferri*[1]
(1)Paul Scherrer Institute, Villigen, Switzerland, (2)EPFL, Lausanne, Switzerland, (3)ETH Zurich, Zurich, Switzerland

Herein, we present an *operando* multi-spectroscopy investigation, complemented by spectroscopic-based kinetic analyses, that unveils mechanistic details of N_2O decomposition over Fe-SSZ-13. We demonstrate the site selectivity of the process, involving the redox of specific Fe ions with the reduction as rate-determining step. These findings advance Fe-zeolite development for after-treatment processes

Aftertreatment System Design for H_2-ICE Using Kinetic Modeling: Promises and Challenges.

Joseph Buttacci*, Keka Mandal, Rajbala Rajbala, Erin Thomson, Manohar Prasad, and Ujjal Das*
Johnson Matthey, Wayne, PA

H_2-ICE is gaining popularity as an alternative to diesel because of carbon free emissions. An aftertreatment system is still required to capture harmful nitrogen oxides. We will highlight the differences between diesel and H_2 emissions and demonstrate the use of kinetic modeling to reduce resources for H_2-ICE system design.

Alloying and Segregation Effects in Palladium-Alloy Catalysts.

Willow Dew[1]*, Sander O. Velle*[1]*, Ingeborg-Helene Svenum*[2]*, and Hilde Venvik*[1]
(1)Chemical Engineering, Norwegian University of Science and Technology, Trondheim, Norway, (2)SINTEF Materials and Nanotechnology, Trondheim, Norway

Supported Pd/Al_2O_3 and $Pd\text{-}Ag/Al_2O_3$ catalysts of varying particle sizes were synthesized and their activity tested in CH_4 oxidation and CO oxidation in comparison with $Pd_{75}Ag_{25}$ (100) and (111) single crystals in order to better understand alloying and segregation effects, using physisorption, chemisorption, X-ray diffraction, X-ray photoelectron spectroscopy, and electron microscopy.

Systematic Studies of Catalyst Structure-Property Relationships in CO_2 Hydrogenation to Methanol.

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

In this work, we demonstrate the influence of various metal coordination environments on catalytic activity and selectivity in CO_2 hydrogenation to methanol, providing insights to guide

the design of tailored catalysts with enhanced performance for utilizing CO_2 as a sustainable carbon feedstock in methanol production.

Determining the Atomistic Structures of Oxy-Carbides and Understanding Their Stability for Oxidative Reactions..

*Tej Choksi[1], **Nurul Farhana Binti Abd Ghaffar**[2], Wen Liu[2], Asmee Prabhu[2], Lavie Rekhi[2], Luan Q. Le[2], and Pieremanuele Canepa[3]*
(1)School of Chemistry, Chemical Engineering and Biotechnology, Nanyang Technological University, Singapore, No State, Singapore, (2)School of Chemistry, Chemical Engineering and Biotechnology, Nanyang Technological University, Singapore, Singapore, (3)Materials Science and Engineering, National University of Singapore, Singapore, Singapore

We develop a physics-based model to determine the most thermodynamically stable oxy-carbide surfaces of VC and TiC across different chemical potential of oxidants (eg: CO_2/CO, H_2O/H_2, and O_2). The model is developed through density functional theory (DFT) calculated co-adsorbate interactions between oxygen atoms on the surface, partitioned into pair-wise interactions.

Automatic Formulation and Exact Solutions to the Master Equation for Multisite Microkinetic Models in Catalysis.

***Jiankai Ge**, Kevin Adams, and Baron Peters*
Chemical and Biomolecular Engineering, University of Illinois at Urbana-Champaign, Urbana, IL

We present master equation microkinetic models (ME-MKMs) that combine the analytic simplicity of mean-field models with the accuracy of kinetic Monte Carlo. ME-MKMs capture adsorbate interactions, surface diffusion, and reaction kinetics, providing accurate rate predictions and parameter estimation capabilities, making them a powerful tool for heterogeneous catalysis studies.

Identification of the Roles of Carbonaceous Species in Pd-Catalyzed Selective Hydrogenation.

*Peng Zhai[1], Divakar Reddy Aireddy[2], Ye Xu[1], and **Kunlun Ding**[1]*
(1)Cain Department of Chemical Engineering, Louisiana State University, Baton Rouge, LA, (2)National Energy Technology Laboratory, Morgantown, WV

In this work, we investigated the roles of carbidic carbon and surface carbonaceous carbon in Pd-catalyzed acetylene hydrogenation. We reveal that the structure of surface carbonaceous species plays a decisive role in hydrogenation selectivity.

Exploring the Role of Oxygen Vacancies in Promoting Electro-Oxidations on NiOOH for Chemical Manufacturing and Water Treatment.

Quy P. Nguyen[1], *Vi Thi Thuy Phan*[2], *Le Thy Thy Ho*[1], *Ian Burgess*[2], *and Bin Wang*[1]
(1)School of Sustainable Chemical, Biological and Materials Engineering, University of Oklahoma, Norman, OK, (2)Department of Chemistry, University of Saskatchewan, Saskatoon, SK, Canada

The fundamental findings reported here is anticipated to comprehend understanding of the mechanistic insights and the structure-activity relationship in electro-catalysis on O/OH-vacant NiOOH, shaping rational guidelines for surface-defect engineering to boost the activity and selectivity for the wide ranges of applications.

CO-Induced Reconstruction of Alumina-Supported Transition Metal Clusters.

Sakshi Satyanand[1], *George Yan*[2], *Dionisios Vlachos*[2], *Stavros Caratzoulas*[2], *Ayman M. Karim*[3], *Raymond Gorte*[4], *and John Vohs*[4]
(1)Chemical and Biomolecular Engineering, University of Delaware, Newark, DE, (2)Delaware Energy Institute, University of Delaware, Newark, DE, (3)Department of Chemical Engineering, Virginia Polytechnic Institute and State University, Blacksburg, VA, (4)Department of Chemical and Biomolecular Engineering, University of Pennsylvania, Philadelphia, PA

We investigate the fundamental question of CO induced restructuring of supported sub-nanometer transition metal clusters on dry and hydroxylated γ-Al_2O_3. We employ *ab initio* simulations to study cluster morphology at cryogenic, room, and high temperatures in different CO coverage.

Towards Understanding Entropic Effects in Multimetallic Catalysts.

Sai Varanasi[1], *Jinwon Oh*[2], *and Matteo Cargnello*[1]
(1)Chemical Engineering, Stanford University, Stanford, CA, (2)Materials Science, Stanford University, Stanford, CA

Fundamentally understanding what specific changes in the geometric and electronic structure make a high entropy alloy active and stable will allow for the ability to efficiently tune catalyst properties. We show a step-by-step approach, investigating the activity of a single metal, bimetallic, trimetallic, tetrametallic, and high entropy alloy pentametallic catalyst.

Leveraging Epitaxial Metal-Support Interface for Structure-Function Relationship Studies in Thermal Catalysis.

Aswathi Rajeevan[1], *Matthew Moegling*[1], *Julia de Barros Dias Moreira*[2], *Libor Kovarik*[2], *Janos Szanyi*[2], *and* ***Linxiao Chen***[1]
(1)Department of Chemical, Biomolecular, and Corrosion Engineering, The University of Akron, Akron, OH, (2)Pacific Northwest National Laboratory, Richland, WA

This work presents a novel epitaxial-growth-based method that allows the rigorous study of particle density effect by isolating it from size and shape effects. Deploying the platform, we demonstrate the effects of multi-particle physisorption of polyolefin chains in hydrogenolysis kinetics.

New Methods for Determining Ad-/Desorption Energies.

Lin Bigom-Eriksen *and* ***Jakob Munkholt Christensen***
Department of Chemical Engineering, Technical University of Denmark, DK-2800 Lyngby, Denmark

We demonstrate new methods for analysis of TPD spectra on the basis of a new adsorption isotherm. We also present new equations for determining both adsorption energies and adsorbate-adsorbate interaction energies on the basis of TPD experiments.

Elucidating Rate Determining Steps in the Presence of Isothermal Multiplicity during Catalytic Oxidation Reactions.

Austin Morales[1], *Jonathan Ratcliff*[1], *Daniel Hodonj*[2], *Patrick Lott*[2], *Olaf Deutschmann*[2], *Michael Harold*[1], *and Praveen Bollini*[1]
(1)William A. Brookshire Department of Chemical and Biomolecular Engineering, University of Houston, Houston, TX, (2)Institute for Chemical Technology and Polymer Chemistry, Karlsruhe Institute of Technology, Karlsruhe, Germany

Recently developed mathematical formalisms for elucidating rate determining steps such as the degree of rate control provide unique insights into the rate governing phenomena behind different branches (solutions) of multivalued rates observed during isothermal methane (CH_4) and carbon monoxide (CO) oxidation over catalyst surfaces.

Understanding Structure Sensitivity and Surface Coverage in the Electrocatalytic Hydrogenation of *Cis,Cis*-Muconic Acid on Palladium.

Deep M. Patel, Prathamesh Prabhu, Jean-Philippe Tessonnier, and ***Luke T. Roling***
Department of Chemical and Biological Engineering, Iowa State University, Ames, IA

The electrocatalytic hydrogenation of *cis,cis*-muconic acid can yield adipic acid from biomass feedstocks. This presentation highlights the importance of Pd terrace sites in enabling adipic acid formation, focusing on fundamentals of surface structure and surface coverage to uncover a tandem mechanism occurring sequentially as outer-sphere and inner-sphere electrochemical processes.

Isotopic Studies of Reaction Pathways within Propylene Epoxidation over Promoted Silver Catalysts.

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

Kinetic and isotopic tracer experiments isolate rate-determining generation of a common oxidant intermediate which readily scrambles with carbon dioxide and initiates either propylene epoxidation or combustion over heavily promoted Ag catalysts. The mechanistic influence of chlorine promotion within propylene epoxidation involves primarily the selectivity-determining step.

Identifying Methanol Adsorbate Geometries on (101)-Faceted Anatase Titania Nanocrystals.

Benjamin Moskowitz[1]*, Carrington Moore*[2]*, Anthony Savoy*[2]*, Mark Engelhard*[1]*, Gregory Collinge*[1]*, Mal Soon Lee*[1]*, Janos Szanyi*[1]*, Feng Gao*[1]*, Simone Raugei*[1,2]*, Jean-Sabin McEwen*[2]*, Huamin Wang*[1,2]*, and Yong Wang*[1,2]
(1)Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA,
(2)The Gene and Linda Voiland School of Chemical Engineering and Bioengineering, Washington State University, Pullman, WA

Understanding the binding of oxygenates to metal oxides at the atomistic level is crucial for efficiently upgrading biomass to fuels and chemicals. We integrate *in situ* diffuse reflectance infrared spectroscopy, density functional theory, and molecular dynamics to reveal the geometries of methanol adsorbates on anatase titania nanocrystals.

Kinetics and Thermodynamics of CO Adsorption Onto Mononuclear Pd Ions Supported on Ceria.

Nicholas Nelson
Catalysis Science, Pacific Northwest National Laboratory, Richland, WA

The variations of CO adsorption kinetics and thermodynamics onto 0.034 wt.% Pd/CeO_2 under different pretreatment conditions reveal structural changes in the coordination sphere of site-isolated metal centers. This provides insight into atom mobility under reaction conditions and can be used to inform rational catalyst design strategies.

Stable CeO_x Nanoglue-Confined Copper Species for CO Oxidation and Water-Gas Shift Reaction.

Ying Zheng *and Jingyue Liu*
Department of Physics, Arizona State University, Tempe, AZ

This work studies the synthesis of atomically dispersed and stable Cu species and how they interact with Ce^{3+}-rich CeO_x nanoislands, peppered onto high-area silica support, to form strongly bound Cu–[O_x]–Ce complexes that act as stable active centers for CO oxidation and water-gas shift reaction.

Molecular-Level Insights into Adsorption and Reaction Sites in Heterogeneous Catalysts from Solid-State NMR.

Zachariah Berkson
Chemical Engineering, Arizona State University, Tempe, AZ

Advanced solid-state NMR techniques provide direct, molecular-level insights into the types, structures, and interactions of surface sites, reaction products, and/or adsorbates in heterogeneous Mo- and W-based olefin metathesis catalysts. In particular, NMR parameters of the transition metal centers (e.g., ^{95}Mo) provide site-specific descriptors for electronic structure and reactivity.

Modeling Solvent Effects on Alcohol Elimination within Zeolite Pores.

Benjamin Jackson[1], *Mal Soon Lee*[1], *Manish Shetty*[1], *Sungmin Kim*[1], *Donald M. Camaioni*[1], *Oliver Gutiérrez-Tinoco*[1], *and Johannes Lercher*[1,2]
(1)Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA, (2)Technical University of Munich, Garching b. München, Germany

The role solvents play in alcohol dehydration and solid-liquid interfaces is poorly understood. Here, cyclohexanol dehydration catalyzed by Brønsted acid sites (BAS) within pores of BEA zeolites is used as a model system to systematically explore the influence of various solvents on the mechanism and rate of dehydration.

SBA-15 Nano Catalysts Evaluated in the Hdo of Phenol As an Oxygen Compound Derived from Bio-Oils.

Luis Jorge Rodriguez Castillo[1], *Franklin J. Méndez*[2], *Jorge García-Macedo*[2], *Lina A. Calzada*[3], *Elim Albiter*[3], *Gabriela Zavala*[4], *Juan A. Alcantara*[4], *Felix Cancino*[4], *Carlos Eduardo Santolalla-Vargas*[4], *and Victor Florencio Santes Hernandez*[4]
(1)Energia, Unidad Profesional Interdisciplinaria en Ingeniería y Tecnologías Avanzadas UPIITA-IPN Avenida Instituto Politécnico Nacional No. 2580, Col. Barrio la Laguna Ticomán, Gustavo A. Madero, Ciudad de México, C.P. 07340., Mexico City, DF, Mexico, (2)Departamento de Estado Sólido, Instituto de Física, Departamento de Estado Sólido, Instituto de Física, Universidad Nacional Autónoma de México, Ciudad Universitaria 04510, Ciudad de México, México., Mexico City, DF, Mexico, (3)Catalisis y Materiales, Laboratorio de Catálisis y Materiales. Instituto Politécnico Nacional-ESIQIE. Zacatenco, C. P. 07738, Ciudad de México, México., Mexico, DF, Mexico, (4)Biociencias e Ingenieria, Departamento de Biociencias e Ingeniería, Centro Interdisciplinario de Investigaciones y Estudios sobre Medio Ambiente y Desarrollo, CIIEMAD-IPN, Instituto Politécnico Nacional, Gustavo A. Madero 07340, Ciudad de México, México., Mexico City, DF, Mexico

This work proposes the synthesis, evaluation and characterization of HDO catalysts. For this, the synthesis of NiMo materials over a SBA15-Gallium supports using the hydrothermal method is described to analyze its catalytic activity and selectivity in the HDO reaction of phenol in order to improve the quality of synthetic biofuels.

Activation of Carbon Monoxide CO in H-Mor Zeolite Via Protonation.

Ja Hun Kwak[1], *Hristiyan A. Aleksandrov*[2], *Nicholas Jaegers*[3], *Georgi Vayssilov*[2], *Janos Szanyi*[4], *and* ***Konstantin Khivantsev***[5]
(1)Ulsan National Institute of Science and Technology, Ulsan, Korea, Republic of (South), (2)Faculty of Chemistry, University of Sofia, 1126 Sofia, Bulgaria, (3)University of California at Berkeley, Berkeley, CA, (4)Pacific Northwest National Laboratory, Richland, WA, (5)Physical and Computational Sciences Directorate and Institute for Integrated Catalysis, Pacific Northwest National Laboratory, Richland, WA

Our study provides insights into reactivity of zeolitic protons. CO forms protonated HCO^+ species, which opens up a new chapter in understanding zeolites and their reactivity.

Adsorption of Azo Dyes Using ZnO/SiO_2 hybrid Aerogels and Xerogels.

Al-Zahraa Fatima El Cheikh[1], *Houssam El-Rassy*[2], *Mohammad Ahmad*[3], *and Witold Kwapinski*[4]
(1)1Department of Chemical and Environmental Science, university of limerick, Limerick, Ireland, (2)Department of Chemistry, American University of Beirut, Beirut, Lebanon, (3)B & W Basstne Department of Chemical Engineering and Advanced Energy, American University of Beirut, Beirut, Lebanon, (4)University of Limerick, Limerick, Ireland

Nano-ZnO/SiO_2 aerogels and xerogels were synthesized via sol-gel co-gelation of zinc and silica precursors. Characterization confirmed nanoporous ZnO crystals dispersed in a 3D silica matrix. The composites adsorbed Congo Red dye (Q_m is up to 100 mg/g), with adsorption following Freundlich and Langmuir isotherms. They exhibited reusability over five cycles.

Tailoring Morphology and Surface Properties of Microporous Carbon Catalysts Derived from Metal-Organic Frameworks.

Akihiro Okada[1], *Shintaro Takeda*[1], *Shin R. Mukai*[2], *and* ***Isao Ogino***[2]
(1)Graduate School of Chemical Sciences and Engineering, Hokkaido University, Sapporo, Japan, (2)Faculty of Engineering, Hokkaido University, Sapporo, Japan

Metal-organic framework materials (MOFs) are promising precursors for synthesizing supported metal electrocatalysts. Using two different types of ZIFs, a sub-class of MOFs, with similar building units but different morphologies, we demonstrate how particle size and shape influence the catalytic properties of the corresponding carbon-based catalysts in the oxygen reduction reaction.

How Local Order Leads to Shape-Selectivity in Disordered Materials: FAU-FER Interzeolite Transformation Intermediates and Its Exceptional Catalytic Properties.

Julia de Souza[1], *Alexandre Young*[2], *Pedro Romano*[3], *Javier García-Martínez*[4], *and João Monnerat*[5]
(1)LIPCAT, Rio de Janeiro, Brazil, (2)LIPCAT (UFRJ), Rio de Janeiro, Rio de Janeiro, Brazil,

(3)Campus D. de Caxias, Federal University of Rio de Janeiro, Rio de Janeiro, Brazil, (4)Molecular Nanotechnology Lab, Department of Inorganic Chemistry, University of Alicante, Alicante, Spain, (5)Chemistry Institute, Federal University of Rio de Janeiro, Rio de Janeiro, Rio de Janeiro, Brazil

This study explores the innovative development of Interzeolite Transformation Intermediates (ITIs) during FAU-to-FER transitions. These hybrid materials combine high mesoporosity with remarkable shape selectivity, enhancing accessibility for bulky reactants. A standout ITI demonstrated tenfold catalytic activity improvements and exceptional stability, revolutionizing applications in energy transition and complex molecule synthesis.

Tuning Zeolite Catalysts Using Organic Additives: Molecular Modelling Studies.

***Matthew Robinson** and Andrew Logsdail*
School of Chemistry, Cardiff University, Cardiff, United Kingdom

Pyridine-based additives can tune the selectivity of the mordenite-catalysed ethanol dehydration reaction, a potential green route from bio-ethanol to ethylene (a highly-demanded chemical feedstock). The additive can also be decorated with other functional groups to further enhance/diminish its adsorptive behaviour and open up wider applications.

Structure-Property Evolution of Metal-Organic Frameworks (MOFs)-Derived Catalysts.

***Bibesh Gauli**[1], Swarit Dwivedi[2], Akshat Tanksale[1], and Alan Chaffee[3]*
(1)Chemical Engineering, Monash University, Clayton, VIC, Australia, (2)Chemical and Biological Engineering, Monash University, Clayton, VIC, Australia, (3)Chemistry, Monash University, Clayton, VIC, Australia

This work aims to study the thermal decomposition mechanisms and understand the structure-activity evolution of ZIF-8-derived catalysts for CO_2 hydrogenation to methanol. The metal-support interactions in these catalysts will be finetuned by adjusting the pyrolysis temperature and environment to enhance catalytic activity.

An Accelerated Approach Towards Predicting Coverage-Dependent Surface Free Energies on Transition Metal Surfaces.

*Asmee Prabhu and **Tej Choksi***
School of Chemistry, Chemical Engineering and Biotechnology, Nanyang Technological University, Singapore, Singapore

Ab initio phase diagrams have a pivotal role in identifying thermodynamically stable surfaces. Yet, exploring the configurational space of adsorbates on surfaces to construct phase diagrams is computationally intractable using density functional theory. We present a physics-based pre-trained model that builds ab initio phase diagrams on-the-fly, for promoter-decorated (hkl) surfaces.

Exploring the Use of Global Optimization and Universal Potentials – CO Oxidation over Pd-Based Alloys.

Tor S. Haugland[1] *and* ***Ingeborg-Helene Svenum***[1,2]
(1)Sintef Industry, Trondheim, Norway, (2)Department of Chemical Engineering, NTNU, Trondheim, Norway

The segregation behavior of Pd-based alloy surfaces under conditions relevant for CO oxidation have been studied using machine-learning potentials together with global optimization methods, which enables a fast and systematic sampling of the surface composition depending on coverage.

The Ratings Concept As a Combined First-Principles and Microkinetic Modeling Tool for an on-Line Optimization of Integrated Carbon Capture and Conversion.

Supareak Praserthdam *and Piyasan Praserthdam*
Chemical Engineering, Chulalongkorn University, Bangkok, -, Thailand

The Ratings concept, based on Density Functional Theory, enhances the efficiency of the Integrated Carbon Capture and Conversion process. It follows a two-step approach: identifying catalysts using reactivity (RT-R) and stability (RT-S) ratings and optimizing performance through on-line adjustments. Sensitivity analysis shows temperature has a greater impact than feed ratio.

Variable Reaction Coordinate Transition State Theory for Computing Rate Constants for Barrierless Desorption.

Youbin Kim[1] *and C Franklin Goldsmith*[2]
(1)Brown University, Providence, RI, (2)School of Engineering, Brown University, Providence, RI

Variational Transition State Theory (VTST), an extension of Transition State Theory, addresses its limitations in predicting reaction rates, particularly for gas-phase molecular dissociation. This study focuses on Variable Reaction Coordinate TST (VRC-TST), highlighting its strengths in evaluating multi-dimensional partition functions for gas-phase and gas-surface reactions.

Novel Algorithms for Efficient Exploration of Potential Energy Surfaces.

Sandra Liz Simon*, Nitin Kaistha, and* ***Vishal Agarwal***
Department of Chemical Engineering, Indian Institute of Technology Kanpur, Kanpur, India

Efficient exploration of potential energy surfaces and discovery of minimum energy paths and transition states are key to understanding chemical reaction mechanisms. However, the high computational cost of quantum mechanical calculations poses a challenge. This work introduces two novel algorithms to reduce this cost and accelerate transition state discovery.

Na-Y Zeolite Water Interaction: A Multimodal Analysis Using Gcmc, Machine Learning Potentials and *Operando* X-Ray Diffraction.

Agnieszka Seremak[1], *Ruben Goeminne*[2], *Izar Capel Berdiell*[1], *Lars Lundegaard*[3], *Pablo Beato*[3], *Veronique Van Speybroeck*[2], *and Stian Svelle*[1]
(1)Department of Chemistry, University of Oslo, Oslo, Oslo, Norway, (2)Ghent University, Ghent, Belgium, (3)Haldor Topsøe A/S, Kgs. Lyngby, Denmark

The study used GCMC and MLP-MD methods to analyze cation distribution and framework dynamics in zeolite Na-Y during dehydration. Results showed framework contraction upon water removal and expansion due to cation migration. Findings matched XRD data, highlighting the approach's accuracy and the need for advanced methods in complex system studies.

Graph Based Grand Canonical Basin Hopping: A Case Study for Global Optimization for Amorphous Oxides and Metal Clusters.

Kaustubh Sawant *and Philippe Sautet*
Chemical and Biomolecular Engineering, University of California, Los Angeles, Los Angeles, CA

Global optimization of periodic atomistic models using DFT/ML methods is challenging, particularly for complex amorphous materials. We developed an open-source Python package that employs graph-based grand canonical basin hopping, featuring a standardized library of structural moves for basin hopping and integration with common modeling codes.

Multi-Scale Modelling of MOF-Derived Catalysts.

Swarit Dwivedi[1], *Rajan Lakshman*[1], *Adri C.T van Duin*[2], *Alan Chaffee*[3], *and* ***Akshat Tanksale***[1]
(1)Chemical and Biological Engineering, Monash University, Clayton, VIC, Australia, (2)Chemical Engineering, The Pennsylvania State University, University Park, PA, (3)Chemistry, Monash University, Clayton, VIC, Australia

We report a multi-scale atomistic simulation methodology to simulate the chemical transformation in MOFs under high temperatures. We report the formation of MOF-derived porous carbon catalysts, including metal-embedded carbonaceous matrix and single/dual-atom catalysts. We report the key descriptors of parent MOF morphologies that govern the structure of MOF-derived materials.

Modeling Interfacial Hydrogen Atom Transfer Kinetics Using a Nonadiabatic Proton-Coupled Electron Transfer Framework.

Noah South[1] *and Robert Warburton*[2]
(1)Chemical and Biomolecular Engineering, Case Western Reserve University, Cleveland, OH, (2)Department of Chemical and Biomolecular Engineering, Case Western Reserve University, Cleveland, OH

This work uses methane decomposition to develop and apply general computational techniques that model kinetics of interfacial hydrogen atom tunneling. Preliminary results indicate that nonadiabatic proton-coupled electron transfer theory best describes the kinetics and supports the assertion that hydrogen atom tunneling is prevalent in thermal catalysis.

Geometrical Restraints for Enhanced Sampling Simulations in Heterogeneous Catalysis.

Gustavo Perez Lemus, *Yinan Xu, Yezhi Jin, Pablo Zubieta, and Juan J. de Pablo*
Pritzker School of Molecular Engineering, University of Chicago, Chicago, IL

By integrating geometric restraints into enhanced ABF methods in PySAGES and leveraging ML-based potentials, we improve convergence and accuracy of free energy calculations for methane activation on Ni surfaces. Overly tight constraints reduce entropic contributions, while selective minimal constraints maintain accuracy and match known free energy results.

Constant Potential Molecular Dynamics for Electrocatalytic Interface.

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

Electrochemical interface is a complex system with a number of factors that are challenging to model at atomic level, such as solvation, surface charge, and their couplings and dynamics. I will present our efforts to solve these problems by developing “constant potential + hybrid solvation + dynamic model” (CP+HS+DM).

Effect of Electric Potential on Electrochemical CO_2 Reduction at Ag(111)-H_2o Interface.

Xiongwei Tian[1,2], *Axel Tosello Gardini*[1], *Umberto Raucci*[1], *Hai Xiao*[2], *Yuqun Zhuo*[2], *and Michele Parrinello*[1]
(1)Italian Institute of Technology, Genova, Italy, (2)Tsinghua University, Beijing, China

Using neural network molecular dynamics and enhanced sampling techniques, we reveal how the applied constant potential conditions uniquely influence interfacial water dynamics and CO_2 electro-reduction process, offering deeper insights into the effect of electric potential on electrocatalytic mechanisms which is crucial for future reaction optimization.

Synthesis–Structure–Function Relationships of Oxide-Supported Ruthenium Catalysts for Ammonia Reforming.

Gabrielle A. Kliegle[1], *Jacob Miller*[1], *Kathleen D. Brown*[1], *Alexander J. Hill*[1], *Matthew M. Yung*[1], *and Nicholas Thornburg*[2]
(1)Catalytic Carbon Transformation and Scaleup Center, National Renewable Energy Laboratory, Golden, CO, (2)Center for Energy Conversion & Storage Systems, National Renewable Energy Laboratory, Golden, CO

In this work, we synthesize ruthenium catalysts to investigate the effects of metal oxide support identity and alkali promotion, uncovering descriptors of ammonia reforming fixed-bed kinetics. These findings enable an alternative hydrogen production pathway by elucidating synthesis–structure–function relationships that inform on rational catalyst design for ammonia decomposition.

Non-Thermal Plasma Ammonia Synthesis over Porous Silica.

Vashanti Storr[1] *and Maria L. Carreon*[2]
(1)Chemical Engineering, University of Arkansas, Fayettevile, AR, (2)Chemical Engineering, University of Arkansas, Fayetteville, AR

This work investigates earth-abundant silica materials with tailored porosity and morphology, including mesoporous and macroporous structures like spheres and gyroids, to elucidate ammonia synthesis pathways under non-thermal plasma. By optimizing textural properties, this study enhances the development of efficient catalysts for sustainable, decentralized ammonia production, particularly suited for remote regions.

Two-Step Transient Catalytic System for NO_x-to-Ammonia.

Masaru Ogura, *You Hatanaka, and Takeshi Ohnishi*
Institute of Industrial Science, The University of Tokyo, Tokyo, Japan

We develop a new technology “reNOx” to recover NOx as a resource of ammonia. NOx enrichment is attained by use of selective NOx adsorbent from combustion exhaust as the first stage of the process, followed by the reNOx process by hydrogen to obtain almost pure ammonia.

Ammonia Cracking for Hydrogen Production – Effect of Promoters on Non-Noble Metal Catalysts.

Ljubiša Gavrilovic, *Jean-Patrick Pinheiro, Saima Sultana Kazi, and Julien Meyer*
Institute for Energy Technology, Kjeller, Oslo, Norway

Series of Ni and Co based catalysts were synthesized using wet impregnation. The catalysts were characterized using H_2 chemisorption, XRD, TPR and BET/BJH. The effect Ce (1-5wt%) promotion on Ni activity, and Mo (1-5wt%) on Co activity were studied. Ammonia cracking was investigated at different temperatures (400-800 °C) and GHSVs.

Promoting Ru Electron Density By Basic Hydroxyapatite Supports for H_2 Storage As NH_3 Under Mild Conditions.

Sabrina Akrour[1], *Alexandre Vimont*[2], *Sandra Casale*[1], *Guylène Costentin*[1], *and* ***Cyril Thomas***[1]
(1)Sorbonne Université, Laboratoire de Réactivité de Surface, Paris, France, (2)Normandie Université, Laboratoire Catalyse et Spectrochimie, Caen, France

These results not only highlight the potential of modified HAps as supports for Ru in NH_3 synthesis, but also provide a clear proof of concept of the critical role of the basic properties of the support on the electronic density of the Ru particles and on the activation of N_2.

Ternary Hydride Catalysts for Low Temperature Ammonia Synthesis.

Selin Ernam, *Anastasiia Karabanova, Xiufu Sun, and Peter Vang Hendriksen*
Energy Conversion and Storage, Technical University of Denmark, Lyngby, Denmark

This study focuses on hydride-based catalysts for low temperature nitrogen activation for ammonia synthesis. We report the catalytic activity and stability of Li_4RuH_6, and a novel quaternary hydride.

Co/Fe Ratio Effect on the Stability of $LaSrCoFeO_3$ Perovskites for Ammonia-Fueled Solid Oxide Fuel Cells.

Alicia San Martin Rueda[1], *Faranak Foroughi*[2], *Ingeborg-Helene Svenum*[1,3], *David Waller*[2], *and Magnus Rønning*[1]
(1)Department of Chemical Engineering, NTNU, Trondheim, Norway, (2)Yara Technology Center, Porsgrunn, Norway, (3)SINTEF Materials and Nanotechnology, Trondheim, Norway

Ammonia-fueled SOFCs have been claimed as an efficient alternative for single-step chemical energy conversion to electricity. Materials with long-term stability are required for this application. LSCF perovskites are viable catalysts for both anode and cathode. Studying these materials can lead to the optimization of suitable catalysts for such purposes.

Economically Competitive Production of Oleo-Furan Sulfonate Detergents from Furfural and Fatty Alcohols.

Truc Phung[1], *Nicholas L. Gadinas*[2], *Kyle B. Reem*[2], *Emily Pond*[2], *and Konstantinos Goulas*[3]
(1)School of Chemical, Biological and Environmental Engineering, Oregon State University, Corvallis, OR, (2)Oregon State University, CORVALLIS, OR, (3)Oregon State University, Corvallis, OR

Oleo-furan sulfonates are advanced detergents derived from fatty acids and furanic derivatives, offering superior properties over petrochemical-based alternatives. Traditional production via furan acylation with fatty acid anhydrides is thermodynamically limited. We propose an alternative pathway using dehydrogenative aldol condensation of fatty alcohols with furfural, coupled with transfer hydrodeoxygenation using isopropanol.

Modified ZIF-67 for CO_2 Capture and Valorization through Cycloaddition: FT-IR ‘Operando’ Studies.

David Villalgordo Hernández[1], *Andrea Jouve*[2], *Silvia Bordiga*[2], *Enrique V. Ramos Fernandez*[1], *and Javier Narciso*[1]

(1)University of Alicante, Alicante, Spain, (2)Department of Chemistry, University of Turin, Turin, Turin, Italy

ZIF-67 affinity towards CO_2 was greatly enhanced through exchanging up to 60% of its ligand with 1,2,4-Triazole without altering its structure. An FT-IR in-depth study has been carried out to better understand this process' coordinating impact. CO_2 cycloaddition reaction was followed in 'operando' conditions to test the reaction's mechanism.

Synthesis of ZIF-8 on Brass Monoliths Prepared By 3D Selective Laser Melting for CO_2 Conversion.

***Leidy Patricia Figueroa Quintero**, Javier Narciso, and Enrique V. Ramos Fernandez*
University Institute of Materials (IUMA), Inorganic Chemistry Department, University of Alicante, Alicante, Spain

This work reports the integration of ZIF-8 into brass monoliths fabricated by 3D-SLM, managing to combine advanced catalytic properties with high mechanical strength. The synthesized materials achieved 90% conversion in CO_2 cycloaddition, underlining their impact as a sustainable and efficient solution for CO_2 capture and valorization.

Na-Promoted Bimetallic Hydroxide Nanoparticles for Aerobic C-H Activation: Catalyst Design Principles and Insights into Reaction Mechanism.

*Beyzanur Erdivan, Eylul Calikyilmaz, Yunus Emre Turkmen, and **Emrah Ozensoy***
Chemistry, Bilkent University, Ankara, Turkey

Na-promoted bimetallic $Fe_xMn_{1-x}(OH)_y$ hydroxides capable of catalyzing aerobic C–H (alkylarene) oxidation reactions at low temperatures were developed, without the need for an initiator. Through a systematic synthetic effort, we scanned a wide nanoparticle synthesis parameter space to lay out a detailed set of catalyst design principles.

Continuous Injection Isothermal Titration Calorimetry for the Determination of Adsorption Kinetics at Solid-Liquid Interfaces.

***Jeong Hwan Lee**[1], Sophia Minadaki[2], Ran Wang[1], Antonios Armaou[1], and Robert Rioux[3,4]*
(1)Chemical Engineering, The Pennsylvania State University, University Park, PA, (2)Chemical Engineering, University of Patras, Patras, Greece, (3)Department of Chemistry, The Pennsylvania State University, University Park, PA, (4)Department of Chemical Engineering, The Pennsylvania State University, University Park, PA

Continuous injection isothermal titration calorimetry (CI-ITC) was developed to determine the kinetic parameters for adsorption processes at the solid-liquid interface. We demonstrated complete characterization of the kinetics and thermodynamics of thiol adsorption to Au nanoparticles. CI-ITC is a novel approach to characterize solid-liquid interfacial kinetics, relevant to heterogeneous catalysis.

Exploring the Growth Kinetics of Carbon Nanotubes Using Transient Pressure Pulsing.

Audrey Dannar[1]*, Jack Peden*[2]*, Adam Boies*[2,3]*, and Christian Reece*[1]
(1)Rowland Institute at Harvard, Harvard University, Cambridge, MA, (2)Cambridge University, Cambridge, United Kingdom, (3)Stanford University, Stanford, CA

Upconversion of hydrocarbons to carbon nanotubes (CNTs) is a promising method of generating CO-free H_2 on the industrial scale. High-quality CNTs could offset the cost of H_2, but fundamental insight is needed to control growth. We utilize *in-situ* kinetic measurements of C_2 gas decomposition to reveal competing CNT growth mechanisms.

Aqueous Phase Reforming (APR) of Glycerol over Platinum Supported on Al_2O_3 Catalyst.

Lioudmila Nossova and ***Gianni Caravaggio***
CanmetENERGY-Ottawa, Natural Resources Canada (NRCan), Ottawa, ON, Canada

The glycerol's APR reaction over 5 wt% Pt/Al_2O_3 catalyst for H_2 production in a batch reactor is investigated in the present work. The effect of the operating parameters (reaction time, temperature, glycerol and catalyst concentration) on the H_2 productivity and selectivity was investigated.

Modification of Metal–Organic Framework: ZIF-8 By Ligand Exchange for the Adsorption and Removal of Mercury.

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

The urgent need to remove mercury from wastewater drives the search for new materials. Sulfur-modified ZIF-8 shows great potential as an adsorbent. This study develops six innovative materials, with Int.Z1.1-1 emerging as the most effective, exhibiting optimal structural and chemical properties for environmental water remediation applications.

Selective Hydrogenation of Furfural on Ptsn Alloy Surfaces.

Mengxiong Qiao[1]*, Wenrui Chai*[2]*, Sharfa Farzandh*[3]*, Sumit Beniwal*[3]*, Fangliang Li*[3]*, Graeme Henkelman*[2]*, and Donna Chen*[4]
(1)Chemistry and biochemistry, University of South Carolina, Columbia, SC, (2)Department of Chemistry and Biochemistry, University of Texas at Austin, Austin, TX, (3)Chemistry and Biochemistry, University of South Carolina, Columbia, SC, (4)Chemistry, University of South Carolina, Coulmbia, SC

Selective hydrogenation of furfural to furfuryl alcohol on PtSn catalysts was investigated by combination of experimental studies on single-crystal surfaces and density functional theory calculations. The ordered Pt_3Sn catalyst has high activity and selectivity to furfuryl alcohol compared with Pt(111), as well as other alloy surfaces with different Sn compositions.

Atomically Precise $Cu_{14}H_1$ Nanoclusters for Electrocatalytic CO_2 Reduction.

Manju Maman[1], *Anik Sarkar*[1], *Beenish Bashir*[2], *John Bacsa*[3], *Zhenming Du*[1], *Guoxiang (Emma) Hu*[2], *Gangli Wang*[1], *and Xuefei Li*[1]
(1)Department of Chemistry, georgia state university, Atlanta, GA, (2)school of chemistry and biochemistry, georgia institute of technology, Atlanta, GA, (3)Department of Chemistry, Emory University, Atlanta, GA

We synthesized atomically precise $Cu_{14}H_1$ nanoclusters and evaluated their performance for electrochemical CO_2 reduction. The clusters exhibit high selectivity over the hydrogen evolution reaction, with preliminary gas chromatography indicating hydrocarbon formation. This study provides fundamental insight into active site structure and supports the design of selective catalysts for CO_2 conversion.

Micro-Scale Reactor Systems for Investigating Biomass/Biooil Upgrading.

Tricia Marchese[1], ***Erica Razook***[1], *Marco Castaldi*[1], *and Lucas Dorazio*[2]
(1)Chemical Engineering, The City College of New York, New York, NY, (2)BASF, Iselin, NJ

The poster summarizes development of a micro-scale lab reactor for testing high concentrations (50% up to 100 wt%) of biooil in gasoil mixtures. The reactor enables evaluation of catalyst performance in impacting coke formation, and addresses limitations of traditional methods in advancing biomass upgrading for renewable fuel production.

Two-Dimensional (2D) Mxene Supported Ruthenium Catalysts for Plastic Waste Hydrogenolysis: Mass Transport Versus Confinement in Interlayer Spacing.

Ali Kamali *and Dongxia Liu*
Department of Chemical and Biomolecular Engineering, University of Delaware, Newark, DE

Two-dimensional MXene supports confine Ru nanoparticles, enhancing accessibility and mass transport for hydrogenolysis of polyethylene into valuable liquid fuels. It further suppresses methane formation, and elevates liquid selectivity, illustrating MXene's promise for efficient, selective thermochemical upcycling of plastic waste.

Thermal Stability Study of Rh Single Atom Catalyst on Titanate Perovskites and TiO_2 thin Films, Al_2O_3 and $MgAl_2O_4$.

Zhanyuan Liu, *Raymond Gorte, and John Vohs*
Department of Chemical and Biomolecular Engineering, University of Pennsylvania, Philadelphia, PA

CO-DRIFTS was employed to investigate the dynamics of the deposited Rh single atoms at temperatures up to 500°C under reducing conditions. This study demonstrated a large variation in the thermal stability of the Rh single atoms on the various supports, which were ranked as: $Al_2O_3>MgAl_2O_4>TiO_2/Al_2O_3>SrTiO_3/MgAl_2O_4>CaTiO_3/Al_2O_3$.

Robust, Thermally Stable and Versatile Single Atom Catalysts Based on Earth Abundant Materials.

Brandon Burnside[1]*, Juliana Bertoldi*[1]*, Ryan Alcala*[1]*, Jesse Larence*[2]*, Shan Jiang*[3]*, Wei Ling Huang*[3]*, Geunho Han*[4]*, Andrew T. DeLaRiva*[5]*, Hien N. Pham*[5]*, Abhaya K. Datye*[1]*, Justin M. Notestein*[4]*, Jeffrey T. Miller*[3]*, and Hua Guo*[6]
(1)Department of Chemical & Biological Engineering and Center for Micro-Engineered Materials, University of New Mexico, Albuquerque, NM, (2)University of New Mexico, Albuquerque, NM, (3)Davidson School of Chemical Engineering, Purdue University, West Lafayette, IN, (4)Department of Chemical & Biological Engineering, Northwestern University, Evanston, IL, (5)Department of Chemical and Biological Engineering and Center for Micro-Engineered Materials, University of New Mexico, Albuquerque, NM, (6)Department of Chemistry, University of New Mexico, Albuquerque, NM

We developed a robust thermally stable single atom catalyst based on earth abundant materials. We show a nickel single atom catalyst that is capable of performing both oxidation and hydrogenation mechanism without needing pretreatment to alter the active site. While also showing excellent selectivity in all tested reactions.

Understanding pH Effects and Intrinsic Reaction Kinetics in Electrocatalysis: The Reference Potential Scale Matters.

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

Understanding the intrinsic kinetics of electrocatalytic processes is essential to develop electrified interfaces with high efficiency and selectivity for energy conversion. Here, we highlight the importance of the potential reference – absolute vs. pH dependent scale in interpreting intrinsic reaction kinetics and mechanisms of multistep electrocatalytic processes.

First Principles Insights into Effect of Charge Condensation on Water Gas Shift Reaction Mechanism.

Venkata Rohit Punyapu[1] *and Rachel Getman*[2]
(1)Chemical and Biomolecular Engineering, The Ohio State University, Columbus, OH, (2)Department of Chemical and Biomolecular Engineering, The Ohio State University, Columbus, OH

We show that surface charge condensation can significantly alter Water Gas Shift reaction energetics on Pt catalysts. Positive charge strengthens intermediate binding and shifts reaction barriers, offering a new strategy for tuning catalytic activity through charge manipulation combined with microkinetic modeling.

Rational Design of Interface-Controlled Materials: Bridging Structure-Property Relationships in Heterogeneous Catalysis.

Jiaqi Yu
Department of Chemistry, Northwestern University, Evanston, IL

In heterogeneous catalysis, catalysts are fundamentally connected with reaction kinetics and thermodynamics. While researchers traditionally leverage this relationship to develop catalysts based on reaction principles, our approach reverses this paradigm by designing materials to unveil deeper mechanistic insights. This poster will present our efforts in this direction.

Comparing Constructions of Supported Nanoparticlesvia Machine Learning Interatomic Potentials.

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Idealized constructions common to nanoparticle analysis are evaluated and we find that all fail relative to direct optimization. This work using MLIPs indicates that researchers must exercise a high level of caution when applying idealized construction to catalytic descriptors for supported nanoparticles when an atomistic model has not been optimized.

Lithium Silicates for Isothermal Sorption-Enhanced Steam Methane Reforming (SE-SMR).

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A novel surfactant-mediated synthesis of lithium orthosilicate which isothermally and reversibly absorbs CO2 at 600 - 650° C has been evaluated in packed-bed reactor studies for sorption-enhanced steam-methane reforming (SE-SMR) show 25 - 30% increase above equilibrium in H_2 production

Seeing Catalysis Dynamics Live at the Atomic Scale: New *in Situ* Transmission Electron Microscopy Workflows Under Reactive Gas Environments.

Lee Casalena
Thermo Fisher Scientific, Portland, OR

Recent advances in environmental TEM enable real-time atomic-scale imaging and spectroscopy under reactive gas environments. New workflows integrate high-stability optics, in situ EELS, pulsed beams, and damage mitigation strategies, allowing researchers to observe dynamic structural and chemical changes in catalysts under near-operando conditions.

Influence of Organocations on the Kinetics and Mechanism of Electrocatalytic Hydrogen Evolution in Alkaline Media.

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Organocations strongly influence alkaline HER rates, yet the mechanistic basis for this effect remains unclear. This study combines mechanism-derived rate expressions with the coverage-dependence of Tafel slopes to discriminate among candidate HER mechanisms, revealing that organocations decrease the rate of the kinetically relevant step without changing the overall HER mechanism.

Scalable Transformation of Pyrolysis Oil into Biographite Anode for Lithium-Ion Batteries.

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This study explored five different pathways to address iron-induced foaming in pyrolysis oil. Following the optimal pathway, the pyrolysis oil was catalytically converted into biographite anode for lithium-ion battery application.

Elucidating Molybdenum Trioxide (MoO_3) Deactivation during the Ambient Pressure Hydrogenation of Lignin-Derived MODEL Compounds.

Mahmudul Khan *and Brent H. Shanks*
Department of Chemical and Biological Engineering, Iowa State University, Ames, IA

Understanding the deactivation of molybdenum trioxide under reaction conditions is crucial for the rational catalyst design for biomass processing. We show that the deactivation kinetics of lignin-derived molecules are oxygenate-dependent, and the catalyst does not remain universally stable, even after the formation of a stable oxycarbohydride phase, limiting pretreatment potential.

Synthesis and Characterization of Pt Single-Atom and Clusters on Transition Metal Carbide Catalyst Supports.

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Transition metal carbides (TMCs) exhibit strong metal-support interaction that is crucial for the long-term stability of Pt single-atom catalysts (SACs). DFT calculations comparing Pt SACs supported on various TMCs were verified experimentally using a case study of Pt/HfC. The results provide guidance on selecting stable Pt SACs supported by TMCs.

Breaking the C-X Bond: A Kinetic Analysis of the Room Temperature Dehalogenation of Halobenzenes Catalyzed By Rh/Al_2O_3.

Olivia De Luca[1], *Lauren Babb*[2], *Maria Blankemeyer*[2], *Charlotte Suh*[2], *Chloe Deitz*[2], *Christian Geci*[3], *Brian Frederick*[3], *Thomas Schwartz*[4], *and Rachel Austin*[2]
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This study examines Rh/Al_2O_3-catalyzed hydrogenolysis of halobenzenes, showing that reaction rates depend on C–X bond strength when Rh is in its metallic form. These findings clarify the catalytic mechanism of C-X bond breakage and inform the design of efficient, earth-abundant metal catalysts for remediating persistent halogenated environmental pollutants.

Effect of Plasma Power on Intermediate Species and Reaction Temperature in the Presence and Absence of Catalysts for Dry Reforming of Methane Application.

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

This study investigates the impact of plasma power on reactor temperature and catalytic reaction pathway in dry methane reforming (DRM). Plasma-induced temperature rise enhances catalytic activity when the catalyst exceeds its thermal activation threshold. The research demonstrates how plasma power influences product distribution, activating new reaction pathways at higher temperatures.

Exploring Catalyst Compositions for Microwave-Assisted Methane Dehydroaromatization.

Biswanath Dutta[1], *Swarom Kanitkar*[1], *Duy Hien Mai*[1], *Evgeniy Myshakin*[1], *and* ***Daniel Haynes***[2]
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Flaring natural gas wastes resources and increases CO_2 emissions. Microwave-assisted methane dehydro-aromatization (MDA) offers a sustainable alternative, converting methane into valuable chemicals. This study enhances CH_4 conversion and selectivity toward aromatics, minimizing coke formation by modifying synthesis methods and incorporating catalytic promoters.