NAM28

# 28th

# North American Catalysis Society Meeting

Providence, RI · June 18–23, 2023

NAM28

The 28th North American Catalysis Society Meeting

June 18 – 23, 2023 ■ Providence, Rhode Island

Greetings!

As Co-Chairs, we welcome you at the 28th North American Meeting of the North American Catalysis Society – NAM28 – to be held at the OMNI Hotel, Providence, RI, USA on June 18-23, 2023. The North American Catalysis Society Meeting is one of the premier scientific events in the field of catalysis. It is a forum for the discussion of relevant technological issues and state of the art research.

The meeting will focus on technological challenges, breakthrough discoveries and state-of-the-art industrial research in catalysis.

Additional information regarding the 28th North American Meeting is available on the North American Catalysis Society Meeting's website: http://www.nam28.org/.

Christopher Landry Steven L. Suib

Scott M. Auerback
Co-Chair
28th North American Catalysis
Society Meeting

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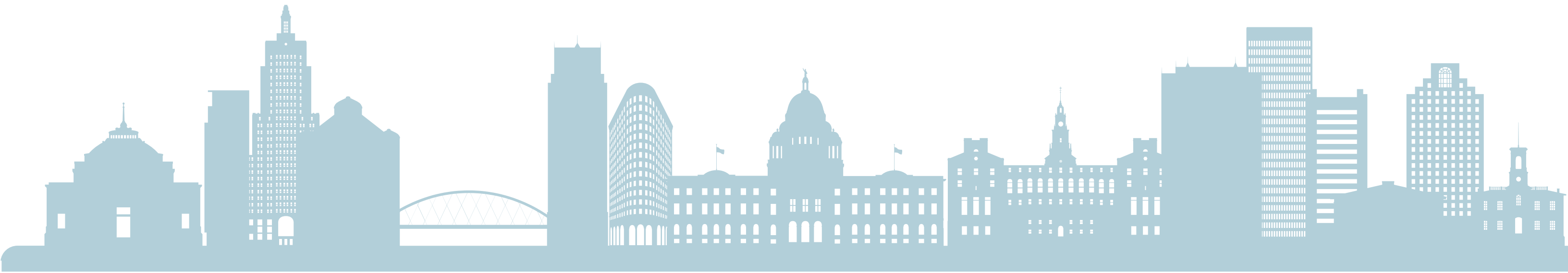

# NAM28 Co-chairs

### Scott M. Auerbach

Professor of Chemistry and Chemical Engineering
Mahoney Family Sponsored Executive Director, UMass iCons Program
University of Massachusetts, Amherst, MA

Scott Auerbach earned a BS in Chemistry from Georgetown in 1988 and a PhD in theoretical chemistry from UC Berkeley in 1993. After an NSF postdoc at UC Santa Barbara, Auerbach began his career in 1995 at UMass Chemistry and was promoted to full professor in 2004. Auerbach's research focuses on simulating nanostructured materials such as zeolites – important to renewable energy technologies including biofuels and fuel cells. Auerbach has developed new semiclassical methods for treating quantum tunneling, molecular dynamics methods for treating microwave heating, and Monte Carlo methods for simulation zeolite crystal formation. Auerbach won an NSF Career Award in 1998, a Sloan Fellowship in 1999, a Dreyfus Teacher-Scholar Award in 1999, and the inaugural Manning Prize for excellent in teaching in 2016.

### Christopher C. Landry

John N. Pomeroy Professor of Chemistry
Materials Science Program
Cellular, Molecular, and Biomedical Program
University of Vermont, Burlington, VT

Christopher Landry received his undergraduate degree from the University of Richmond and completed his Ph.D. at Harvard University before working as a post-doctoral associate with Galen Stucky at the University of California, Santa Barbara. He is a former Chair of the Chemistry Department at UVM and has been recognized as a University Scholar. He is a member of the Vermont Academy of Science and Engineering, and received a Fulbright Senior Research Award to study at the Instituto de Tecnología Química in Valencia, Spain. Professor Landry's research is focused on the synthesis and applications of nanomaterials. Over the years he has published numerous articles on porous nanoparticles in filtration and as catalytic supports; he has also extensively explored the use of these materials as drug delivery vehicles. Current work includes preparing porous tungsten oxide nanoparticles for oxidative photocatalysis and developing a diagnostic test for prostate cancer using the nanoparticle protein corona.

### Steven L. Suib

Board of Trustees Distinguished Professor of Chemistry
Director, Institute of Materials Science
University of Connecticut, Storrs, CT

Steve Suib did his undergraduate work at the State University of New York at Fredonia where he received a Bachelor of Sciences Double Major in Chemistry and Geology. He obtained his Ph.D. at the University of Illinois at Urbana Champaign. After a postdoctoral position at the University of Illinois at Urbana Champaign he joined the faculty at the University of Connecticut. His research in the area of heterogeneous catalysis involves synthesis and use of porous transition metal oxides; selective oxidations; activation of small molecules; and use of various activation methods in catalysis including thermal, photochemical, ultrasound, microwave, and combinations of these. Characterization of these systems with in situ and in operando methods is being done with a variety of microscopic, spectroscopic, surface, bulk, magnetic, optical, and structural methods.

# NAM28 Honorary Chair

**Gary L. Haller**

Henry Prentiss Becton Professor of Engineering and Applied Science
Yale University
New Haven, CT

Professor Haller received a B.S. degree in mathematics and chemistry from the University of Nebraska at Kearney. His Ph.D. work was in physical chemistry at Northwestern University. After a NATO Post-doctoral Fellowship at Oxford University, he joined Yale University where he was Chair of the Department of Chemical Engineering, Chair of the Council of Engineering, and Deputy Provost for Physical Sciences and Engineering. Professor Haller was Master of Jonathan Edwards College. He is currently Director of the Koerner Center for Emeritus Faculty. His professional service has included co-Editor of the Journal of Catalysis, and the editorial boards of several journals. His alma mater has honored him with the Donald E. Fox Chemistry Lectureship and Outstanding Alumni Award and he has received the Meritorious Service Award of the Yale Science and Engineering Association. Professor Haller's research is known for being of the highest quality focusing on molecular understanding of heterogeneous catalysts.

# NAM28 Organizing Committee

| | | |
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| | Chris Landry | University of Vermont |
| | Steve Suib | University of Connecticut |
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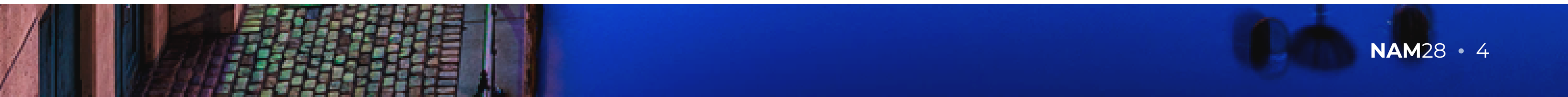


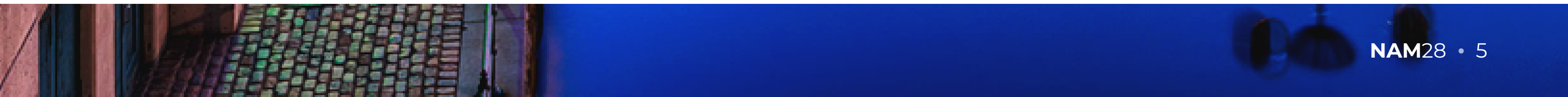
# NAM28 Acknowledgments

## The 28th NAM organizing committee would like to thank the following:

- The **North American Catalysis Society** for their support of NAM28
- The **National Science Foundation, US Department of Energy, the North American Catalysis Society, and the University of Massachusetts at Amherst** for their support of the Richard J. Kokes Student Travel Awards program
- The NAM27 organizing committee for their support, help, and guidance
- Dr. Jingguang Chen, President of NACS, for his steady counsel and wise assistance with finances
- The many reviewers who helped us with evaluating Extended Abstract submissions for NAM28
- Jennifer Whiting, and the team at Meeting Solutions, Inc. for their invaluable help during the entire planning process and with all aspects of running the meeting onsite
- Ami Coli from Confex for assistance managing the abstracts and presentations
- Kaitlyn Cullen from the University of Connecticut for outstanding administrative support
- The fantastic staff of the OMNI Providence

## Sponsors of the NAM28 Awards:

- The **Haldor Topsøe Company** as the sponsor of the Michel Boudart Award for the Advancement of Catalysis, presented jointly by the North American Catalysis Society and the European Federation of Catalysis Societies. Congratulations to **Johannes Lercher**.
- **Johnson Matthey** for sponsoring The Robert Burwell Lectureship in Catalysis Award, administered by The North American Catalysis Society. Congratulations to **Umit Ozkan**.
- **W.R. Grace and Company** for sponsoring the Paul H. Emmett Award in Fundamental Catalysis. Congratulations to **Aditya Bhan** and **Yuriy Román-Leshkov**.
- **Clariant** for sponsoring the Eugene J. Houdry Award in Applied Catalysis. Congratulations to **Stephen Schmidt**.
- **ExxonMobil Research and Engineering** and **Clariant** for sponsoring the NACS Award for Distinguished Service in the Advancement of Catalysis. Congratulations to **Stuart Soled**.



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# 28th NAM Kokes Award Winners

*The Kokes Awards are sponsored by the North American Catalysis Society and administered by the North American Meetings (NAM) organization. The objective of the Richard J. Kokes Travel Award program is to encourage the participation of students in the biennial North American Meetings. The Kokes Award covers a portion of the lodging and conference registration costs.*

## Congratulations to the following Kokes Award Winners!

| Name | Institution | Country |
|---|---|---|
| Monica Abdallah | Columbia University | USA |
| Mona Abdelgaid | University of Pittsburgh | USA |
| Husain Adamji | Massachusetts Institute of Technology | USA |
| Alexander Adogwa | Clemson University | USA |
| Jesús Ariel Aguirre Escalante | National Autonomous University of Mexico | Mexico |
| Ryan Alcala | University of New Mexico | Mexico |
| Cameron Armstrong | Worcester Polytechnic Institute | USA |
| Selin Bac Bilgi | University of Southern California | USA |
| Ezra Baghdady | University of Colorado, Boulder | USA |
| Dishari Basu | The Ohio State University | USA |
| Mubarak Bello | University of South Carolina | USA |
| Maya Bhat | Carnegie Mellon University | USA |
| Elizabeth Bickel | Purdue University | USA |
| Zachary Blanchette | University of Colorado, Boulder | USA |
| Victor Brandão | Georgia Institute of Technology | USA |
| Anna Brenner | Massachusetts Institute of Technology | USA |
| William Broomhead | University of Toronto | USA |
| Sean Brown | West Virginia University | USA |
| Brandon Burnside | University of New Mexico | USA |
| Jason Chalmers | University of California, Santa Barbara | USA |
| Jian Chang | University of Pennsylvania | USA |
| Xiuting Chen | Clemson University | USA |
| Saumil Chheda | University of Minnesota, Twin Cities | USA |
| Amish Chovatiya | University of Notre Dame | USA |
| Minju Chung | Massachusetts Institute of Technology | USA |
| Bradie Crandall | University of Delaware | USA |
| Natalia Diaz Montenegro | University of Virginia | USA |
| Berkay Ekinci | Penn State University | USA |
| Joseph Esposito | University of Minnesota | USA |
| Jordan Finzel | University of California, Santa Barbara | USA |
| Leah Ford | The Ohio State University | USA |
| Jesús Eduardo García Rodríguez | Universidad Autónoma de San Luis Potosí | Mexico |
| Kaivalya Gawande | University of Massachusetts, Amherst | USA |
| Raka Ghosh Dastidar | University of Wisconsin, Madison | USA |
| Laura Alejandra Gomez | University of Oklahoma | USA |
| FNU Gorky | University of Massachusetts, Lowell | USA |
| Jinyu Guo | Stanford University | USA |
| Piyush Haluai | Arizona State University | USA |
| Ahmed Maged Aly Hamed | Penn State University | USA |
| Xue Han | Brookhaven National Laboratory | USA |

# 28th NAM Kokes Award Winners

| Name | Institution | Country |
|---|---|---|
| Sevy Harris | Northeastern University | USA |
| Mohammad Hasibul Hasan | Clarkson University | USA |
| Daniel Hernández López | Metropolitan Autonomous University | Mexico |
| Isabel Hortal-Sanchez | University of Puerto Rico | USA |
| Jeremy Hu | The Pennsylvania State University | USA |
| Phillips Hutchison | Yale University | USA |
| Sherafghan Iftikhar | North Carolina State University | USA |
| Haldrian Iriawan | Massachusetts Institute of Technology | USA |
| Ana Carolina Jerdy | University of Oklahoma | USA |
| Olusola Johnson | University of South Florida | USA |
| Seongjoo Jung | University of Minnesota | USA |
| Gaurav Kamat | Stanford University | USA |
| Lance Kavalsky | Carnegie Mellon University | USA |
| Andrew Kohler | Iowa State University | USA |
| Jakub Konkol | Rutgers, the State University of New Jersey | USA |
| Stephen Kristy | Oregon State University | USA |
| Ajibola Lawal | University of Massachusetts, Amherst | USA |
| Kaitlyn Lawrence | The City College of New York | USA |
| Tien Le | University of Oklahoma | USA |
| Edgard Lebron Rodriguez | University of Wisconsin-Madison | USA |
| Mo Li | NJIT | USA |
| Gennaro Liccardo | Stanford University | USA |
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| Max Mortensen | University of Tennessee | USA |
| Tianyou Mou | Virginia Polytechnic Institute and State University | USA |
| Jinwoong Nam | Rutgers University | USA |
| Hoan Nguyen | Oregon State University | USA |
| Gregory Novotny | Tufts University | USA |
| Isaac Ogabiela | University of Massachusetts, Amherst | USA |
| Samuel Ojo | Case Western Reserve University | USA |
| Isaac Olowookere | University of Connecticut | USA |
| Samuel Olusegun | Texas Tech University | USA |
| Ayodeji Omoniyi | Stevens Institute of Technology | USA |
| Isaac Onyango | Washington State University | USA |
| Hope Otor | University of Notre Dame | USA |

# 28th NAM Kokes Award Winners

| Name | Institution | Country |
|---|---|---|
| Deep Patel | Iowa State University | USA |
| William Porter | Columbia University | USA |
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| Laura Proano | Georgia Institute of Technology | USA |
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| Samantha Roenigk | University of Pittsburgh | USA |
| Roshni Sajiv Kumar | University of Alberta | Canada |
| Fuat Sakirler | University of Massachusetts, Lowell | USA |
| Usman Salahuddin | University of Connecticut | USA |
| Anthony Savoy | Washington State University | USA |
| Adhika Setiawan | Lehigh University | USA |
| Kai Shen | University of Pennsylvania | USA |
| Luolin Shi | Stony Brook University | USA |
| Kumari Shilpa | University of Houston | USA |
| Anukriti Shrestha | University of Virginia | USA |
| Odiri Siakpebru | University of Kansas | USA |
| Erin Sobchinsky | Lehigh University | USA |
| Sayed Abu Sufyan | University of Utah | USA |
| Jiyu Sun | University of Connecticut | USA |
| Roshaan Surendhran | University of Delaware | USA |
| Jun Zhi Tan | Princeton University | USA |
| Mayank Tanwar | University of Minnesota | USA |
| Brook Wander | Carnegie Mellon University | USA |
| Guanhua Wang | Northwestern University | USA |
| Haodong Wang | Stony Brook University | USA |
| Min Wang | University of Maine | USA |
| Andrew Wong | Penn State University | USA |
| Yantao Xia | University of California, Los Angeles | USA |
| Yuting Xu | University of Massachusetts, Lowell | USA |
| Arash Yahyazadeh | University of Saskatchewan | Canada |
| Carissa Yim | University of Michigan | USA |
| Md Raian Yousuf | Virginia Polytechnic Institute and State University | USA |
| Tae Yong Yun | Penn State University | USA |
| Emigdio Zamora | Autonomous Metropolitan University, Azapotzalco | Mexico |
| Hong Zhang | Stony Brook University | USA |
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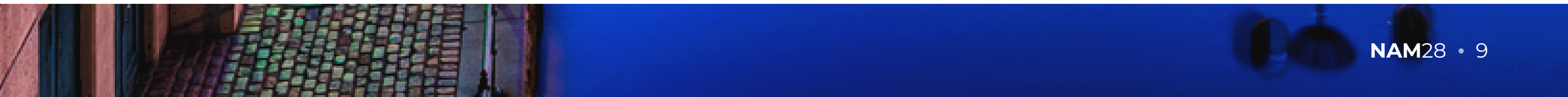

# 28th NAM Kokes Award Winners

# NAM28 Exhibitors

| Company | Booth |
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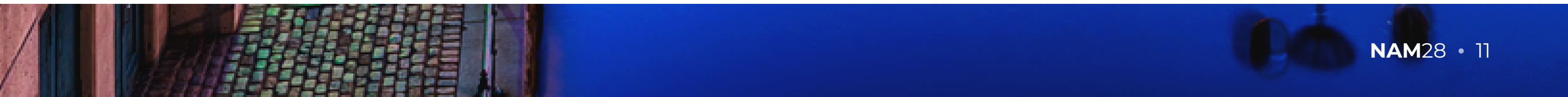

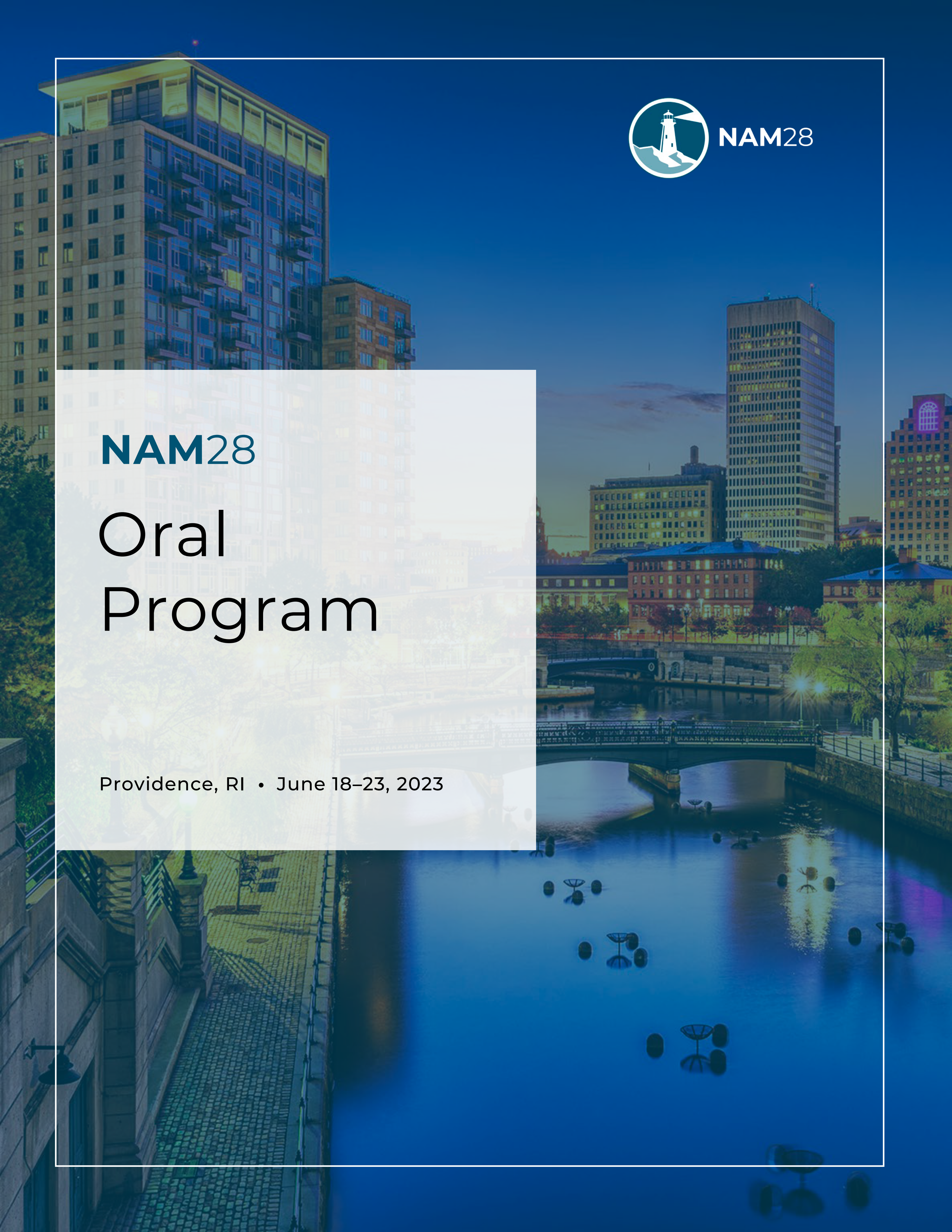

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# NAM28

# Oral Program

Providence, RI • June 18–23, 2023

# Monday, June 19, 2023

## Ballroom A-E

### MONDAY MORNING

*2023 Paul H. Emmett Award Lecture: Aditya Bhan*
Session Chairs: Christopher Landry, *University of Vermont, USA* and Matthew Neurock, *University of Minnesota, Twin Cities, USA*

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8:05 AM All That Most Maddens and Torments in Catalytic C1 Conversion.
**Aditya Bhan**, *University of Minnesota, Twin Cities, USA*.

## 551 AB

### Reaction Mechanisms

Session Chairs: Alyssa Love, *ExxonMobil Research and Engineering, USA* and Dionysios Vlachos, *University of Delaware, USA*.

---

9:30 AM **Mon-551AB-0930** Elementary Steps and Bifunctional Scavenging Pathways in Methylcyclohexane Dehydrogenation on Dispersed Pt Nanoparticles.
Sai Chen[1], Zhongyao Zhang[1], **Trenton Otto**[2] and Enrique Iglesia[1], *(1)University of California, Berkeley, USA, (2)Chevron Energy Technology Co., USA*.

**Short Summary:**
These findings shed light on the elementary steps and mechanistic origins of bifunctional scavenging pathway in metal-oxide systems via scavenging molecular shuttles at support surface beyond electronic effects or bifunctional reactions at metal-support interfaces

---

9:50 AM **Mon-551AB-0950** Hydride-Driven Chemoselective C-H Bond Formation of Benzoic Acid on Anatase $TiO_2$.
**Jeremy Hu**, Michael Janik and Konstantinos Alexopoulos, *The Pennsylvania State University, USA*.

**Short Summary:**
The chemoselective hydrogenation of benzoic acid to aromatic products is studied on anatase $TiO_2$ using DFT and kinetic modeling. A novel hydride-mediated mechanism is proposed for C-H bond formation on $TiO_2$, with consistently favorable reaction energies between surface hydrides and negatively-charged intermediate ligands coadsorbed in oxygen vacancies.

---

10:10 AM **Mon-551AB-1010** Toward Mechanistic Understanding of Methanol Synthesis on an $In_2O_3$ Catalyst.
**Yong Yang**[1], Liang Zhu[1], Yang Liu[1], Yulu Cai[1], Zhehao Qiu[1], Junyu Lang[1] and Li Shenggang[1,2], *(1)ShanghaiTech University, China, (2)Shanghai Advanced Research Institute, CAS,, China*.

**Short Summary:**
$In_2O_3$ catalyst have been proved to have a high activity for $CO_2$ hydrogenation to methanol. Isotope transients ($D_2$+$CO_2$->$H_2$+$CO_2$, *in situ* time resolved FT-IR and XPS (200-270°C, 1-16 bar) are applied in this study to understand the kinetics and spectroscopic fundamental of this reaction under industrial conditions.

---

10:30 AM **Mon-551AB-1030** Magnetic Induction Heating Changes the Intrinsic Thermal Catalytic Behavior of Pt/$Fe_3O_4$ Catalyst for CO Oxidation.
**Alexander Adogwa**[1], Ewa Chukwu[1], Owen Chamness[1], Rachel Getman[1], Sungsik Lee[2], Michael Zachman[3], Alexander Malaj[1], Thompson Mefford[1] and Ming Yang[1], *(1)Clemson University, USA, (2)Argonne National Laboratory, USA, (3)Oak Ridge National Laboratory, Oak Ridge, TN, USA*.

**Short Summary:**
The kinetics of CO oxidation reaction is demonstrated to be significantly influenced by magnetic induction heating. The presence of an alternating magnetic field greatly enhanced the electronic interaction between the platinum-centric site and the $O_2$ intermediate, resulting in a distinctive Langmuir-Hinshelwood reaction pathway that aided CO oxidation catalysis.

---

10:50 AM **Mon-551AB-1050** Active Site Entropies Can Influence Catalytic Kinetics: Mobile Atomically Dispersed Rh Catalysts on $Al_2O_3$
Gregory Zakem, Emily Schroeder and **Phil Christopher**, *University of California, Santa Barbara, USA*.

**Short Summary:**
The rates of CO desorption and ethylene hydroformylation on Rh/$Al_2O_3$ are influenced by the entropy of Rh on $Al_2O_3$. Active site entropy was modified by alkyl phosphonic acid functionalization of $Al_2O_3$, which immobilized Rh. This demonstrates control of catalytic reactivity by influencing active site entropy – a rarely considered approach.

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11:10 AM **Mon-551AB-1110** Metal-Modified Molybdenum Nitride As Selective Catalysts for Ethanol Reforming and Dehydrogenation.
**Zhexi Lin**[1], William Porter[1], Steven Denny[1], Nongnuch Artrith[2] and Jingguang Chen[1], *(1)Columbia University, USA, (2)Utrecht University, Netherlands*.

**Short Summary:**
The abundant bioethanol can be upgraded through two promising pathways: reforming and dehydrogenation. This study sheds light on the design principle of efficient ethanol reforming and dehydrogenation catalysts using metal-modified $Mo_2N$, with accelerated catalyst design based on machine learning predictions, which are verified by experimental evaluation.

11:30 AM **Mon-551AB-1130** Understanding Reaction Mechanisms for Electrochemical Biomass Valorization.
**Nitish Govindarajan**[1], Sihang Liu[2] and Karen Chan[2], *(1)Lawrence Livermore National Laboratory, USA, (2)Technical University of Denmark, Denmark*.

**Short Summary:**
A detailed understanding of reaction mechanisms for electrochemical processes involved in biomass conversion is crucial for the design and development of efficient and selective electrocatalysts. Here we focus on two important reactions related to biomass valorization: Kolbe electrolysis on Pt oxides, and alkaline CO electro-oxidation on Cu single crystal surfaces.

## MONDAY AFTERNOON

## Fundamental Insights into Kinetics and Mechanisms

Session Chairs: Neil Schweitzer, *Northwestern University, USA* and Zhexi Lin, *Columbia University, USA*.

1:20 PM **Mon-551AB-1320** Quantitative Thermodynamics of Hydrogen Spillover: How Entropy and Surface Hydroxyl H+ Transfer Chemistry Drive $H_2$ Adsorption and Spillover on Au/$TiO_2$.
Akbar Mahdavi-Shakib[1], Todd Whittaker[2], Tae Yong Yun[1] and **Bert Chandler**[1,3], *(1)The Pennsylvania State University, USA, (2)University of Colorado Boulder, USA, (3)Pennsylvania State University, USA*.

**Short Summary:**
We report the quantification of hydrogen adsorption and spillover on Au/$TiO_2$ catalysts, showing hydrogen spillover is an entropy-driven process associated with zwitterionic hydroxyl pairs on the titania surface. Spillover increases with temperature due to increasing numbers of these zwitterionic pairs, which give rise to larger configurational surface entropy contributions.

1:40 PM **Mon-551AB-1340** Interrogating Size-Dependent Intrinsic Kinetics for Pt Nanoparticles.
**Taek-Seung Kim** and Christian Reece, *Harvard University, USA*.

**Short Summary:**
Utilizing the TAP reactor, it becomes possible to accurately calculate the kinetics of individual steps of the LH mechanism while also being highly sensitive to the distribution of sites on the CO catalyst. By performing these experiments of 2–15 nm-sized Pt, we can deconvolute the site-dependent kinetics for CO oxidation.

2:00 PM **Mon-551AB-1400** Taming of Transition States on Nanohybrid Polymer-Metal Catalysts.
Pengcheng Huang[1], Rick Baldenhofer[2], Ricardo Pinto Enes Martinho[2], Leon Lefferts[2] and **Jimmy Faria**[2], *(1)MESA + Institute for Nanotechnology, Netherlands, (2)University of Twente, Netherlands*.

**Short Summary:**
Here, we describe a strategy using stimulus-responsive polymers to control the activity and selectivity of Pd catalysts during reductive removal nitrites in drinking water. We found for the first time that depending on the polymer solvation state it is possible to tune the energetics of the transition state.

2:20 PM **Mon-551AB-1420** An Electrochemical Approach to Understanding Thermochemical Catalysis.
William Howland, Jaeyune Ryu, Thejas Wesley, Yuriy Roman and **Yogesh Surendranath**, *Massachusetts Institute of Technology, USA*.

**Short Summary:**
Electrochemical paradigms provide a powerful framework for understanding and controlling thermochemical catalysis at solid-liquid interfaces.

2:40 PM ***KEYNOTE*** **Mon-551AB-1440 High-Precision Kinetics of Elementary Surface Reactions: A New Tool for Understanding Heterogeneous Catalysis.**
**Alec Wodtke**[1,2,3], Dmitriy Borodin[1,2], Michael Schwarzer[1,2], Jan Fingerhut[1,2], Florian Nitz[1,2], Hua Guo[4] and Theofanis Kitsopoulos[1,2,5], *(1)University of Goettingen, Germany, (2)Max Planck Institute for Multidisciplinary Sciences, Germany, (3)Institute for Advanced Studies of Energy Conversion (ICASEC), Germany, (4)University of New Mexico, USA, (5)University of Krete, Greece*.

**Short Summary:**
Velocity Resolved Kinetics yields more accurate thermal rate constants for elementary reactions involved in heterogeneous catalysis. For the first time, meaningful comparison of theoretically predicted and experimentally derived rate constants is possible, from which catalytic active sites can be identified.

## Microkinetic Modeling

Session Chairs: Peng Bai, *University of Massachusetts Amherst, USA* and John R. Kitchin, *Carnegie Mellon University, USA*.

3:45 PM **Mon-551AB-1545** Application of Machine-Learning Techniques to Reproduce a Microkinetic Model for the Methanol Synthesis.
**Bruno Lacerda de Oliveira Campos**[1], Esly Ferreira da Costa Junior[2], Karla Herrera-Delgado[1], Andréa Oliveira Souza da Costa[2], Stephan Pitter[1] and Jörg Sauer[1], *(1)Karlsruhe Institute of Technology (KIT), Germany, (2)Federal University of Minas Gerais (UFMG), Brazil*.

**Short Summary:**
A methodology is proposed here to transfer information from a detailed microkinetic model (MM) of the methanol synthesis to an artificial neural network (ANN), taking into account *a priori* information of thermodynamic equilibrium equations. The developed ANN accurately reproduced the MM, and is adequate for various model-based applications.

4:05 PM **Mon-551AB-1605** Microkinetic Modeling of Multifaceted Catalysts in Cantera.
**Gandhali Kogekar**, Bjarne Kreitz and Franklin Goldsmith, *Brown University, USA*.

**Short Summary:**
The effect of a molecular diffusion on multifaceted catalysts is studied using Cantera. A stirred-reactor model is implemented to simulate the temperature-programmed desorption (TPD) of $CO_2^+$ from supported Ni catalyst. This newly implemented capability enables the modeling of a molecular diffusion across multiple surfaces or facets for various chemical processes.

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4:25 PM **Mon-551AB-1625** Efficient Implementation of Detailed Surface Kinetics By Neural Network Representations of the Rate-Determining Steps.
**Felix Döppel**[1] and Martin Votsmeier[1,2], *(1)Technical University of Darmstadt, Germany, (2)Umicore Ag & Co. KG., Germany*.

**Short Summary:**
Solving for detailed kinetics presents a severe bottleneck in multi-scale modeling, rendering it infeasible. Surrogate models can circumvent this bottleneck but are limited to specific use cases. We present a new modeling approach based on interpolating the forward- and reverse rates of the rate-determining reactions and thus overcoming this limitation.

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4:45 PM **Mon-551AB-1645** Extracting Knowledge from Transient Kinetic Data Using Kinetics-Informed Neural Networks.
**Andrew Medford** and Gabriel Gusmão, *Georgia Institute of Technology, USA*.

**Short Summary:**
This talk presents “kinetics-informed neural networks” (KINNs) that combines numerical techniques from machine learning with a bespoke architecture to handle the structure of micro-kinetic equations. Topological constraints are used to satisfy site conservation, and the loss function contains terms to simultaneously fit kinetic data and kinetic rate parameters.

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5:05 PM **Mon-551AB-1705** Pynta: A Workflow Software for Automatic Calculation of Surface and Gas-Surface Kinetics.
**Matthew S. Johnson**[1], Maciej Gierada[1], Eric D. Hermes[1], David Bross[2], Khachik Sargsyan[1], Habib Najm[1] and Judit Zádor[1], *(1)Sandia National Laboratories, USA, (2)Argonne National Laboratory, USA*.

**Short Summary:**
We present Pynta, a software for automating calculation of surface reaction kinetic parameters. We demonstrate Pynta on 12 reactions involving gas-phase, monodentate and bidentate species and a low-index and a high-index surface. We show different saddle points (SPs) can vary significantly in energy emphasizing the importance of SP search approaches.

## 552 AB

### MONDAY MORNING

### Biomass-Derived Alcohol Valorization

Session Chairs: Christopher Nicholas, *Låkril Technologies Corporation, USA* and Yomaira Pagan Torres, *University of Puerto Rico - Mayagüez, PR*.

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9:30 AM **Mon-552AB-0930** TAP Study of Renewable Ethanol Upgrading to Butanol on Lanthanide Oxides Supported on Activated Carbon.
**Joachim Pasel**, Johannes Häusler and Ralf Peters, *Forschungszentrum Jülich GmbH, Germany*.

**Short Summary:**
The catalytic upgrading of $CO_2$-based ethanol into higher alcohols is of increasing interest. A synthesis towards n-butanol is the aldol condensation, which was investigated using the TAP methodology on $Dy_2O_3/C$, $Eu_2O_3/C$, $Er_2O_3/C$. In addition to the aldol condensation of acetaldehyde yielding butanol, its decomposition into CO, $CH_4$, and $H_2$ occurred.

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9:50 AM **Mon-552AB-0950** Catalytic Upgrading of Ethanol into Diesel-Fuel Range C10+ Ethers.
**Emmanuel Canales**[1] and George Huber[2], *(1)University of Wisconsin - Madison, USA, (2)University of Wisconsin Madison, USA*.

**Short Summary:**
Diesel fuel demand is projected to continue to increase. Long-chain mono C10+ ethers have high cetane numbers and appropriate physical properties to be blended into diesel fuel. In our ethanol to diesel approach, We will show the catalytic chemistry, engine and physical measurements, and techno-economic analysis of our process.

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10:10 AM **Mon-552AB-1010** The Role of the Oxygen Vacancies and Zn in the Isobutene Synthesis from Ethanol Employing Zn Zr Based Catalysts..
Mariana G. S. Pinheiro[1,2], **Luciano H. Chagas**[3], Priscila C. Zonetti[3], Guilherme G. Gonzalez[3], Odivaldo C. Alves[4], Luiz E. P. Borges1, Liane Rossi[5] and Lucia Gorenstin Appel[3], *(1)Instituto Militar de Engenharia, Brazil, (2)CBPF, Brazil, (3)Instituto Nacional de Tecnologia, Brazil, (4)Universidade Federal Fluminense, Brazil, (5)University of São Paulo, Brazil*.

**Short Summary:**
Isobutene can be generated in one-pot synthesis from ethanol employing Zn-Zr based catalysts. When $Zn^{+2}$ replaces $Zr^{4+}$ in the $ZrO_2$ monoclinic lattice oxygen vacancies are formed. These species promote the redox properties and basicity of the catalyst favoring all steps of the isobutene generation from ethanol.

10:30 AM **Mon-552AB-1030** Elucidation of Catalyst Structure and Reaction Pathway for the Ethanol-to-Butadiene Reaction.
**Sang-Ho Chung**, Teng Li, Tuiana Shoinkhorova, Sarah Komaty, Adrian Ramirez, Ildar Mukhambetov, Edy Abou-Hamad, Genrikh Shterk, Selvedin Telaovic, Alla Dikhtiarenko, Polina Lavrik, Xinqi Tang, Jorge Gascon and Javier Ruiz-Martinez, *King Abdullah University of Science and Technology (KAUST), Saudi Arabia*.

**Short Summary:**
We elucidate the origin of catalytically active sites of wet-kneaded silica–magnesia catalyst for Lebedev process, which has been black box over 70 years. From directly observed relations of beneficial/detrimental magnesium silicates on ethanol-to-butadiene process, this study opens a new possibility for development of the next generation Lebedev catalysts.

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10:50 AM **Mon-552AB-1050** Selective Conversion of 2,3-Butanediol to C4+ Olefins Using Dioxolane Intermediates.
**Michael Cordon**[1], Claire Yang[2], Cameron Moore[2], Zhenglong Li[1] and Andrew Sutton[1], *(1)Oak Ridge National Laboratory, USA, (2)Los Alamos National Laboratory, USA*.

**Short Summary:**
2,3-butanediol separation from aqueous media like fermentation broths is possible via reaction with an aldehyde over Amberlyst-15 to form a dioxolane species. These dioxolanes can then be converted over Cu/ZSM-5 into olefin-rich product streams as key intermediates for aviation fuel generation from renewable 2,3-butanediol.

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11:10 AM **Mon-552AB-1110** Improving the Regenerability of Copper-Containing Catalysts through Atom-Trapping in Zeolite Defects.
**Stephen Purdy**[1], Gregory Collinge[2], Junyan Zhang[1], Shivangi Borate[3], Kinga A. Unocic[1], Qiyuan Wu[4], Evan C. Wegener[5], Nohor Samad[3], Susan Habas[4], Theodore Krause[5], James Harris[3], Mal-Soon Lee[2], Vassiliki-Alexandra Glezakou[2], Rodger Rousseau[2], Andrew Sutton[1] and Zhenglong Li[1], *(1)Oak Ridge National Laboratory, USA, (2)Pacific Northwest National Laboratory, USA, (3)The University of Alabama, USA, (4)National Renewable Energy Laboratory, USA, (5)Argonne National Laboratory, USA*.

**Short Summary:**
Silanol nests in dealuminated beta zeolite are capable of trapping single atom Cu, which allows Cu to be redispersed to single sites from metal nanoparticles. This allows for full regeneration of catalytic activity of Cu-Zn-Y/Beta in ethanol upgrading.

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11:30 AM **Mon-552AB-1130** Biomass Conversion to Renewable Fuels.
**Christopher Keturakis**, Ruben Barajas, Suheil Abdo, Dave Mackowiak and Amanda Hickman, *Honeywell UOP, USA*.

**Short Summary:**
This talk discusses UOP's progress in developing commercially viable biomass conversion to renewable fuel processes.

## MONDAY AFTERNOON

### Design and Synthesis of Bimetallic Catalysts I

Session Chairs: John Regalbuto, *University of South Carolina, USA* and Paul Dauenhauer, *University of Minnesota, USA*.

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1:20 PM **Mon-552AB-1320** Modularly Designed Heterogeneous Catalysts Control Selectivity *Via* Interparticle Distance.
**Kang Rui Garrick Lim**[1], Selina K. Kaiser[1], Haichao Wu[1], Sadhya Garg[1], Marta Perxés Perich[2], Jessi E.S. van der Hoeven[2], Michael Aizenberg[1] and Joanna Aizenberg[1], *(1)Harvard University, USA, (2)Utrecht University, Netherlands*.

**Short Summary:**
In thermal catalysis, the impact of interparticle distance on selectivity is often confounded by concomitant changes in the NP size distribution, another key catalytic descriptor. Herein, we use a modular raspberry colloid templating method to ensuring a preserved NP size distribution during synthesis and catalysis.

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1:40 PM **Mon-552AB-1340** Biphasic 'Janus' Pt-Pd Particles Show Self-Healing Characteristics in Diesel Oxidation Catalysts.
Stephen Porter[1], Arnab Ghosh[1,2], Hien Pham[1], Chih Han Liu[3], Chase Thompson[1], Andrew De La Riva[1], Eric J. Peterson[1], Eleni Kyriakidou[3] and **Abhaya Datye**[1], *(1)University of New Mexico, USA, (2)Carus, USA, (3)University at Buffalo (SUNY), USA*.

**Short Summary:**
This work addresses the remarkable thermal stability of Pt-Pd diesel oxidation catalysts, after aging in air at 800 C. We find that the thermodynamically stable state of the Pt-Pd particles involves a biphasic structure, with an epitaxial growth of the oxide on the metal.

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2:00 PM **Mon-552AB-1400** Effects of Stoichiometry and Structure in Bimetallic Nanoparticle Catalysts for the Liquid-Phase Semihydrogenation of Diphenylacetylene.
Si Chen[1], Xiaohui Huang[2,3], Di Wang[2], Christian Kuebel[2,3] and **Silke Behrens**[1], *(1)Karlsruhe Institute of Technology (KIT), Germany, (2)Karlsruhe Institute of Technology, Germany, (3)Technische Universität Darmstadt, Germany*.

**Short Summary:**
Intermetallic Pd-In nanoparticles with different stoichiometry and phase composition were received by colloidal synthesis in ionic liquids and used as catalysts in the liquid-phase, semi-hydrogenation of diphenylacetylene. Notably, intermetallic PdIn nanoparticles reveal both high activity and selectivity to cis-stilbene even at full conversion.

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2:20 PM **Mon-552AB-1420** Identifying Active Sites for Stabilizing Fe-ZSM-5 for CO Hydrogenation.
**Jane Agwara**[1] and Marc Porosoff[2], *(1)Porosoff Lab, University of Rochester, USA, (2)University of Rochester, USA*.

**Short Summary:**
Fe is an abundant and cost-effective catalyst for CO conversion to valuable hydrocarbons. However, catalyst deactivation remains a challenge for Fe supported on ZSM-5. Fe-ZSM-5 was synthesized via a grinding synthesis method resulting in predominantly $Fe^{3+}$ species confined within the zeolite, which are active and stable during CO hydrogenation reaction.

2:40 PM **Mon-552AB-1440** Catalytic Trends on Transition Metal Phosphide Catalysts: A Hydrodeoxygenation Case Study.
**Carrie Farberow**, *National Renewable Energy Laboratory, USA*.

**Short Summary:**
Controlled solution phase synthesis, advanced characterization techniques, and atomic-scale simulations are applied to understand the changes in experimental hydrodeoxygenation selectivity on a series of ternary transition metal phosphide (TMP) nanoparticle catalysts. The heterogeneity of surface sites in TMPs demonstrates the unique challenges in identifying a single, robust TMP catalytic descriptor.

3:00 PM **Mon-552AB-1500** An Electrochemical Approach for Designing Thermochemical Bimetallic Nitrate Hydrogenation Catalysts.
**Kunal Lodaya**, Bryan Tang, Ryan Bisbey, Sophia Weng, Karl Westendorff, Wei Lun Toh and Yogesh Surendranath, *Massachusetts Institute of Technology, USA*.

**Short Summary:**
Nitrate hydrogenation at bimetallic catalysts proceeds via the coupling of electrochemical half-reactions at distinct metal sites. New metal pairs are identified and tested for this reaction based on this mechanism. In contrast to atomistic interaction, we provide a new framework for bimetallic catalyst design centered around segregated electrochemical coupling reactivity.

## Design and Synthesis of Bimetallic Catalysts II

Session Chairs: Francisco Zaera, *University of California Riverside, USA* and Umit Ozkan, *The Ohio State University, USA*.

3:45 PM **Mon-552AB-1545** Unravelling Metal Segregation Phenomena in Supported Pd-Ni-Based Catalysts.
**Florian Zand**[1], Suzanne Hangx[1], Christopher Spiers[1], Jonathan D. Poplawsky[2], Florian Meirer[1], Matteo Monai[1] and Bert M. Weckhuysen[1], *(1)Utrecht University, Netherlands, (2)Oak Ridge National Laboratory, USA*.

**Short Summary:**
Avoiding metal segregation phenomena during industrially-relevant preparation techniques is crucial to obtain uniform catalyst materials offering optimal catalytic performance, and limited use of scarce resources such as noble metals. We show during which steps metal segregation predominately occurs, as well as how it can be prevented and identified.

4:05 PM **Mon-552AB-1605** Boosting Low-Temperature Dry Reforming of Methane on Supported Intermetallic Ni-Zn Nanocatalysts.
**Olusola Johnson**[1], Yang He[2], Babu Joseph[1] and John Kuhn[1], *(1)University of South Florida, USA, (2)Oak Ridge National Laboratory, USA*.

**Short Summary:**
The electronic and surface environment modulation of intermetallic nanocatalysts for low-temperature methane reforming was explored in the study. The surface chemistry optimization of Ni-Zn nanocatalysts increased catalytic activity and stability while limiting coke formation, which is thermodynamically favorable.

4:25 PM **Mon-552AB-1625** Synthesis and Characterization of Core-Shell Cu-Ru, Cu-Rh, and Cu-Ir Nanoparticles.
**Alexandre Foucher**[1] and Eric Stach[2], *(1)Massachusetts Institute of Technology, USA, (2)University of Pennsylvania, USA*.

**Short Summary:**
We report the synthesis and characterization of core-shell Cu-Ru, Cu-Rh and Cu-Ir particles to optimize the use of platinum-group metals (PGMs). The Cu core can be etched to obtain promising Ru, Rh and Ir nanoshells with high stability and activity for CO oxidation.

4:45 PM **Mon-552AB-1645** Core-Shell Au@Pd Catalysts Surpasses the Activity of AuPd Alloy Catalysts for Alcohol Oxidation.
**Adriano Braga**[1], Liane Rossi[2], Johnatan Fiorio[3], Ofelia Yang[2], Karla Caetano[2], Simon Bare[4] and Adam Hoffman[4], *(1)Purdue University, USA, (2)University of São Paulo, Brazil, (3)Technische Universität Dresden, Germany, (4)SLAC National Accelerator Laboratory, USA*.

**Short Summary:**
Herein we added increasing amounts of palladium to titania-supported gold nanoparticles with average sizes between 2 and 10 nm for testing in benzyl alcohol oxidation. The activity increases by addition of Pd, reaching a plateau, and decreases with the further addition of Pd, thus resulting in a volcano-like curve.

5:05 PM **Mon-552AB-1705** Development of Highly Controlled Bimetallic Catalysts Using Galvanic Displacement.
**Haiying Zhou**, Yanjiao Yi, John Meynard Tengco and John R. Monnier, *University of South Carolina, USA*.

**Short Summary:**
Highly dispersed/single-site Cu-Ni and Ag-Ni catalysts can be synthesized by galvanic displacement. It is a simple and scalable method. The amount of deposition is controllable and measurable.

# 555 AB

## MONDAY MORNING

### Integrated Syngas Chemistry

Session Chairs: Juan Jimenez, *Brookhaven National Laboratory, USA* and Marc Porosoff, *University of Rochester, USA*.

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9:30 AM **Mon-555AB-0930** Portable Process Development for Methanol Synthesis from Stranded Methane.
**Hsiang-Sheng Chen**[1], Paul Yelvington[2], Nazim Muradov[1] and Edwin Yik[2], *(1)University of Central Florida, USA, (2)M2X Energy Inc., USA*.

**Short Summary:**
Uneconomic flaring (or outright venting) of stranded natural gas results in greenhouse gas emissions that today are very large in aggregate. This project emphasizes the unconventional technological approach to economically viable and environmentally sustainable valorization of stranded methane using portable modular units that converts stranded methane to energy-dense methanol.

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9:50 AM **Mon-555AB-0950** Direct Synthesis of Acetone from Syngas and Dimethyl Ether V*ia* Tandem Carbonylation-Ketonization Catalysis.
**Eva Andrés**, Raquel Peláez, Adrián Rielves, Wilson Henao, Marcos G. Farpón and Gonzalo Prieto, *Instituto de Tecnología Química (ITQ UPV-CSIC), Spain*.

**Short Summary:**
The selective chain propagation from $C_1$ building blocks to specifically $C_3$ compounds remains an important challenge for heterogeneous catalysis. Here we report how the tandem integration of carbonylation and ketonization reaction steps on a multifunctional catalyst provides a novel route for the direct synthesis of acetone from $C^1$ building blocks.

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10:10 AM ***KEYNOTE*** **Mon-555AB-1010 Oxygenate-Mediated Conversion of $H_2/CO_x$ to Hydrocarbons: Influence of Heteroatom and Gas Composition on Zeotype Performance. Unni Olsbye**, *University of Oslo, Norway; University of Oslo, Norway*.

**Short Summary:**
Valorisation of syngas-containing off-gas streams from point sources is a key technology for the post-fossil society, where it will enable production of consumer goods with properties equal to those obtained by converting fossil carbon, as well as liquid fuels for energy storage.

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10:50 AM **Mon-555AB-1050** Catalytic Activity for Direct $CO_2$ Hydrogenation to Dimethyl Ether with Different Proximity on Bifunctional Cu-ZnO-$Al_2O_3$@Ferrierite.
Xu Wang, So Yun Jeong, Hyun Seung Jung and **Jong Wook Bae**, *Sungkyunkwan University, Korea, Republic of (South)*.

**Short Summary:**
Core-shell structured integrations of Cu-ZnO-$Al_2O_3$ and ferrierite zeolite (FER) are investigated for direct $CO_2$ hydrogenation to DME. The detrimental surface properties formed by possible ion-exchange of FER surfaces with the relatively volatile metal ions from Cu-ZnO-$Al_2O_3$ surfaces were effectively suppressed by applying the physically coating interlayers with $SiO_2$.

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11:10 AM **Mon-555AB-1110** Reactive Separations of CO/$CO_2$ Mixtures over Ru-Co Single Atom Alloys.
**Renjie Liu** and Marc Porosoff, *University of Rochester, USA*.

**Short Summary:**
We study a Ru-Co single-atom alloy for reactive CO/$CO_2$ separations to produce $C_{5+}$ hydrocarbons. The catalyst shows a superior Fischer-Tropsch activity at 200 °C without converting $CO_2$. Unlike most research, Ru atoms preserve Co in a reduced phase during reaction, instead of enhancing the hydrogenation activity or the olefins desorption.

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11:30 AM **Mon-555AB-1130** Intensification of Heat Transfer in Tubular Packed Bed Reactors for the Fischer-Tropsch Synthesis By the Adoption of Conductive Cellular Internals: A Pilot-Scale Study.
Martino Panzeri, **Carlo Giorgio Visconti**, Gianpiero Groppi and Enrico Tronconi, *Politecnico di Milano, Italy*.

**Short Summary:**
For all the conductive (Al) internals tested at the pilot reactor scale, demonstrates the effective intensification of heat transfer in FTs with respect to the packed bed configuration. The enhanced heat transfer through the adoption of conductive cellular internals promises a breakthrough for FTs in compact reactors.

## MONDAY AFTERNOON

### Carbon Dioxide Methanation

Session Chairs: Carsten Sievers, *Georgia Institute of Technology, USA* and Xunhua Mo, *Johnson Matthey, USA*.

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1:20 PM **Mon-555AB-1320** Catalytic Activity at the MgO-Ni Interface for $CO_2$ Methanation.
**Yufei Xie**, Thomas Van De Moere, Hilde Poelman and Vladimir V Galvita, *Ghent University, Belgium*.

**Short Summary:**
Modifying Ni/$Al_2O_3$ with MgO, either on support or on Ni, has great impact on $CO_2$ methanation. When impregnated on $Al_2O_3$ support, MgO weakens the MSI and increases NiO reducibility. When impregnated on Ni, MgO creates a new MgO/Ni interface with strong interaction, which is proposed to provide highly active sites.

1:40 PM **Mon-555AB-1340** Importance of Chlorine Removal from Ru/$TiO_2$ Methanation Catalysts.
**James Crawford**[1], Brittney E. Petel[1], Mathew Rasmussen[1], Mike Griffin[1], Thomas Ludwig[2], Simon H. Pang[2] and Matthew M. Yung[1], *(1)National Renewable Energy Laboratory, USA, (2)Lawrence Livermore National Laboratory, USA*.

**Short Summary:**
Combining green $H_2$ and direct air capture $CO_2$ provides a pathway to renewable natural gas. Ru/$TiO_2$ is a well-studied catalyst for low temperature (<200°C) methanation of $CO_2$. Chlorine contamination, owed to commonly employed $RuCl_3$ precursor, is demonstrated to have a detrimental impact on methanation activity.

2:00 PM **Mon-555AB-1400** Results from the Operation of an Industrial-Scale Plate-Type Methanation Reactor: Optimal Blend of Catalyst and Reactor Design.
**Emanuele Moioli**, *Hitachi Zosen Inova, Switzerland*.

**Short Summary:**
We present the results from the operation of an industrial-scale plate-type methanation reactor, operated with a Ni-$ZrO_2$ catalyst

2:20 PM **Mon-555AB-1420** Cross-Talking of Ni Metal Nanoparticle Facets Explains the Structuresensitivity of the $CO_2$ Methanation Reaction.
Matteo Ferri[1], Raffaele Cheula[1], Matteo Monai[2], Bert M. Weckhuysen[2] and **Matteo Maestri**[1], *(1)Politecnico di Milano, Italy, (2)Utrecht University, Netherlands*.

**Short Summary:**
We provide theoretical underpinnings that the cross-talking of Ni metal nanoparticle facets explains the structure sensitivity of the $CO_2$ methanation reaction.

2:40 PM **Mon-555AB-1440** Intensification of Ru/$Al_2O_3$ Catalysts for $CO_2$ Methanation.
**Clara Larghi**, Alessandro Porta, Carlo Giorgio Visconti and Luca Lietti, *Politecnico di Milano, Italy*.

**Short Summary:**
This work provides an optimized formulation for Ru/$Al_2O_3$ catalyst for $CO_2$ methanation exploiting structure-activity relations. However, the highly active catalyst incurred in diffusional limitations that need to be carefully considered in view of the process industrialization.

3:00 PM **Mon-555AB-1500** Ce- and La- Modified Ni- Based Catalysts for $CO_2$ Hydrogenation to Methane.
Paola Riani, Elena Spennati, Riccardo Freccero and **Gabriella Garbarino**, *University of Genova, Italy*.

**Short Summary:**
$CO_2$ hydrogenation is recognised as key-process to reduce $CO_2$ emission and among products $CH_4$ is suitable to be introduced in natural gas grid. The target of this work is to promote the $CO_2$ conversion and selectivity performances of Ni-based catalyst doped with La and Ce by using different synthetic routes.

## Methane Reforming I (Steam & Dry)

Session Chairs: Kewei Huang, *Shell, USA* and Oz Gazit, *Israel Institute of Technology -Technion, Israel*.

3:45 PM **Mon-555AB-1545** Steam Methane Reforming with EARTH®.
**Yeping Cai**, *Clariant Corporation, BU Catalysts, USA*.

**Short Summary:**
EARTH®, **E**nhanced **A**nnular **R**eformer **T**ube for **H**ydrogen and Syngas, is a removable annular structure installed inside reformer tubes to achieve simultaneously higher catalytic activity and heat recovery. Another important feature of the EARTH® design is its low pressure drop, allowing to increase syngas productivity.

4:05 PM **Mon-555AB-1605** Joule Heated Foams for Methane Steam Reforming: An Experimental and Modelling Study.
Matteo Ambrosetti, Lei Zheng, Francesca Zaio, Alessandra Beretta, **Gianpiero Groppi** and Enrico Tronconi, *Politecnico di Milano, Italy*.

**Short Summary:**
We demonstrate experimentally the feasibility of running methane steam reforming over a Joule heated structured foam catalyst. A mathematical model of the electrified methane steam reformer is validated against the data and used for preliminary scale-up calculations, which show the potential of compact eMSRs with superior hydrogen productivities.

4:25 PM **Mon-555AB-1625** Plasma Catalyst Bi-Reforming of Synthetic Biogas at Mild Conditions Using Ceria over Ni-Based La-Perovskite Catalyst.
Diego Gonzalez, **Sahanaz Parvin**, Srinivas Rangarajan and Jonas Baltrusaitis, *Lehigh University, USA*.

**Short Summary:**
DBD plasma bi-reforming reaction on perovskite via Response Surface Methodology

4:45 PM **Mon-555AB-1645** Role of Geometric Structure Materials and Coated $Al_2O_3$ Layer on Ni-Based Catalyst for Combined Steam and $CO_2$ Reforming with $CH_4$.
**Young Gul Hur**, *Hyundai Motor Company, Korea, Republic of (South)*.

**Short Summary:**
In this study, a catalyst development concept was reported that grafted a catalyst with excellent thermal stability to a geometric structure with an excellent thermal conductivity as a way to overcome the temperature gradient in a highly endothermic reaction system such as a reforming reaction.

5:05 PM **Mon-555AB-1705** Identification of Highly Selective Surface Pathways for Methane Dry Reforming Using Mechano-Chemical Synthesis of Pd-$CeO_2$.
**Juan Jimenez**[1], Luis E. Betancourt[1], Maila Danielis[2], Hong Zhang[1], Ping Liu[1,3], Alessandro Trovarelli[2], Jose Rodriguez[3], Sara Colussi[2] and Sanjaya D. Senanayake[1], *(1)Brookhaven National Laboratory, USA, (2)University of Udine and INSTM, Italy, (3)Stony Brook University, USA*.

**Short Summary:**
The reaction mechanism for methane dry reforming was explored over mechano-chemically prepared $PdAcCeO_2M$ catalysts. Isotopically labeled DRIFTS highlighted that intermediate $CO_2$ hydrogenation steps played a key role in the overall DRM mechanism. Catalyst structure via in situ XRD and XPS discerned the structure/function evolution for $PdAcCeO_2$ during DRM.

## 556 AB

### MONDAY MORNING

### C-C Bond Formation

Session Chairs: Joseph DeWilde, *The Dow Chemical Company, USA* and Brent H. Shanks, *Center for Biorenewable Chemicals (CBiRC), USA*.

9:30 AM **Mon-556AB-0930** Upgrading Biomass through the Aldol Condensation Using Cooperative Interactions in Aminosilica Materials: Discovering Different Types of Catalytic Sites in Aminosilica Materials and the Stability.
**Jee-Yee Chen** and Nick Brunelli, *The Ohio State University, USA*.

**Short Summary:**
Site quantification experiments successfully revealed complexity of the aminosilica catalytic materials which have four types of sites, and the fraction of each site depends on the surface loading. Recycled catalysts have shown high activity sites transformed into lower activity sites. Elucidating synthesis-structure-function relationships aminosilica materials for the aldol reaction.

9:50 AM **Mon-556AB-0950** Controlling Aldolization over Mg-Al Mixed Oxides Derived from Alkali-Free Layered Double Hydroxides.
**Davi Petrolini**, Ho-Yi Lam, Prashant Deshlahra and Nat Eagan, *Tufts University, USA*.

**Short Summary:**
Mixed oxides of magnesium and aluminum were prepared via alkali-free methods to produce aldolization-active materials of comparable structure across varied pretreatment conditions. Ex-situ characterizations, kinetic modeling of reactor data, and in-situ titrations unveil details about site requirements. Comparable quantum chemistry simulations further explain the role aluminum plays in these materials.

10:10 AM **Mon-556AB-1010** Mechanistic Insights on C-C Coupling Reactions Catalyzed By Uio-66 Acid Catalysts.
**Julian Schmid**, Oliver Y. Gutierrez and Johannes A. Lercher, *Pacific Northwest National Laboratory, USA*.

**Short Summary:**
The modification of missing-linker defects in MOFs increased their activity for C-C coupling reactions using both renewable and fossil feedstocks (aldol condensation and oligomerization of light olefins). We harness the high degree of periodicity of MOFs on a molecular level to provide structure-reactivity correlations and detailed mechanisms proposals.

10:30 AM **Mon-556AB-1030** Assessing the Mechanism and Active Sites in Alkene Dimerization on Ni Grafted within Mesoporous Solids: (Ni–OH)+ Centers and C–C Coupling Mediated By Lewis Acid-Base Pairs.
Nicholas Jaegers, Iker Agirrezabal-Telleria and **Enrique Iglesia**, *University of California, Berkeley, USA*.

**Short Summary:**
Alkene dimerization proceeds with low activation barriers via concerted interactions at $(Ni–OH)^+$ acid-base pairs. Such pathways have not been previously considered and differ in the nature of the steps, the active sites required, and the need for co-catalysts or activators from metallacyle and Cossee-Arlman routes that prevail on molecular catalysts.

10:50 AM **Mon-556AB-1050** Influence of Lewis Acidity and Confinement on Aldehyde Enolization and C-C Coupling in Beta Zeolites.
Wenlin He[1], David Potts[2], David Flaherty[2] and **Viktor Cybulskis**[1], *(1)Syracuse University, USA, (2)University of Illinois Urbana-Champaign, USA*.

**Short Summary:**
Isolated metal sites in M-*BEA catalyze competitive condensation events between bound enolates and carbonyls compounds ($C_3$, $C_{10}$) with rate differences that are influenced by the functional Lewis acid strength of the metal center and interactions between reacting molecules and the surrounding voids.

11:10 AM **Mon-556AB-1110** Insights into the Catalytic Promotion of Propylene Metathesis over Silica-Supported Molybdenum Oxide Using Substituted Olefins.
**Ran Zhu**1, Husain Adamji[1], Zachariah Berkson[2], Jie Zhu1, Ashley Head[3], Heather Kulik[4], Christophe Copéret[2] and Yuriy Roman[1], *(1)Massachusetts Institute of Technology, USA, (2)ETH Zürich, Switzerland, (3)Brookhaven National Laboratory, USA, (4)MIT, USA*.

**Short Summary:**
Co-feeding 1 mol% 2,3-dimethyl-2-butene (4ME), we observed a 10-100x increase in the steady state rate of propylene metathesis on $MoO_x/SiO_2$. Based on our kinetic and spectroscopic results, we propose that the promoter facilitates the active site formation via a 1,2-proton shift mechanism, explaining the promotion effect in the steady-state rate.

11:30 AM **Mon-556AB-1130** Oleofurans As Intermediates to High Value Products: Synthesis and Conversion Pathways.
Nicholas Gadinas[1], Shawn Eady[2], Kyle Reem[1], Christoph Krumm[2] and **Kostas Goulas**[1], *(1)Oregon State University, USA, (2)Sironix Renewables, USA*.

**Short Summary:**
Oleofurans are molecules that are produced via C-C bond formation reactions between furanic molecules and long-chain oxygenates. Their cost-competitive production is achieved via a two-step aldol condensation and hydrodeoxygenation process. The oleofurans are then converted to sulfonate detergents.

## MONDAY AFTERNOON

### New Carbon Dioxide Activation Methods

Session Chairs: Elizabeth Biddinger, *The City College of New York, CUNY, USA* and Stephen Schuyten, *Johnson Matthey, USA*.

1:20 PM **Mon-556AB-1320** Eager for the Spotlight: TiN As a Plasmonic Support for Photothermal $CO_2$ Methanation.
**Yi Fen Zhu**, Bingqiao Xie, Rose Amal, Emma Lovell and Jason Scott, *University of New South Wales, Australia*.

**Short Summary:**
TiN was implemented as a plasmonic support for a Ni catalyst to promote high $CH_4$ selectivity for $CO_2$ methanation. The catalyst configuration preserves the high hydrogenation ability of Ni, which is critical for $CH_4$ synthesis, while imposing the plasmonic phenomenon via the TiN as well as possible charge participation.

1:40 PM **Mon-556AB-1340** Sunlight Powered Continuous Flow $CO_2$ Reduction to CO Using a Plasmonic Nanocatalyst.
Pau Martinez Molina[1], Koen W. Bossers[1], Jelle Rohlfs[1], Nicole Meulendijks[1], Marcel Verheijen[2], Pascal Buskens[3] and **Francesc Sastre**[1], *(1)The Netherlands Organisation for Applied Scientific Research, Netherlands, (2)Eurofins Materials Science, Netherlands, (3)Hasselt University, Netherlands*.

**Short Summary:**
Continuous flow experiment under solar light illumination (14 suns) without any external heating showed a CO production rate of $4086 mmol\cdot m^{-2}\cdot h^{-1}$ with an apparent quantum efficiency (AQE) 3.2%. We provide a catalyst bed thickness optimization to elucidate the different irradiations regimes and get a deeper understanding of the light illumination effect.

2:00 PM **Mon-556AB-1400** Plasma-Assisted Catalytic Hydrogenation of Carbon Dioxide to Higher Hydrocarbons: Significance of Support Dielectric Constant.
**Berkay Ekinci**, Xiaoxing Wang, Sean Knecht and Sven Bilén, *The Pennsylvania State University, USA*.

**Short Summary:**
A promising recent approach to $CO_2$ conversion and utilization is the incorporation of low-temperature plasma (LTP) technology to enhance the catalytic process. We have investigated plasma-catalytic $CO_2$ hydrogenation over a series of catalyst-and-support combinations and report a combination that promotes C2+ selectivity/production at relatively lower steady-state voltage.

2:20 PM **Mon-556AB-1420** Carbon Dioxide Valorization: Using Visible Light to Enhance Thermal Catalysis.
Sana Ullah, Yi Fen Zhu, George O'Connell, Jason Scott, Rose Amal and **Emma Lovell**, *University of New South Wales, Australia*.

**Short Summary:**
The valorization $CO_2$ to value added products is of great interest. To capture the benefits of visible light illumination, to offset thermal energy requirements, the surface basicity and defect density of the support is vital. This work provides a pathway for future directions in catalyst design for photo-thermal conversions.

2:40 PM **Mon-556AB-1440** Electrified Catalytic Processes for $CO_2$ Valorization: Joule-Heated $CO_2$ Reforming of Methane and Reverse Water-Gas Shift.
**Lei Zheng**, Federico Nicolini, Matteo Ambrosetti, Alessandra Beretta, Gianpiero Groppi and Enrico Tronconi, *Politecnico di Milano, Italy*.

**Short Summary:**
Joule-heated $CO_2$ reforming of methane and reverse water-gas shift could drastically reduce the carbon footprint of hydrogen and syngas production by consuming $CO_2$ as a feedstock, and by replacing fuel combustion heating with Joule heating based on renewable electric energy.

3:00 PM **Mon-556AB-1500** A Critical View on Direct Syngas to Aromatics over Combined Zinc Oxide on Zirconia and H-ZSM-5.
**Michael Nikolajsen**[1], Martin Høj[1], Jakob M. Christensen[1], Niels Christian Schjødt[2], Uffe V. Mentzel[2] and Jens Sehested ,
*(1)Technical University of Denmark, Denmark, (2)Haldor Topsøe A/S, Denmark, (3)Haldor Topsoe A/S, Denmark*.

**Short Summary:**
Zinc oxide supported on zirconia combined with ZSM-5 has been tested for the direct conversion of $CO_2$ to aromatics. The findings question the possibility of producing aromatics with a selectivity above 70%. The competition between olefin hydrogenation and aromatization reactions and the high hydrogen partial pressure limits aromatic selectivity.

## Operando and In Situ Techniques

Session Chairs: Israel Wachs, *Lehigh University, USA* and Peter Crozier, *Arizona State University, USA*.

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3:45 PM **Mon-556AB-1545** Shedding Light on the Deactivation Pathways of a CrO$_x$/Al$_2$O$_3$ Dehydrogenation Catalyst with Emission Spectroscopy.
**Jason Malizia** and Rebecca Fushimi, *Idaho National Laboratory, USA*.

**Short Summary:**
This work shows photoluminescence spectroscopy as a novel approach to directly detect the onset and acceleration of Cr$^{3+}$ solid state diffusion, a critical physical deactivation pathway that limits the lifetime of the CrO$_x$/Al$_2$O$_3$ propane dehydrogenation catalyst used in the commercial Catofin process.

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4:05 PM **Mon-556AB-1605** Fluorescent-Probe Characterization for Pore-Space Mapping via Single-Particle Tracking.
**Rafael Mayorga Gonzalez** and Florian Meirer, *Utrecht University, Netherlands*.

**Short Summary:**
Single particle tracking can be used to characterize porous materials. However, diffusion in catalysts involves complex probe-host interactions. We developed a well-defined model-pore to track individual probes as they diffuse within it. This will allow us to catalogue their behavior in confinement before using them to characterize real-life catalysts.

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4:25 PM **Mon-556AB-1625** Coupling Catalytic Reactions and In-Situ Bulk Characterization to Track Surface Evolution during Synthesis of Pd-Zn Alloy Catalysts.
**Ahmed Maged Aly Hamed** and Rob Rioux, *Pennsylvania State University, USA*.

**Short Summary:**
The Pd-Zn bimetallic system is characterized by numerous alloys and intermetallic structures with distinct catalytic active sites and well-studied kinetic parameters that can distinguish the surface of these structures. Coupled with in-situ XRD the relationship between bulk and surface alloying of Pd and Zn is explored.

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4:45 PM **Mon-556AB-1645** Crystallite Size Dependent Oxidation of Ni Catalysts Revealed By *in Situ* Magnetometry.
**Dominic de Oliveira**[1], Nico Fischer[2], Michael Higham[3], C. Richard A. Catlow[4] and Michael Claeys[1], *(1)University of Cape Town, South Africa, (2)Catalysis Institute and c*change (DSI-NRF Centre of Excellence in Catalysis), University of Cape Town, South Africa, (3)University College London, United Kingdom, (4)Cardiff University, United Kingdom*.

**Short Summary:**
This work shows the importance of in situ characterization and specifically the advantage of in situ magnetic characterization, with the live observation of the oxidation of Ni being detected under working conditions without the exposure of these air sensitive materials to air.

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5:05 PM **Mon-556AB-1705** Transient PRBS Gas Injections for Determination of Robust Heterogeneous Catalytic Reaction Mechanisms.
**Zayne Weber**[1], Ran Wang[1], Antonios Armaou[1], Michael Janik[2] and Rob Rioux[1], *(1)Pennsylvania State University, USA, (2)The Pennsylvania State University, USA*.

**Short Summary:**
Determination of elementary rate constants of complex catalytic mechanisms is achieved through transient pseudo random binary sequence (PRBS) gas pulse experiments. This method leads to reduced experimental time, while also supplying microkinetic models with a more robust data stream leading to rate constants calculated with higher confidence.

# Ballroom A

### MONDAY MORNING

## Applications of In Situ Microscopy

Session Chairs: Nina Genz, *Paul-Scherrer-Institut, Switzerland* and Adam Hoffman, *SLAC National Accelerator Laboratory, USA*.

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9:30 AM **Mon-BLRMA-0930** Restructuring of TiO$_x$ Overlayers over Ni Nanoparticles during Catalysis.
**Matteo Monai**[1], Kellie Jenkinson[2], Angela Melcherts[1], Jaap Louwen[1], Ece Irmak[2], Sandra Van Aert[2], Thomas Altantzis[3], Charlotte Vogt[4], Ward van der Stam[1], Tomáš Duchoň[5], Břetislav Šmíd[6], Esther Groeneveld[7], Peter Berben[7], Sara Bals[2] and Bert M. Weckhuysen[1], *(1)Utrecht University, Netherlands, (2)EMAT and NANOlab Center of Excellence, University of Antwerp, Belgium, (3)ELCAT, University of Antwerp, Belgium, (4)Technion - Israel Institute of Technology, Israel, (5)Peter-Grünberg-Institut 6, Forschungszentrum Jülich GmbH, Germany, (6)Charles University, V Holešovičkách 2, Czech Republic, (7)BASF Nederland B.V., Netherlands*.

**Short Summary:**
Using multiscale *operando* techniques, this study reveals that strong metal-support interaction in Ni/TiO$_2$ restructures under CO$_2$ hydrogenation conditions, leading to (partial) re-exposure and modification of active sites, and a performance that strongly depends on the reduction temperature.

9:50 AM **Mon-BLRMA-0950** Structure-Reactivity Relationships in Zinc-Based Bifunctional Catalysts for Direct Syngas Conversion to Olefins.
**David Yancey**[1], Vera Santos[2], Glenn Pollefeyt[2], Alexey Kirilin[2], Adam Chojecki[2], Davy Nieskens[2] and Andre Malek[2], *(1)The Dow Chemical Company, USA, (2)The Dow Chemical Company, Netherlands*.

**Short Summary:**
Advanced characterization tools are used to understand the structure of zinc-based methanol catalysts used in bifunctional conversion of syngas to hydrocarbons. Understanding of catalyst activity, selectivity and deactivation mechanisms are achieved and discussed.

10:10 AM **Mon-BLRMA-1010** Atomic Level Fluxional Behavior and Activity of $CeO_2$-Supported Pt Catalysts for CO Oxidation.
**Peter Crozier**, *Arizona State University, USA*.

**Short Summary:**
We investigate the structural dynamics taking place on a Pt/$CeO_2$ catalyst performing CO oxidation. Using operando TEM, we are able to show that fluxional behavior in the Pt nanoparticles and nearby $CeO_2$ surface increases with the turnover frequency.

10:30 AM **Mon-BLRMA-1030** Dynamics of Nanoparticle Motion and Metal-Oxide Support in Redox-Reactive Gases.
**Arik Beck**[1], Hannes Frey[1], Xing Huang[2], Jeroen A. van Bokhoven[1] and Marc-Georg Willinger[3], *(1)ETH Zürich, Switzerland, (2)Fuzhou University, China, (3)TU Munich, Germany*.

**Short Summary:**
Operando TEM revealed that the strong metal-support interaction (SMSI)–induced encapsulation of platinum particles on titania observed under reducing conditions is lost and nanoparticle dynamics start once the system is exposed to a redox-reactive environment.

10:50 AM **Mon-BLRMA-1050** MEMS-Based Microreactor for *in-Situ/Operando* High-Resolution 3D X-Ray Microscopy of Single Catalyst Particles.
**Luca Carnevale**[1], Alessia Broccoli[1], Rafael Mayorga Gonzalez[2], Thomas P. van Swieten[2], Jarno Groenesteijn[1], Kechun Ma[1], Remco J. Wiegerink[1], Bert M. Weckhuysen[2], Florian Meirer[2], Wouter Olthuis[1] and Mathieu Odijk[1], *(1)University of Twente, Netherlands, (2)Utrecht University, Netherlands*.

**Short Summary:**
A new MEMS-based microreactor for *in-situ/operando* X-ray imaging is proposed. Our device allows to trap and study an individual catalyst particle of up to ~100 micrometers in size under real process conditions (temperature up to 400 °C and pressure up to 30 bar).

11:10 AM ***KEYNOTE* Mon-BLRMA-1110 Understanding Catalysts using Advanced Methods in the Transmission Electron Microscope. Ilke Arslan**, *Argonne National Laboratory, USA*.

**Short Summary:**
Electron microscopy is a key method used in the characterization of catalysts due to the spatial resolution achievable with electrons. Using advanced methods in the TEM, catalysts can be characterized more accurately with 3-D imaging, and more closely to their native environments with in-situ imaging.

## MONDAY AFTERNOON

### Catalyst Manufacturing

Session Chairs: Karen Wilson, *Griffith University, Australia* and Maureen Bricker, , .

1:20 PM ***KEYNOTE* Mon-BLRMA-1320 Catalyst Manufacturing Science - Challenges and Opportunities. Jean Beeckman**, *retired, USA*.

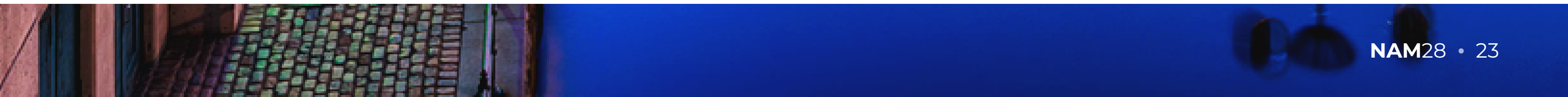
**Short Summary:**
Discussed first are general methods of catalyst manufacture. Thereafter, catalyst bending strength is applied in the prediction of the length to diameter ratio of catalyst extrudates in commercial plants. Very deep networks (VDN) are shown to realistically represent the pore spare of commercial catalysts.

2:00 PM **Mon-BLRMA-1400** Industrial Aspects of Catalyst Manufacturing..
**Raimond Bonné**, *Euro Support Catalyst Group BV, Netherlands*.

**Short Summary:**
A short overview of industrial aspects of successful catalyst manufacturing is presented in which a few examples of manufacturing process steps and their impact on catalyst quality are highlighted.

2:20 PM **Mon-BLRMA-1420** Natural Gas Reforming to Syngas Using Additively Manufactured Catalysts.
**Matthew Ide**, *ExxonMobil, USA*.

**Short Summary:**
Advanced manufacturing is a transformative approach that enables the rapid synthesis of any geometry composed of a wide range of materials. Many technologies in the energy industry suffer from coking and subsequent deactivation. This work discusses manufacturing materials capable of switching between two different environments with enhanced catalytic activity.



2:40 PM **Mon-BLRMA-1440** Interfacial Restructuring Behavior of Copper Oxides/Fluorite-Structured High-Entropy Oxides upon Heterostructure Construction Towards Enhanced Catalysis.
**Meijia Li**[1], Zhenzhen Yang[2] and Sheng Dai[2], *(1)Oak Ridge National Laboratory, USA, (2)Oak Ridge National laboratory, USA*.

**Short Summary:**
A facile method to activate and stabilize the conventional CuO catalyst via heterostructure construction with high entropy fluorite oxide is introduced. The high energetic ball milling procedure was proved to be an effective method to create abundant oxygen vacancies and active species in CuO-HEFO composite.

3:00 PM **Mon-BLRMA-1500** Citral to Menthol Transformations in Flow over Extruded Catalysts.
Zuzana Vajglova[1], Irina L. Simakova[1,2], Narendra Kumar[1], Päivi Mäki-Arvela[1], Kari Eränen[1] and **Dmitry Murzin**[1], *(1)Åbo Akademi University, Finland, (2)Boreskov Institute of Catalysis, Russian Federation*.

**Short Summary:**
One-pot continuous synthesis of menthols from citral was performed in a trickle bed reactor over bifunctional catalysts shaped to extrudates with different binders. Catalytic behavior was dependent on the metal type, location, acidity and binder. Ni supported on MCM-41 and shaped with sepiolite afforded high selectivity to menthols of 75%.

## New Concepts in Electrocatalysis I

Session Chairs: Adam Holewinski, *University of Colorado at Boulder, USA* and Christopher Muhich, *Arizona State University, USA*.

3:45 PM **Mon-BLRMA-1545** Strain and Buckling of Pt(111) during Chronoamperometry between 0.6 and 1.1 $V_{RHE}$.
**Arthur Shih**[1,2], Kasinath Ojha[1], Mingchuan Luo[1], Xiaoting Chen[1], Guangdong Liu[3], Zhiqin Liang[1], Matias Villalba[1], Francesc Valls Mascaró[1], Hassan Javed[1], Rafaël Vos[1], Huiqiu Deng[3], Jeffrey Greeley[4], Zhenhua Zeng[4] and Marc Koper[1], *(1)Leiden University, Netherlands, (2)Northwestern University, USA, (3)Hunan University, China, (4)Purdue University, USA*.

**Short Summary:**
An anomalous reduction feature at ~0.53 $V_{RHE}$ in the Pt(111) cyclic voltammogram after chronoamperometry in the PtOH region (0.6 to 1.1 $V_{RHE}$) in Ar-saturated $HClO_4$ is observed. We attribute this to thermodynamically-stable $PtO_xH_y$ (x, y = 0, 1, 2) and discuss implications on CO oxidation and oxygen reduction.

4:05 PM **Mon-BLRMA-1605** Restructuring and Activation of Cu (111) Under Electrocatalytic Reduction Conditions.
**Dongfang Cheng**1, Anastassia Alexandrova[1] and Philippe Sautet[1,2], *(1)University of California, Los Angeles, USA, (2)University of California Los Angeles, USA*.

**Short Summary:**
We unravel the potential- and pH-dependent restructuring of Cu (111) in acidic electrolyte by joint first-principles calculations and operando ECSTM experiments. At reductive potential, Cu (111) is covered by a high density of H atoms, and below a threshold potential, Cu adatoms are formed on the surface, in (4×4) superstructure.

4:25 PM ***KEYNOTE*** **Mon-BLRMA-1625 Platinum Group Metal-free Electrocatalysts for Hydrogen Generation and Conversion.**
Luigi Osmieri, Hanguang Zhang, Wilton Kort-Kamp, Edward Holby and **Piotr Zelenay**, *Los Alamos National Laboratory, USA*.

**Short Summary:**
In this presentation, we summarize recent progress in the development of platinum group metal-free electrocatalysts for oxygen reduction reaction in polymer electrolyte fuel cells, and oxygen and hydrogen evolution reactions in low-temperature electrolyzers operating with anion exchange membrane. The presentation covers both experimental and theoretical parts of the effort.

5:05 PM **Mon-BLRMA-1705** Activation Energies of Reactions at Electrochemical Interface.
**Yuanyue Liu**, *University of Texas at Austin, USA*.

**Short Summary:**
There is very limited information about the activation energies of heterogeneous electrochemistry. Here we present a atomistic model to simulate the reaction kinetics at electrochemical interface, and its application to elucidate the kinetic mechanisms of single metal atom in graphene for catalyzing carbon dioxide and oxygen reductions.

# Ballroom BC

### MONDAY MORNING

## Catalysis for Aquatic Environment Remediation

Session Chairs: Rohil Daya, *Cummins Inc., USA* and Arthur Shih, *Northwestern University, USA*.

9:30 AM **Mon-BLRMBC-0930** Understanding the Stability and Performance of (earth-abundant) MOFs in Oxidative Degradation of Aqueous Pollutants.
**Samuel Moore** and Michele Sarazen, *Princeton University, USA*.

**Short Summary:**
In a wider effort to understand structure-functional relationships on earth-abundant MOFs for use in aqueous pollutant degradation, this study qualifies previous reports by showing that while MIL-101(Fe) outperforms MIL-88B(Fe) in the breakdown of methylene blue dye on an iron-normalized basis, leaching is present in the aqueous-phase.

9:50 AM **Mon-BLRMBC-0950** Catalytic Remediation of Chlorophenolic Compounds in Drinking Water: Understanding the Reaction Mechanism Using DFT Simulations.
**Chaitra Shenoy**[1], Shelaka Gupta[2], Tuhin S. Khan[3], Mayank Agrawal[4] and M. Ali Haider[1], *(1)Indian Institute of Technology Delhi, India, (2)Indian Institute of Technology Hyderabad, India, (3)CSIR-Indian Institute of Petroleum, India, (4)Brown University, USA*.

**Short Summary:**
For the hydrodechlorination (HDC) reaction, it is of utmost importance to design catalysts that can resist severe deactivation effects due to chlorine poisoning. The present study is an attempt to gain insights into the reaction mechanism of 4-chlorophenol over Pd (111) surface.

10:10 AM **Mon-BLRMBC-1010** From "Single" to "It's Complicated": Single Atom Ensembles for Selective Dehalogenation.
**Kali Rigby**[1], Chiheng Chu[1], Dahong Huang[1], Christopher Muhich[2], Jaehong Kim[1] and Eli Stavitski[3], *(1)Yale University, USA, (2)Arizona State University, USA, (3)Brookhaven National Laboratory, USA*.

**Short Summary:**
Single atom catalysts (SAC) exhibit superior selectivity over nanoparticulate catalysts for many catalytic reactions. However, selectively is often accompanied by loss of activity. Here we demonstrate that neighboring Pd SACs retain selectivity, while the cooperative interactions between neighboring atoms greatly enhance the activity for hydrogenation of carbon-halogen bonds.

10:30 AM **Mon-BLRMBC-1030** Catalysts for the on-Demand Production of Green Oxidants in the Treatment, Purification and Reuse of Produced Water..
**Michael Reynolds**[1], Christian L. Coonrod[2] and Michael S. Wong[2], *(1)Shell USA, Inc, USA, (2)Rice University, USA*.

**Short Summary:**
Recovering hydrocarbons from shale reservoirs is a water intensive process that uses 10.5 MM gallons/well of water. These volumes justify the need for water recycle and reuse. This presentation will describe a joint industry and academia effort to treat and reuse produced water through the catalytic production of green oxidants.

10:50 AM **Mon-BLRMBC-1050** Catalytic Reduction of Nitrate to Nitrous Oxide with a Rhenium(V) Complex.
**Joerg Schachner**, *University of Graz, Austria*.

**Short Summary:**
The oxidorhenium(V) complex ReOCl(dmoz)2 shows promising activity in the catalytic reduction of nitrate to $N_2$. It catalyzes the reduction of nitrate via nitrite to NO in aqueous environment. Further reduction is not inhibited, as the Re(V) complex does not form a stable nitrosyl complex, based on its high oxidation state.

11:10 AM **Mon-BLRMBC-1110** Assessing Nitrate Reduction Molecular Electrocatalysis in Real Wastewaters for Reactive Separation of Ammonia.
**Dean Miller**[1], Matthew Liu[1], Jinyu Guo[1], Brandon Clark[1] and William Tarpeh[1,2], *(1)Stanford University, USA, (2)SLAC National Accelerator Laboratory, USA*.

**Short Summary:**
Wastewater nitrate valorization via electrochemical nitrate reduction requires separation of produced ammonia from the catalyst and treated wastewater, and operation in complex electrolytes with dilute nitrate concentrations. We evaluate a homogeneous molecular electrocatalyst in reactive separations architectures to interrogate catalyst inhibition mechanisms and controls to enhance performance in real wastewaters.

11:30 AM **Mon-BLRMBC-1130** Electrodialysis and Nitrate Reduction to Enable Distributed Ammonia Manufacturing from Wastewaters.
Jinyu Guo[1], Matthew Liu[1], Chloe Laguna[1], Sarah Blair[1], Brandon Clark[1], Kuai Fang[1], Dean Miller[1], Zach Perzan[1], Corisa Wong[1], Adam Nielander[1,2], David Lobell[1], Meagan Mauter[1], Kate Maher[1], Thomas F. Jaramillo[1,2] and **William Tarpeh**[1,2], *(1)Stanford University, USA, (2)SLAC National Accelerator Laboratory, USA*.

**Short Summary:**
We propose a novel electrochemical reactive separation process, Electrodialysis and Nitrate Reduction (EDNR) to efficiently couple water purification and ammonia production from reactive N-polluted wastewaters. By engineering the reaction environment and operation parameters, we recovered close to 100% influent nitrate and ammonium pollutants as ammonia.

## MONDAY AFTERNOON

## Photocatalysis I

Session Chairs: Eranda Nikolla, *University of Michigan,* and Pu-Xian Gao, *University of Connecticut, USA*.

1:20 PM **Mon-BLRMBC-1320** Analysis of the Role of Electrocatalyst/Semiconductor Interfaces in Solar Water Splitting.
**Ahmet Sert**, Aarti Mathur, John Hemmerling and Suljo Linic, *University of Michigan, USA*.

**Short Summary:**
We experimentally and computationally demonstrated significant photovoltage enhancements in metal–insulator–semiconductor (MIS) photoelectrocatalysts by precisely modulating the thickness of the insulator layer, which tunes the charge carrier fluxes and recombination. The competing recombination mechanisms and the upper performance limits for MIS photoelectrocatalysts were quantified.

1:40 PM **Mon-BLRMBC-1340** Design of Metal-Organic Frameworks and Reaction Systems for Efficient Photocatalytic $H_2O_2$ Production.
**Hiromi Yamashita**[1], Yoshifumi Kondo[1], Yasutaka Kuwahara[1,2] and Kohsuke Mori[1], *(1)Osaka University, Japan, (2)JST, Japan*.

**Short Summary:**
The design flexibility of MOFs not only enables the development of highly efficient photocatalysts but also constructs rational reaction systems for photocatalytic $H_2O_2$ production. The modifications of MOFs with co-catalyst Ni and missing-linker defects and the utilization of two-phase reaction system are effective for efficient photocatalytic $H_2O_2$ production.

2:00 PM **Mon-BLRMBC-1400** Photocatalytic Reduction of $CO_2$ to CO in Water Using a CNQD·[Fe-p-TMA] Hybrid Assembly.
Liam Mistry, Long Le-Quang, Gerard Masdeu, Wilma Björkman, **Hanna Härelind** and Maria Abrahamsson, *Chalmers University of Technology, Sweden*.

**Short Summary:**
We present an efficient and selective water-soluble photocatalytic system with an iron-porphyrin catalyst electrostatically coupled to functionalized carbon nitride quantum dots for the reduction of $CO_2$-to-CO, using visible light. The hybrid assembly shows excellent performance under mild conditions with high TON and selectivity around 96 % in water.

2:20 PM **Mon-BLRMBC-1420** Towards Elucidating the Structure-Performance Relationship in Nanoscale Photocatalysts for Environmental Methane Oxidation.
**Max Kessler**, Richard Randall, Eddie Sun, Gang Wan and Arun Majumdar, *Stanford University, USA*.

**Short Summary:**
Total oxidation of methane is gaining attention as a means to draw down this highly potent greenhouse gas in the atmosphere. We elucidate the structure-performance relationship of titanium dioxide and co-catalysts for the photocatalytic oxidation of methane and investigate the effect of other reactive molecules often present in the atmosphere.

2:40 PM **Mon-BLRMBC-1440** Thermo-Photo Catalytic Oxidation of Methane on Hematite Nanosheets Functionalized with Silver Nanoparticles.
**Jake Heinlein**, Gaukhar Alzhanova, Manav Singh, Shu Hu and Lisa Pfefferle, *Yale University, USA*.

**Short Summary:**
Hematite ($\alpha$-$Fe_2O_3$) nanosheets functionalized with silver nanoparticles (AgNPs) were synthesized and shown to improve the performance of the bare nanosheets for the methane oxidation reaction by incorporating both light and heat energy. Mechanistic studies show the effect of varying temperature and light intensity on fundamental methane activation and conversion.

3:00 PM **Mon-BLRMBC-1500** Kinetic Studies on Using Plasmonic Photocatalytic Coatings for Autogenously Improving Indoor Air Quality By Removing Volatile Organic Compound.
**Samuel Ojo** and (Bill) Yu Xiong, *Case Western Reserve University, USA*.

**Short Summary:**
An holistic finite element model (FEM) simulations to evaluate the performance of plasmonic photocatalyst in air quality improvements and compare that with C-/N- doped-$TiO_2$.

## Photocatalysis II

Session Chairs: Siddharth Deshpande, *University of Delaware, USA* and Raul Lobo, *University of Delaware, USA*.

3:45 PM ***KEYNOTE*** **Mon-BLRMBC-1545 Defects for the Enhancement of Photocatalytic Activity. Akira Yamakata**, *Okayama University, Japan*.

**Short Summary:**
Powder defects control the photocatalytic activity since they sometimes accelerate the recombination but sometimes decelerate the recombination: the difference is determined by the distance among the defects.

4:25 PM **Mon-BLRMBC-1625** Direct Evidence for Sulfur Induced Deep Electron and Hole Traps in Titania.
Amir Rahmani-Chokanlu[1], Akbar Mahdavi[1,2], Liping Yu[1], Thomas J. Schwartz[1], Rachel Austin[2] and **Brian Frederick**[1], *(1)University of Maine, USA, (2)Barnard College, USA*.

**Short Summary:**
The effect of sulfating titania on photocatalytic activity is contradictory, as both electron and hole traps have been proposed. We report partially unoccupied states ~2.8 eV below the CBM, assigned to S5+ on a titanium lattice site in non-stoichiometric $TiO_2$+x, which explains their role as both electron and hole traps.

4:45 PM **Mon-BLRMBC-1645** Photon and Charge Carrier Utilization in Photo-Enhanced Ammonia Synthesis.
**Carissa S. Yim**, Andrew J. Gayle, Alexander J. Hill, Sijun Seong, Xiwen Gong, Neil P. Dasgupta, Galen B. Fisher, Andrej Lenert and Johannes W. Schwank, *University of Michigan-Ann Arbor, USA*.

**Short Summary:**
This work examines photoluminescence (PL) as a characterization tool to optimize Ru/$TiO_2$ photocatalysts for carbon-free, small scale ammonia synthesis. PL shows that parasitic absorption of light by Ru is a substantial photon loss mechanism in the system and indicates that charge-carrier lifetime decreases with increasing temperature.

5:05 PM **Mon-BLRMBC-1705** Plasmon-Assisted Direct Charge Transfer Drives Surface Reactions.
Taha Salavati Fard, Tien Le and **Bin Wang**, *University of Oklahoma, USA*.

**Short Summary:**
In this contribution, we take advantage of previous experiments that were performed with relatively simple reactions under well-controlled conditions and benchmark first-principles calculations of the excitation energy, through which we report that direct interfacial charge transfer between metal and the empty molecular orbitals can quantitatively explain the experimental observations.

## Ballroom DE

### MONDAY MORNING

### New Directions in $NH_3$ Synthesis

Session Chairs: William Schneider, *University of Notre Dame, USA* and Feng Gao, *Pacific Northwest National Laboratory, USA*.

9:30 AM ***KEYNOTE*** **Mon-BLRMDE-0930 Electrochemical Activation of Molecular Nitrogen to Ammonia: Scaling up. Ib Chorkendorff**, *Technical University of Denmark, Denmark*.

**Short Summary:**
In this presentation a short review of the current background and status of the field of electrochemical ammonia synthesis shall be given. The path towards an up-scaling of the process using a fuel cell design will be discussed along with recent progress.

10:10 AM **Mon-BLRMDE-1010** Synthesis of Transition Metal Nitride Catalysts for Mechanocatalytic Ammonia Production.
**Jacob DeWitt**, Erin Phillips, Karoline Lena Hebisch, Andrew Tricker and Carsten Sievers, *Georgia Institute of Technology, USA*.

**Short Summary:**
Mechanocatalytic ammonia synthesis is a novel approach toward ammonia synthesis under mild conditions. To this end, the nitride phase formation and structural evolution of an *in-situ* synthesized titanium nitride catalyst is explored and compared to other meta-stable transition metal nitrides for optimization of mechanochemical synthesis.

10:30 AM **Mon-BLRMDE-1030** In Operando Investigations of the Solid Electrolyte Interphase (SEI) Layer in the Electrochemical Li-Mediated Ammonia Synthesis.
**Niklas Henrik Deissler** and Ib Chorkendorff, *Technical University of Denmark, Denmark*.

**Short Summary:**
The components, formation, and changes of the SEI in the Li mediated nitrogen reduction were studied in operando by GI WAXS in a synchrotron setup. This allows for a time resolution in the seconds range, enabling the detection of temporarily present species and fluctuations of deposits on the electrode surface.

10:50 AM **Mon-BLRMDE-1050** Exploring Catalytic Systems in Microwave Mediated Reactions for Carbon Intensive Industries.
**Biswanath Dutta**[1,2], Chris Marin[3], Christina Wildfire[3], Douglas Kauffman[4] and Dushyant Shekhawat[3], *(1)National Energy Technology Laboratories, USA, (2)Leidos, USA, (3)National Energy Technology Laboratory, USA, (4)National Energy Technology Laboratory, DOE, USA*.

**Short Summary:**
Microwave-assisted ammonia synthesis and methane-dry-reforming are promising alternatives to the carbon-intensive Haber-Bosch and conventional methane-dry-reforming reactions. In this work, we report the catalytic performance of mixed-metal oxide/nitride catalysts under microwave conditions for these reactions, their active sites, and identify the root-cause of their catalytic-deactivation using kinetic and surface analysis studies

11:10 AM **Mon-BLRMDE-1110** Cation Additive Effects on Lithium-Mediated Nitrogen Reduction to Ammonia.
**Valerie Niemann**[1,2], Peter Benedek[1,2], Eric McShane[1], Adam Nielander[2], William Tarpeh[1,2] and Thomas F. Jaramillo[1,2], *(1)Stanford University, USA, (2)SLAC National Accelerator Laboratory, USA*.

**Short Summary:**
Our work demonstrates the effect of cation additives on the performance of lithium-mediated $N_2$ reduction to ammonia. We employ surface characterization methods to understand solid-electrolyte interphase (SEI) and catalyst composition-performance relationships.

11:30 AM **Mon-BLRMDE-1130** Cs-Promoted Ru Catalysts for Intermittent $NH_3$ Synthesis.
**Shih-Yuan Chen**, *National Institute of Advanced Science and Technology (AIST), Japan*.

**Short Summary:**
The Cs-Ru/SGCNT catalyst with active components of Cs-promoted Ru nanoparticles are highly active and durable in $NH_3$ synthesis under intermittent operation conditions. It would be a potential candidate for eHB $NH_3$ synthesis with which the electrolytic hydrogen production is varied by the supply of renewable electricity.

## Three-Way Catalysis and NOx Abatement I

Session Chairs: Annette Trunschke, *Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany* and Janos Szanyi, *Pacific Northwest National Laboratory, USA*.

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1:20 PM **Mon-BLRMDE-1320** Intra -Catalyst $CH_4$ Oxidation Pathways of a Pd/$Al_2O_3$-Based Commercial Catalyst and Implications on NOx Conversion Profiles for a Natural Gas Vehicle Exhaust Under Lambda Dithering.
**Dhruba Deka**[1], Calvin R. Thomas[2], Josh Pihl[1] and William Partridge[1], *(1)Oak Ridge National Laboratory, USA, (2)General Motors, USA*.

**Short Summary:**
Spatiotemporal measurement of natural gas engine exhaust pollutant concentrations along the flow channels of a Pd-based commercial three-way catalyst was performed with Spaci-MS. Measurements done under a wide range of lambda dithering conditions at multiple intra-catalyst locations shed light on $CH_4$ conversion pathways and their effect on NOx conversion.

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1:40 PM **Mon-BLRMDE-1340** Understanding the Nature of Pt-Rh Synergy for Three-Way Conversion Catalysis.
**Yuejin Li**[1], Ke-Bin Low[1], Andreas Sundermann[2], Haiyang Zhu[1], Luis Betancourt[1], Shaohua Xie[3] and Fudong Liu[3], *(1)BASF Corporation, USA, (2)hte GmbH, Germany, (3)University of Central Florida, USA*.

**Short Summary:**
The nature of Pt-Rh synergy for TWC was investigated using a variety of characterization tools. On Pt-Rh catalysts, more surface Rh species are formed relative to the Rh reference, some directly on the Pt particles. These surface Rh species are more reduced and responsible for the increased activity.

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2:00 PM **Mon-BLRMDE-1400** Spatio-Temporal Investigation of NO Reduction and CO Oxidation on Pt/$Al_2O_3$.
**Sui Wan**, Thomas Häber, Patrick Lott, Rainer Suntz and Olaf Deutschmann, *Karlsruhe Institute of Technology (KIT), Germany*.

**Short Summary:**
The spatially and temporally resolved absolute NO concentrations during NO reduction by CO over Pt/$Al_2O_3$ are obtained with quenching corrected PLIF. Reaction temperature and NO/CO ratio are associated with the deactivation of NO/CO reaction. The importance of the spatially resolved data is demonstrated via the comparisons of NO concentration gradients.

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2:20 PM **Mon-BLRMDE-1420** Emissions Control Catalyst Tolerance to Renewable Fuel-Based Phosphorous.
**Todd Toops**, Dhruba Deka and Jonathan Willocks, *Oak Ridge National Laboratory, USA*.

**Short Summary:**
To decarbonize the transportation industry renewable low-lifecycle carbon fuels can be used, but most contain some level of bio-based phosphorous (P) which impacts durability. Our efforts illustrate the impact through two emissions control configurations for both hydrocarbon oxidation and $NO_x$ reduction, but CO oxidation is not impacted.

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2:40 PM **Mon-BLRMDE-1440** NO Reduction By CO Kinetics on Rh/$Al_2O_3$: The Effect of Water and $NH_3$.
**Silvia Marino**, Sugandha Verma and William Epling, *University of Virginia, USA*.

**Short Summary:**
Combined kinetics and spectroscopy studies are used to study the effect of $H_2O$ and $NH_3$ on NO + CO reaction over a supported Rh catalyst. We observe that $H_2O$ (and $NH_3$) alters the apparent activation energy depending on the NO/CO ratio.

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3:00 PM WITHDRAWN: Zinc Stabilized Manganese Iron Spinel with High Oxygen Storage Capacity.
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## Three-Way Catalysis and NOx Abatement II

Session Chairs: Josh Pihl, *Oak Ridge National Laboratory, USA* and Nianqiang Wu, *University of Massachusetts Amherst, USA*.

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3:45 PM **Mon-BLRMDE-1545** Modeling NOx Reduction Using Surface Descriptors.
**Michael Tang**[1], Joakim Stenlid[1], Jinyu Guo[2], Elizabeth Corson[2], Milenia Mendoza[2], Matthew Liu[2], William Tarpeh[1] and Frank Abild-Pedersen[1], *(1)SLAC National Accelerator Laboratory, USA, (2)Stanford University, USA*.

**Short Summary:**
A microkinetic model of nitrate reduction in acidic conditions is presented to show how O* and H* surface descriptors are capable of mapping the activity of electrocatalysts for the reaction, alongside hydrogen evolution reaction. The role of proton concentration in the early steps of nitrate reduction is highlighted.

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4:05 PM **Mon-BLRMDE-1605** Atomically Dispersed Ruthenium on Reduced Ceria Surface Enables Low-Temperature $N_2o$ Reduction with CO.
**Inhak Song**, Yong Wang, Konstantin Khivantsev and Janos Szanyi, *Pacific Northwest National Laboratory, USA*.

**Short Summary:**
Atomically dispersed Ru on a ceria support can readily reduce $N_2O$ with CO at low temperatures below 200° C, which outperforms the atomically dispersed Rh/Ceria catalysts.

4:25 PM **Mon-BLRMDE-1625** Combined Experimental and Microkinetic Analysis for the Low-Temperature Formation of Nitrous Oxide on Pt/$Al_2O_3$.
**Sugandha Verma**, Silvia Marino, Carlos Weiler, Robert Davis, William Epling and Chris Paolucci, *University of Virginia, USA*.

**Short Summary:**
In this work, concerted kinetic experiments and molecular simulations reveal that low temperature $N_2O$ formation occurs on undercoordinated catalyst sites. The structure sensitive nature of this reaction can be utilized to design catalysts that reduce $N_2O$ emissions.

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4:45 PM **Mon-BLRMDE-1645** $N_2o$ Emissions Control in Nitric Acid Plant: Fe-FER Catalyst.
**Alberto Garbujo**[1], Fabio Oldani[1], Roberto Lanza[2], Emmanuel Rohart[3], Arnaud Lahougue[3] and Pierdomenico Biasi[1], *(1)Casale SA, Switzerland, (2)Verdant Chemical Technologies AB, Sweden, (3)EnerCat - ALSYS Group, France*.

**Short Summary:**
The fertilizer production was the largest source of $N_2O$ emissions in US. Laboratory results showed that Fe-FER is selective towards $N_2O$ conversion even after severe ageing. The study will contribute to the understanding of catalyst performance during the SoR and EoR which are essential aspects for reducing overall emissions.

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5:05 PM **Mon-BLRMDE-1705** Mechanistic Insights of Pd-Based Catalyst for $H_2$-SCR of Hydrogen-Fueled Engines.
**Kevin Keller**[1,2], Sui Wan[2], Michael Borchers[2], Thomas Häber[2], Rainer Suntz[1], Patrick Lott[2] and Olaf Deutschmann[2], *(1)Karlsruhe Institute of Technology, Germany, (2)Karlsruhe Institute of Technology (KIT), Germany*.

**Short Summary:**
The selective catalytic reduction of NOx with hydrogen as an onboard-reductant is considered an auspicious strategy for effective exhaust gas after-treatment of hydrogen-fueled combustion engines. Our study reveals the interactions between the catalyst formulation, influence of temperature, and exhaust gas composition on the catalysts' performance towards NO reduction during $H_2$-SCR.

## Rotunda

### MONDAY MORNING

### Electrosynthesis of Organic Compounds

Session Chairs: Mike Janik, *The Pennsylvania State University,* and Yuanyue Liu, *The University of Texas at Austin, USA*.

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9:30 AM **Mon-RTND-0930** Electrocatalytic Reduction for Electrochemical Synthesis.
**Matthew Neurock**, Sagar Udyavara, Sahithi Gorthy, Ashwin Chemburkar and Stuart Winikoff, *University of Minnesota, Twin Cities, USA*.

**Short Summary:**
The mechanisms for the electrocatalytic reduction of phenol-ethanol, model Birch reduction, and draws direct analogies to electrocatalytic $CO_2$ reduction and the importance of the electrolyte. Self-assembly of cationic intermediates near the negatively charged cathode facilitate the adsorption, electron and proton transfer by providing stabilizing 3D environment similar to enzymes.

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9:50 AM **Mon-RTND-0950** Selective Electrooxidation of Toluene to Benzyl Alcohol Catalyzed By Laser-Made [NiFe]-Layered Double Hydroxide Nanoparticles.
**Astrid Mueller**, *University of Rochester, USA*.

**Short Summary:**
Selective oxidation of toluene to benzyl alcohol, catalyzed by laser-made nickel–iron-layered double hydroxide nanosheets, was achieved in wet organic electrolytes by systematic variation of applied potential, reaction time, and electrolyte composition. Bivariate analysis of product selectivities enabled mechanistic insights into which solution species control selectivity for the alcohol.

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10:10 AM **Mon-RTND-1010** Synergistic Effects of Platinum and Transition Metal Carbides for Enhancing Glycerol Electrooxidation.
**Hansen Mou**[1], Qiaowan Chang[1], Shyam Kattel[2] and Jingguang Chen[1], *(1)Columbia University, USA, (2)Florida A&M University, USA*.

**Short Summary:**
Utilizing the synergy between platinum (Pt) and transition metal carbides (TMC), Pt/TMC catalysts in this work demonstrated enhanced glycerol oxidation activity and C-C bond cleavage selectivity compared to commercial Pt/C. This marked a promising step towards the application of glycerol as a fuel in direct alcohol fuel cells.

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10:30 AM **Mon-RTND-1030** Understanding the Mechanism of Electrocatalytic Glycolic Acid Oxidation.
**Mohammad Hasibul Hasan** and Ian McCrum, *Clarkson University, USA*.

**Short Summary:**
Understanding the mechanism of electrocatalytic oxidation will help us in better catalyst design for many important reaction. In this work, the electrocatalytic glycolic acid oxidation has been studied on Pt (111) surface. The oxidation reaction rate was found linearly correlated to the product of both adsorbed glycolate and OH coverage.

10:50 AM **Mon-RTND-1050** Electrified C–C Bond Formation at Hydroformylation Catalysts.
**Joy Zeng**[1], Chenyu Jiang[2], Jason Adams[2], Yuriy Roman[1] and Karthish Manthiram[2], *(1)Massachusetts Institute of Technology, USA, (2)California Institute of Technology, USA.*

**Short Summary:**
Rh-based hydroformylation catalysts are imported onto electrode surfaces to unlock an electrochemical hydroformylation reaction. The voltage-driven reaction is found to proceed more readily than its thermochemical analog at ambient temperatures. This work leverages a well-known thermochemical reaction to develop a new system for electrochemical C–C bond formation.

11:10 AM **Mon-RTND-1110** Single-Atom Doping on Manganese Oxide for Selective Alkene Epoxidation Via Electrochemical Water Activation.
**Minju Chung**[1], Kyoungsuk Jin[1] and Karthish Manthiram[2], *(1)Massachusetts Institute of Technology, USA, (2)California Institute of Technology, USA.*

**Short Summary:**
Galvanic replacement reactions were utilized for tuning Ir single-atoms on manganese oxide nanoparticles, which improved rate and Faradaic efficiency toward alkene epoxidation. Operando X-ray absorption spectroscopy revealed that Mn vacancies generated during galvanic replacement allowed the nanoparticles more susceptible to metal oxidation and catalyst reconstruction under an applied anodic potential.

11:30 AM **Mon-RTND-1130** Continuous Flow Electrochemical Alkene Epoxidations in Aqueous-Organic Electrolyte.
**Richa Ghosh**, Drew Hollyfield, Andrew Gewirth and David Flaherty, *University of Illinois Urbana-Champaign, USA.*

**Short Summary:**
We perform bulk electrolysis of $C_6H_{12}$ in aqueous-organic electrolytes with varying reactant ($C_6H_{12}$, $H_2O$) concentrations and potential coupled with in situ Raman spectroscopy to provide insight into the mechanism and influence of surface structure and coverage on rates and FE for steady-state electrochemical alkene epoxidations.

## MONDAY AFTERNOON

## Catalysis for Functionalization I

Session Chairs: Bruce Gates, *University of California Davis, USA* and Jingguang Chen, *Columbia University, USA.*

1:20 PM **Mon-RTND-1320** The Role of Surface Chlorine in Propylene Epoxidation on $Ag/CaCO_3$.
**Joseph Esposito** and Aditya Bhan, *University of Minnesota, USA.*

**Short Summary:**
Propylene epoxidation flow reactions over promoted $Ag/CaCO_3$ coupled with surface titration unravel critical impacts of latent propylene oxychlorination—a parallel pathway to propylene oxidation initiated via cleavage of allylic C-H bonds, forming allyl chloride and substantially reducing oxidation selectivity by lowering steady-state coverages of promoting Cl from the Ag surface.

1:40 PM **Mon-RTND-1340** Hydroformylation with Re-Rh Silica-Supported Bimetallic Catalysts.
**Stuart Soled**, Sara Yacob, Alyssa Love, Aaron Sattler and Michael Caulfield, *ExxonMobil Technology and Engineering Center, USA.*

**Short Summary:**
This work scopes out the advances in heterogeneously catalyzed hydroformylation with silica-supported Rh-Re catalysts. We discuss the impressive synergy of Rh with Re, the importance of keeping Re in the +4 oxidation state as a host for reduced Rh and the desire for more linear aldehyde products.

2:00 PM ***KEYNOTE* Mon-RTND-1400 Gold-Based Catalysts for Oxidation. Richard J. Lewis** and Graham J. Hutchings, *Cardiff University, United Kingdom.*

**Short Summary:**
This presentation will describe and discuss recent research at the Cardiff Catalysis Institute. Including (1) cooperative redox enhancement between Au and Pd in alcohol oxidation (2) the oxidation of methane, (3) the use of in-situ hydrogen peroxide generation as a means of producing Nylon-6 and (4) the disinfection of water.

2:40 PM **Mon-RTND-1440** Fundamental Understanding of Non-Noble Metal Intermetallic Compound Surface Chemistry to Achieve the Selective Hydrogenation of Unsaturated Aldehydes to Unsaturated Alcohols.
**Sijie Guo** and Siris Laursen, *University of Tennessee, USA.*

**Short Summary:**
Selective hydrogenation of cinnamaldehyde was used as a probe reaction. Late 1st-row TM+B-group IMCs were used as catalysts to investigate the effect of TM and B-group element selection and stoichiometry on surface and catalytic chemistry.

3:00 PM **Mon-RTND-1500** BASF Green Precious Metal Catalysts Platform – a Responsible, Novel and Unique $CO_2$ Neutral New Technology.
**Radu Craciun**, *BASF Corporation, USA.*

**Short Summary:**
The new low precious metal loading “edge-coated” catalysts with high metal dispersion provides key advantages over conventional catalysts: i) highly metal concentration on the surface of the support, ii) higher activity and hence iii) improved metal efficiency; iv) high selectivity for reactions involving bulky substrate molecules; v) easy catalyst regenerations/reuse.

## Carbonylation and Oxidation of Hydrocarbon Feedstocks

Session Chairs: Jostein Gabrielsen, *Haldor Topsoe A/S, Denmark* and Ilke Arslan, *Argonne National Laboratory, USA*.

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3:45 PM **Mon-RTND-1545** Fully-Selective Gas-Phase Ethylene Hydroformylation on a Rh1/SnO2 Single-Atom Catalyst.
**Marcos G. Farpón**[1], Wilson Henao[1], Philipp N. Plessow[2], Eva Andrés[1], Raúl Arenal[3], Carlo Marini[4], Giovanni Agostini[4], Felix Studt[2] and Gonzalo Prieto[1], *(1)Instituto de Tecnología Química (ITQ UPV-CSIC), Spain, (2)Karlsruhe Institute of Technology, Germany, (3)Instituto de Ciencias de Materiales de Aragón CSIC-UNIZAR, Spain, (4)ALBA Synchrotron Light Source, Spain*.

**Short Summary:**
In this work, we have studied metal oxide modulation effects on Rh single atom catalysts in the gas-phase hydroformylation of ethylene. We report a system consisting of atomically-dispersed Rh atoms on oxygen-defective SnO2, which combines high activity and full selectivity values, hitherto exclusive for molecular catalysts in solution.

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4:05 PM **Mon-RTND-1605** Tandem Reactions of $CO_2$ and Ethane for Production of $C_3$ Oxygenates via CO Bond Insertion.
**Zhenhua Xie**[1,2], Shyam Kattel[3] and Jingguang Chen[1,2], *(1)Columbia University, USA, (2)Brookhaven National Laboratory, USA, (3)Florida A&M University, USA*.

**Short Summary:**
Nowadays, there is still a lack of feasible strategy to directly produce oxygenates from $CO_2$ and shale gas, especially at ambient pressure. Herein, the proposed strategy provides an opportunity for upgrading the underutilized light alkanes in shale gas by reacting with green-house gas $CO_2$ to produce aldehydes and alcohols.

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4:25 PM **Mon-RTND-1625** An Expanded Reaction Network of Ethylene Oxidation on Partially Oxidized Ag Surface.
**Adhika Setiawan**, Tiancheng Pu, Israel Wachs and Srinivas Rangarajan, *Lehigh University, USA*.

**Short Summary:**
The recent paradigm shift towards partially oxidized Ag catalysts for ethylene oxidation(EO) introduces additional complexities in surface representations, relevant chemical species, and relevant reaction mechanisms. The current study proposes a MKM featuring an extended mechanism, supported by DFT experiments, and encompassing both unpromoted and sequentially-promoted catalysts.

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4:45 PM **Mon-RTND-1645** Investigating the Activity and Stability of Pt/Si-Doped $TiO_2$ for Total Propane Oxidation.
**Max Tigwell**, *Cardiff University, United Kingdom*.

**Short Summary:**
A systematic study investigating the influence of Si incorporation on the support effects for total propane oxidation. The presence of Si is crucial for high moisture resistance as well as enhanced activity.

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5:05 PM **Mon-RTND-1705** The Role of Microporous Channels of M1 Phase Mixed Oxides in the Selective Oxidation of Propane and Propylene.
**Adam Twombly**, Yilang Liu and Prashant Deshlahra, *Tufts University, USA*.

**Short Summary:**
M1-phase mixed metal oxides exhibit unique, well-known properties for selective oxidation of small hydrocarbons. We identify roles of micropores and H-abstraction strength of lattice O-atoms of these oxides in controlling selectivity using measured alkane-size-dependent rate ratios, kinetic data for propane and propene feeds, and DFT calculations.

# Tuesday, June 20, 2023

## Ballroom A-E

### TUESDAY MORNING

### 2024 Paul H. Emmett Award Lecture: Yuriy Román-Leshkov

Session Chairs: Steven Suib, *University of Connecticut, USA* and Christopher W. Jones, *Georgia Institute of Technology, USA*

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8:05 AM Electric Fields, Confinement, and Cooperativity as Unique Handles to Promote Turnover in Solid Acid Catalysts.
**Yuriy Román-Leshkov**, *Massachusetts Institute of Technology, USA*.

## 551 AB

## Zeolite Catalysis

Session Chairs: Nicholas Thornburg, *National Renewable Energy Laboratory, USA* and Anand Ramanathan, *Chevron Phillips Chemical Company LP, .*

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9:30 AM **Tue-551AB-0930** Tuning Active Site Distributions in Zeolite Catalysts for Regioselective Toluene Methylation to *Para*-Xylene.
**Sopuruchukwu Ezenwa**[1], Deng (DY) Jan[2] and Raj Gounder[1], *(1)Purdue University, USA, (2)Honeywell UOP, USA*.

**Short Summary:**
We use different structure-directing agents to bias the distribution of active sites within MFI zeolite voids and demonstrate the consequences for regioselective toluene methylation to *para*-xylene under kinetically controlled conditions that minimize the influence of side reactions and intracrystalline diffusional constraints on xylenes product distribution.

9:50 AM **Tue-551AB-0950** Structural Evolution of Molybdenum and Brønsted Acid Sites on MFI during Methane Dehydroaromatization Reaction-Regeneration Cycles.
**Angel Santiago-Colon** and Raj Gounder, *Purdue University, USA*.

**Short Summary:**
Quantitative characterization and kinetic measurements are used to determine the structural changes of Mo and $H^+$ species in zeolites after exposure to successive methane dehydroaromatization reaction-regeneration cycles, which leads to irreversible deactivation. These findings provide guidance on synthetic and regeneration strategies to improve Mo-MFI catalyst lifetime for methane dehydroaromatization.

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10:10 AM **Tue-551AB-1010** Mechanisms and Kinetics of $C_6$-$C_8$ ring Dehydrogenation Toward Aromatics in H-MFI.
**Hansel Montalvo-Castro**, Mykela Deluca, Lauren Kilburn and David Hibbitts, *University of Florida, USA*.

**Short Summary:**
During methanol-to-olefins (MTO) chemistries, aromatic compounds act as co-catalysts that predominantly form ethylene over propylene products, but they participate in subsequent deactivation reactions that hinders MTO from becoming an economically feasible route. Using density functional theory, we elucidated the dehydrogenation routes that form aromatics from cyclization product intermediates.

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10:30 AM **Tue-551AB-1030** Kinetic Investigation on Solvating Alkylamine Hofmann Elimination over Brønsted Acidic Zeolites.
**Han Chen** and Omar Abdelrahman, *University of Massachusetts Amherst, USA*.

**Short Summary:**
Effect of solvents on catalytic reaction over Brønsted acid site in zeolite was investigated using Hofmann elimination of *tert*-butylamine (TBA) as probe chemistry. A reversible kinetic inhibition was observed in the presence of solvent, and the formation of solvent-TBA adsorption complex was proposed to cause the inhibition.

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10:50 AM **Tue-551AB-1050** Kinetic, Spectroscopic, and Theoretical Study of Toluene Alkylation with Light Alkenes on Acidic Mordenite Zeolites.
**Stephanie Kwon**, *Colorado School of Mines, USA*.

**Short Summary:**
Alkylations of aromatics with light alkenes are important industrial processes to produce cumene, ethylbenzene and ethyltoluene. This work combines kinetic, spectroscopic, and theoretical methods to assess elementary steps and the role of microporous environments on reaction pathways by using toluene alkylation with ethylene on acidic mordenite as a model system.

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11:10 AM **Tue-551AB-1110** Distribution of Deactivating Carbonaceous Species Formed in Hierarchical Zeolites during Conversion of Bulky Hydrocarbons.
Hayat Adawi, Jun Zhi Tan and **Michele Sarazen**, *Princeton University, USA*.

**Short Summary:**
Reactions of (poly)substituted aromatics and polyolefins on solid acid zeolites suffer from severe diffusional barriers within narrow micropores. Reaction-diffusion-deactivation analysis of competitive reactions on hierarchical zeolites containing larger, mesoporous voids provides fundamental insight into the potential for more atom-efficient conversions of bulky hydrocarbon species.

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11:30 AM **Tue-551AB-1130** Manipulating Inner and Outer Sphere Environments in Zeolites to Control Regioselectivity of Epoxide Methanolysis.
**David Potts**, Jessica Komar and David Flaherty, *University of Illinois Urbana-Champaign, USA*.

**Short Summary:**
We show that the rates, mechanism, and selectivity of 1,2-epoxybutane ring-opening depend on the active metal, nucleophile choice, and nature of the active site (Lewis vs Bronsted acid site) through changes in the stability of reactive species. These findings provide opportunities to increase ring-opening rates and selectivities to desired products.

## TUESDAY AFTERNOON

## Dynamics in Catalytic Processes

Session Chairs: Linxiao Chen, *Pacific Northwest National Laboratory, USA* and Siwen Wang, *Toyota Research Institute of North America, USA*.

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1:20 PM **Tue-551AB-1320** Dynamic Evolution of Nanoparticle Heterogeneous Catalysts Using Machine Learned Force Fields from First Principles.
**Cameron J. Owen**[1], Nicholas Marcella[2], Yu Xie[1], Anders Johansson[1], Jin Soo Lim[1], Lixin Sun[1], Anatoly Frenkel[3,4], Ralph Nuzzo[2] and Boris Kozinsky[1,5], *(1)Harvard University, USA, (2)University of Illinois, USA, (3)Stony Brook University, USA, (4)Brookhaven National Laboratory, USA, (5)Bosch Research, USA*.

**Short Summary:**
This work demonstrates the power of machine learned force fields (MLFFs) from first principles in providing atomistic understanding of nanoparticle catalyst evolution at quantum mechanical accuracy. Direct observation of these dynamic phenomenona have been largely inaccessible until now, due to experimental resolutions and previous model inaccuracies.

1:40 PM **Tue-551AB-1340** First Principles and Data-Driven Analysis of Tungsten Oxide Structure on Defective Transition Metal Catalysts.
**Siddharth Deshpande** and Dionysios Vlachos, *University of Delaware, USA*.

**Short Summary:**
Metal-metal oxide (M-MO) inverse catalysts are central to many vital reactions owing to cooperative catalysis amongst different active sites. A remaining challenge in their design is understanding their in-situ structure and stability. Herein we present data-based comprehensive atomic models for tungsten oxide (WOx) on platinum nanoparticles.

2:00 PM **Tue-551AB-1400** Plasma Oxidation of Copper: Molecular Dynamics Study with Neural Network Potentials.
**Yantao Xia** and Philippe Sautet, *University of California, Los Angeles, USA*.

**Short Summary:**
A machine learning potential is trained to cover the entire range of PES from metallic copper, epitaxial oxide, full oxide, and the interaction of their surfaces with energetic atomic and molecular oxygen ions. MD simulation unveils potential mechanism for oxide growth under plasma, leading to proposals for optimized oxidation conditions.

2:20 PM **Tue-551AB-1420** Towards Swift Predictions of Metal Ad-Atom Diffusion Barriers and Surface/Segregation Energies for Enhanced Understanding of Sintering and Catalysts Durability.
**Shyam Deo**[1,2], Joakim Halldin Stenlid[1,2], Shikha Saini[1,2] and Frank Abild-Pedersen[2], *(1)Stanford University, USA, (2)SLAC National Accelerator Laboratory, USA*.

**Short Summary:**
Our work leads to effective screening of thermodynamic stabilities of alloy metal nanoparticles(MNPs), by integrating coordination schemes with structural and site information. The resulting models can then be applied to calculate the energetics of any nanoparticle morphology and chemical composition, thus significantly accelerating design of durable nanoalloys.

2:40 PM **Tue-551AB-1440** Over-Oxidative Effects of the Side-Product, Hydrogen Peroxide, on the NPGM-Based Fe-N-C Catalysts during ORR.
**Ankita Morankar**[1], Siddharth Deshpande[1], Plamen Atanassov[2] and Jeffrey Greeley[1], *(1)Purdue University, USA, (2)University of California, Irvine, USA*.

**Short Summary:**
Thermodynamics and kinetics for oxidative attack of Fe-N-C catalyst by the side-product, $H_2O_2$, formed during ORR is probed. The process is feasible at room temperature, is independent of applied voltage, and can induce deactivation by poisoning in some cases, while also leaving the possibility of carbon corrosion post over-oxidation.

3:00 PM **Tue-551AB-1500** Support Polarization Control of Catalysts: Elucidating and Breaking Scaling Relations.
**Seongjoo Jung**[1], Cristina Pizzolitto[2], Pierdomenico Biasi[2], Paul Dauenhauer[3] and Turan Birol[1], *(1)University of Minnesota, Twin Cities, USA, (2)CASALE SA, Switzerland, (3)University of Minnesota, USA*.

**Short Summary:**
We explore catalyst control by support polarization as a potential method to break the Sabatier limit. Using the constrained-forces method, Pt/PbTiO3 heterostructure was modelled at fixed polarizations. We elucidate the scaling relations between the adsorption energies and the breaking of the transition-state scaling relations, relating to surface electronic structure modifications.

## Computational Elucidation of Reaction Mechanisms

Session Chairs: Florian Goeltl, *The University of Arizona, USA* and Ping Liu, *Brookhaven National Laboratory, USA*.

3:45 PM **Tue-551AB-1545** Propane Dehydrogenation Mechanism on PtxSny (x, y ≤ 4) Clusters on $Al_2O_3$(110).
**Yilang Liu**[1], Xue Zong[2], Stavros Caratzoulas[1] and Dionysios Vlachos[1], *(1)University of Delaware, USA, (2)RAPID Manufacturing Institute, University of Delaware, USA*.

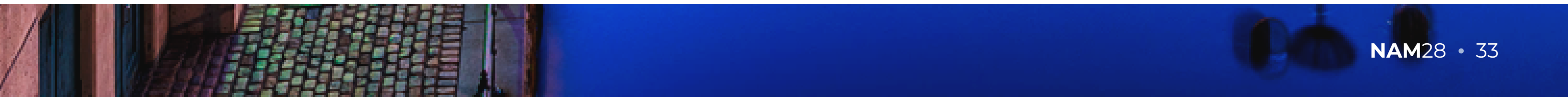
**Short Summary:**
We have elucidated the effects of Pt nuclearity and Sn heteroatom on sub-nanometer Pt cluster catalysts on $\gamma$-$Al_2O_3$(110) for propane dehydrogenation, which advances the understanding of structure-property relationships and provides guidance for the design of this type of catalysts.

4:05 PM **Tue-551AB-1605** Optimization of Catalytic Reaction Mechanism Parameters Using Basin-Hopping.
**Rinu Chacko**, Kevin Keller, Steffen Tischer, Akash B. Shirsath, Patrick Lott and Olaf Deutschmann, *Karlsruhe Institute of Technology (KIT), Germany*.

**Short Summary:**
This work focusses on automated optimization of catalytic reaction mechanism parameters while maintaining thermodynamic consistency, using the global optimization algorithm Basin-Hopping. The Python-based automated workflow and use of the simulation software DETCHEM facilitates acceleration of microkinetic model development as opposed to a manual approach of iteratively fine-tuning kinetic models.

4:25 PM **Tue-551AB-1625** Reaction-Driven Selective $CO_2$ Hydrogenation to Formic Acid on Pd(111).
**Hong Zhang**[1], Xuelong Wang[2] and Ping Liu[1,2], *(1)Stony Brook University, USA, (2)Brookhaven National Laboratory, USA*.

**Short Summary:**
This work investigates the Pd(111) surface composition under typical hydrogenation environments, the surface is covered with 1 monolayer of chemisorbed hydrogens. The hydrogens not only facilitate the activation of $CO_2$, but also modified the reaction mechanism to selectively promote *HOCO as an intermediate that leads to HCOOH.



4:45 PM **Tue-551AB-1645** Revealing Interfacial Kinetics of Electrochemical Urea Production from First-Principles Molecular Dynamics.
**Tianyou Mou**, Xue Han, Huiyuan Zhu and Hongliang Xin, *Virginia Polytechnic Institute and State University, USA*.

**Short Summary:**
We developed and employed a constant-potential AIMD approach for modeling electrokinetics of urea production from $CO_2$ and nitrate coupling at the surface-electrolyte interface. We uncover governing factors of rate-determining steps, which shed light on design rules of C-N coupling toward value-added chemicals.

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5:05 PM **Tue-551AB-1705** $CO_2$ and $H_2O$ Activation at Au(100)-Water Interfaces.
Xueping Qin, Tejs Vegge and **Heine Anton Hansen**, *Technical University of Denmark, Denmark*.

**Short Summary:**
We present ab initio molecular dynamics simulations of the $CO_2$ electroreduction and the competing hydrogen evolution reaction at charged interfaces between gold and liquid water. The impact of non-covalent interactions and the hydrogen bond network on reaction selectivity caused by $K^+$ and $H^+$ ions is analyzed.

## 552 AB

### TUESDAY MORNING

### Conversion of Biomass-Derived Oxygenates I

Session Chairs: Anurag Kumar, *Phillips 66, USA* and Dan Ruddy, *National Renewable Energy Laboratory, USA*.

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9:30 AM **Tue-552AB-0930** Highly Selective Conversion of Lactic Acid to Renewable Acrylic Acid over Na-ZSM-5: The Critical Role of Hidden Basic Sites of NaOx.
**Jichan Kim**[1], Jungup Bang[2], Jae-Soon Choi[1], Dong-Ha Lim[3] and Jungho Jae[1], *(1)Pusan National University, Korea, Republic of (South), (2)LG Chem Ltd, Korea, Republic of (South), (3)Korea Institute of Industrial Technology, Korea, Republic of (South)*.

**Short Summary:**
In this study, we disclose for the first time the crucial role of the residual alkali metal oxides in the alkali-exchanged zeolite catalysts in modifying the catalyst selectivity for the dehydration of lactic acid to renewable acrylic acid.

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9:50 AM **Tue-552AB-0950** A Zeolite Encapsulated Hydrogenation Catalyst for the Direct Conversion of Glucose to Ethylene Glycol.
**Roshaan Surendhran** and Marat Orazov, *University of Delaware, USA*.

**Short Summary:**
Direct conversion of biomass to ethylene glycol (EG) is a promising alternative to current methods of EG production. This work focuses on improving the yield and selectivity to EG by utilizing a zeolite-encapsulated Ni catalyst for size-selective hydrogenation by excluding glucose and minimizing hexitol production.

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10:10 AM **Tue-552AB-1010** Biomass Conversion into Neo Acids.
**Erha Andini**, Kristin Paragian, Sunitha Sadula and Dionysios Vlachos, *University of Delaware, USA*.

**Short Summary:**
This work provides a novel strategy to synthesize bio-based neo acids from lignocellulosic biomass derivatives in two-steps, C-C coupling of furans with keto acids through hydroxyalkylation/alkylation (HAA), followed by ring-opening of furans through hydrodeoxygenation (HDO). This work enables multiple opportunities for producing renewable commodity chemicals with diverse industrial applications.

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10:30 AM **Tue-552AB-1030** Highly Selective Production of Bio-Based Polymeric Monomer Tetrahydrofuran-2,5-Dimethanol from 5-Hydroxymethylfurfural over Ni@U-Silicalite-1 Catalysts.
**Xiangcheng Li**, *SINOPEC Shanghai Research Institute of Petrochemical Technology, State Key Laboratory of Green Chemical Engineering and Industrial Catalysis, China*.

**Short Summary:**
Ni@U-Silicalite-1 catalysts efficiently stabilize the nickel ions by Silicalite-1 zeolite, and show potential application for selectively conversion of 5-hydroxymethylfurfural (HMF) into tetrahydrofuran-2,5-dimethanol (THFDM).

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10:50 AM **Tue-552AB-1050** Electrocatalytic Conversion of Phenol to Cyclohexane.
**Jeffrey Page**, Stoyan Bliznakov and Julia Valla, *University of Connecticut, USA*.

**Short Summary:**
Electrochemical hydrogenation represents a mild method for the production of biofuels from bio-oils. Promotion of deoxygenation reactions remains a key barrier in its commercial viability. The objective of this study is to demonstrate electrocatalytic hydrogenation of phenol to cyclohexane and understand the factors influencing product yields and selectivities.

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11:10 AM **Tue-552AB-1110** Quantification of Active Sites for Ethanol Upgrading over Yttrium-Containing Beta Zeotypes.
Shivangi Borate[1], Nohor Samad[1], Junyan Zhang[2], Stephen Purdy[2], Michael Cordon[2], Meijun Li[2], Andrew Sutton[2], Zhenglong Li[3] and **James Harris**[1], *(1)The University of Alabama, USA, (2)Oak Ridge National Laboratory, USA, (3)ORNL, USA*.

**Short Summary:**
Copper, zinc, and yttrium containing Beta zeotypes produce $C_3$+ olefins at ~90% yield. The C-C coupling rate is driven by the number of yttrium Lewis acid sites. These sites were quantified by *ex situ* FTIR and *in situ* titration. *Ex situ* chemisorption FTIR accurately quantifies the number of active sites.

11:30 AM **Tue-552AB-1130** Hydrogenation of Bio-Oil Oxygenates at Ambient Conditions Via a Two-Step Redox Cycle.
**Chongyan Ruan** and Fanxing Li, *North Carolina State University, USA*.

**Short Summary:**
We report here a two-step solar thermochemical hydrogenation process, sourcing hydrogen directly from water and concentrated solar radiation for furfural and bio-oils upgrading. Superior catalytic performance was achieved at room temperature and atmospheric pressure, with up to two orders of magnitude higher H2 utilization efficiency compared to state-of-the-art catalytic hydrogenation.

## TUESDAY AFTERNOON

### Hydrodeoxygenation and Hydrogenolysis

Session Chairs: Mike Griffin, *National Renewable Energy Laboratory, USA* and Ravi Joshi, *Phillips 66, USA*.

1:20 PM **Tue-552AB-1320** A Tandem Catalytic Dehydration–Hydrogenation of Glycerol to n-Propanol.
Thanasak Solos[1], Kittisak Choojun[2] and **Tawan Sooknoi**[1], *(1)King Mongkut's Institute of Technology Ladkrabang, Thailand, (2)King Mongkut's Institute of Technology Ladkrabang, Thailand*.

**Short Summary:**
The direct conversion of glycerol to n-propanol can be achieved over a tandem catalytic system using HZSM-5 and supported Ni catalysts under atmospheric H2. A complete conversion of glycerol over HZSM-5 yield mainly acrolein that can be subsequently hydrogenated to n-propanol over supported Ni catalysts under atmospheric H2 pressure.

1:40 PM **Tue-552AB-1340** Metal Clusters on Ru-Ti-Aerogel Catalyst for the Improved Hydrodeoxygenation.
**Jisong Kang**[1,2], Jae-Wook Choi[1], Dong Jin Suh[1], Chun-Jae Yoo[1], Kyeongsu Kim[1], Choi Jungkyu[2], Hyung Chul Ham[3] and Jeong-Myeong Ha[1,4], *(1)Korea Institute of Science and Technology, Korea, Republic of (South), (2)Korea University, Korea, Republic of (South), (3)Inha University, Korea, Republic of (South), (4)Korea University of Science and Technology, Korea, Republic of (South)*.

**Short Summary:**
The Ru-Ti-aerogel catalyst was prepared with highly dispersed Ru clusters, which exhibited the excellent hydrodeoxygenation activity. Catalyst characterization and DFT calculation were conducted to clarify the reaction mechanisms for understanding HDO activity.

2:00 PM **Tue-552AB-1400** Effect of Pt-Metal Interaction on the Direct Reduction of Esters to Ethers with $H_2$ over Pt-M on Mordenite.
**Jieun Lee**[1], Claudia Berdugo-Díaz[1], Yangsik Yun[1], Jing Luo[2], David Barton[2], Ida Chen[2] and David Flaherty[1], *(1)University of Illinois Urbana-Champaign, USA, (2)The Dow Chemical Company, USA*.

**Short Summary:**
We characterize and kinetically examine catalysts comprising Pt and Pt-based bimetallic nanoparticles within mordenite (Pt-M-MOR) for esters reduction to ethers with hydrogen. Among these, Pt-Ru-MOR shows a higher ether-formation rate than monometallic and other bimetallic combinations, likely because Ru affects the Pt dispersion and increases the hemiacetal concentrations within pores.

2:20 PM **Tue-552AB-1420** Ru, Ni and Pd Catalysts Deposited Onto Zeolites and Mesoporous Molecular Sieves for Hydrogenation and Hydrocracking of Biomass-Derived Compounds.
German Araujo-Barahona[1], Roman Barakov[2], Ivan Kopa[2], Mark Martinez-Klimov[1], Tapio Salmi[1], Nataliya Shcherban[2] and **Dmitry Murzin**[1], *(1)Åbo Akademi University, Finland, (2)L.V. Pisarzhevsky Institute of Physical Chemistry, National Academy of Sciences of Ukraine, Ukraine*.

**Short Summary:**
Highly dispersed Ru, Ni and Pd catalysts deposited onto conventional and hierarchical beta zeolites and MCF, MCM and SBA type mesoporous molecular sieves were prepared. Supported Ru catalysts demonstrated superior catalytic performance (conversion and selectivity > 99%) in hydrogenation of D-xylose.

2:40 PM ***KEYNOTE*** **Tue-552AB-1440 Development of Heterogeneous Deoxydehydration Catalysts for Production of Biomass-Based Chemicals. Keiichi Tomishige**, *Tohoku University, Japan*.

**Short Summary:**
The combination of high valent Re species on cerium oxide and noble metals with high $H_2$ activation ability has been applied to the development of heterogenous deoxydehydration catalysts enabling $H_2$ reductant, and $ReO_x$-Ag/$CeO_2$ has high deoxydehydration activity and low hydrogenation activity of C-C double bond.

### Lignin and Bio-Oil Conversion I

Session Chairs: Manish Shetty, *Texas A&M University, USA* and Matt Wulfers, *Phillips 66, USA*.

3:45 PM **Tue-552AB-1545** Boosting Metal Efficiency of Ru/$TiO_2$ for the Liquid Phase Guaiacol Hydrogenation Via Hydrogen Spillover.
**Hyungjoo Kim**[1], Seungdo Yang[1], Yong Hyun Lim[1], Jaeha Lee[1], Jeong-Myeong Ha[2] and Do Heui Kim[1], *(1)Seoul National University, Korea, Republic of (South), (2)Korea University, Korea, Republic of (South)*.

**Short Summary:**
The lowered metal efficiency of Ru/$TiO_2$ catalysts with high Ru loading driven by low Ru dispersion could be enhanced simply by the incorporation of Ru-free $TiO_2$, which played a role as additional active sites for hydrogenation reaction generated by hydrogen spillover in the liquid phase.

4:05 PM **Tue-552AB-1605** Impact of Catalytic Hydrotreatment of Simulated Pyrolysis Oil for Bio-Char Formation.
Elham Nejadmoghadam[1], Abdenour Achour[1], Olov Öhrman[2], Prakhar Arora[2], **Louise Olsson**[1] and Derek Creaser[1], *(1)Chalmers University of Technology, Sweden, (2)Preem AB Sweden, Sweden*.

**Short Summary:**
Catalytic hydrotreating improves pyrolysis oil properties for its application in fuels. However, during heating, side-reactions forming solids can cause rapid deactivation of catalysts. In this study, we aim to minimize and understand the nature of solids formed from different oxygenate compounds during mild hydrotreatment over various alumina supported catalysts.

4:25 PM **Tue-552AB-1625** Co-Hydroliquefaction of Kraft Lignin and Bio-Derived Oxygenates over Unsupported Nimos Catalyst: A Strategy for Char Suppression.
You Wayne Cheah[1], Rawipa Intakul[1], Muhammad Abdus Salam[1], Joby Sebastian[1], Phuoc Hoang Ho[1], Olov Öhrman[2], Prakhar Arora[2], **Derek Creaser**[1] and Louise Olsson[1], *(1)Chalmers University of Technology, Sweden, (2)Preem AB Sweden, Sweden*.

**Short Summary:**
The hydroliquefaction of Kraft lignin with bio-derived oxygenated co-reactants and NiMoS catalyst is presented as a strategy to suppress char formation with higher total yields of bio-oil product. The possible mechanistic roles of the functional groups of co-reactants and their influence on char formation is also investigated.

4:45 PM **Tue-552AB-1645** Site-Specificity of Oxide-Limited Strong Metal-Support Interaction in $WO_x$/Pt Catalysts Drives Selective HDO Towards Aromatics.
**Justin Marlowe**[1], Siddharth Deshpande[2], Dionysios Vlachos[2], Mahdi M. Abu-Omar[1] and Phil Christopher[1], *(1)University of California, Santa Barbara, USA, (2)University of Delaware, USA*.

**Short Summary:**
A combination of *in-situ* spectroscopy and hydrodeoxygenation (HDO) reaction analysis of WOx-modified Pt/$SiO_2$ elucidates the role of well-coordinated metal sites in facilitating ring hydrogenation. Preferential titration of these sites by dynamic $WO_x$ restructuring under reaction conditions is responsible for the remarkable aromatics selectivity of these catalysts in HDO of phenolics.

5:05 PM **Wed-552AB-1705** Highly Selective Cross Ketonization of Renewable Acids over Magnesium Oxide.
**Tejas Goculdas**[1], Sunitha Sadula[1], Siddharth Deshpande[1], Weiqing Zheng[1], Raymond J. Gorte[2] and Dionysios Vlachos[1], *(1)University of Delaware, USA, (2)University of Pennsylvania, USA*.

**Short Summary:**
Biomass derived OFS exhibit superior performance compared with petroleum sourced LAS but are synthesized using homogenous catalysts. We demonstrate a heterogeneously catalyzed selective route to circumvent the homogenously catalyzed step in the synthesis while using similar biomass derived raw materials. We reveal the mechanism through combined computational and experimental studies.

## 555 AB

### TUESDAY MORNING

### Methane Reforming II (Dry)

Session Chairs: Matthew M. Yung, *National Renewable Energy Laboratory, USA* and Jason Malizia, *Idaho National Laboratory, USA*.

9:30 AM **Tue-555AB-0930** Impacts of Catalyst and Process Parameters on Ni-Catalyzed Methane Dry Reforming Via Interpretable Machine Learning.
Keerthana Vellayappan, Yifei Yue, **Kang Hui Lim**, Terry Z. H. Gani, Iftekhar A. Karimi and Sibudjing Kawi, *National University of Singapore, Singapore*.

**Short Summary:**
Gray-box machine learning model was implemented for catalyst performance prediction in Dry Reforming of Methane, and subsequently apply model interpretation techniques specifically for tuning $H_2$/CO ratio and hence $H_2$ yield. We uncover unexpected and divergent effects of Ni particle size and Ni loading on the $H_2$/CO ratio and reactant conversion.

9:50 AM **Tue-555AB-0950** High Performance DRM Catalysis by Ni at Heterointerfaces between Thin MgAlOx and Bulk $ZrO_2$.
**Jin Wang**[1] and Oz Gazit[2], *(1)Technion Institute of technology, Israel, (2)Israel Institute of Technology -Technion, Israel*.

**Short Summary:**
The effect of MSI for Ni at different locations in hierarchical support consisting of $MgAlO_x$ nanosheet on $ZrO_2$ was examined. Mainly two types of active sites were identified, residing either at the interface of MAZ or on top of MAZ. The balance between those sites created active and stable catalysts.

10:10 AM **Tue-555AB-1010** Improving Selectivity and Stability in Methane Dry Reforming by Atomic Layer Deposition onto Ni-$CeO_2$-$ZrO_2$/$Al_2O_3$ Catalysts.
**Kerry Dooley**[1], Jonathan Lucas[2], James Dorman[1], Kunlun Ding[1] and David Cullen[3], *(1)Louisiana State University, USA, (2)LSU, USA, (3)Oak Ridge National Laboratory, USA*.

**Short Summary:**
The addition of an ALD layer to Ni/CZO catalysts is shown in this work to greatly improve the stability during methane reforming, achieve a ~1 H2/CO ratio, lower coking rates, and greatly increased operation times are seen.

10:30 AM **Tue-555AB-1030** Reactivity and Structure Evolution of High Entropy Oxides in Dry Reforming of Methane (DRM).
Junyan Zhang[1], Meijia Li[1], Aditya Savara[1], Yuanyuan Li[1], Zili Wu[1], Zhenzhen Yang[1], **Felipe Polo-Garzon**[1] and Sheng Dai[1,2], *(1)Oak Ridge National Laboratory, USA, (2)University of Tennessee, USA*.

**Short Summary:**
Dry reforming of methane (DRM) consists of converting $CH_4$ and $CO_2$ into CO and $H_2$. This reaction requires thermally stable catalysts. High entropy oxides (HEOs) are thermally stable solid solutions, owing their stability to maximizing the entropy of mixture. Structure-performance relationships of HEOs for catalyzing DRM will be presented.

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10:50 AM **Tue-555AB-1050** Single Atom Ni Catalyst for Converting Greenhouse Gases $CO_2$ & $CH_4$ to Fuels and Chemicals.
**Brandon Burnside**[1], Abhaya Datye[1], David Dean[2], Jeffrey T. Miller[3] and Stephen Porter[1], *(1)University of New Mexico, USA, (2)University of Purdue, USA, (3)Davidson School of Chemical Engineering, Purdue University, USA*.

**Short Summary:**
The work presented investigates Ni single atoms doped into a ceria host lattice for use in the dry reforming of methane. During testing excellent performance and stability was observed. In addition that samples show excellent selectivity as only trace amounts of carbon deposition could be detected via *in-situ* TPO.

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11:10 AM **Tue-555AB-1110** Dry Reforming of Methane on Bimetallic Ni-Co Catalysts Produced Via Spray-Drying.
**Gerrit Küchen**[1], Vinzent Olszok[1], Bjarne Kreitz[2], Thomas Turek[1], Alfred Weber[1] and Gregor D. Wehinger[1], *(1)Clausthal University of Technology, Germany, (2)Brown University, USA*.

**Short Summary:**
Bimetallic nanoparticle catalysts produced via spray-drying, where one metal is ferromagnetic to allow for induction heating and the other is catalytically active, are a promising application for electrified reactors. Several temperature programmed measurements are conducted to examine catalyst compositions achieving optimal activities while enabling sufficient induction heating capabilities.

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11:30 AM **Tue-555AB-1130** Tuning the Performance of Ru-Ni-Mg/Ceria-Zirconia Dry Reforming Catalysts through Strategic Reduction Conditions and Ru Loading.
Yetunde Oluwatosin Sokefun and **John Kuhn**, *University of South Florida, USA*.

**Short Summary:**
Ru based catalyst samples were used for low temperature (450-510°C) dry reforming experiments. The addition of greater than 0.02 wt% Ru to the Ni-Mg-CZO samples significantly influenced the reactants' conversion. The modulation of catalytic properties and activity by the Ru loading amount, presence of promoter, reduction temperature was also evaluated.

## TUESDAY AFTERNOON

### Carbon Dioxide Conversion to Methanol I

Session Chairs: Ning Yan, *National University of Singapore, Singapore* and Unni Olsbye, *University of Oslo, Norway*.

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1:20 PM **Tue-555AB-1320** Effect of Pre-Treatment on the Support Effect in Catalytic Methanol Synthesis.
Jonas Abitz Boysen, **Jakob M. Christensen** and Anker D. Jensen, *Technical University of Denmark, Denmark*.

**Short Summary:**
The active site of the industrial $Cu/ZnO/Al_2O_3$ catalyst used for $CO_2$ hydrogenation to methanol is not fully understood due to contradicting observations. The aim of this work is to further enhance the understanding of the active site.

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1:40 PM **Tue-555AB-1340** Unique Role of Novel Titanate Nanorod Support in $Cu\text{-}ZnO\text{-}Al_2O_3$ Catalyst for $CO_2$ Hydrogenation to Methanol.
**Usman Salahuddin**, Pu-Xian Gao, Jiyu Sun, Chunxiang Zhu and Xingxu Lu, *University of Connecticut, USA*.

**Short Summary:**
The anti-sintering effect of titanate nanorods has been investigated, in correlations with the design, fabrication, and testing of these LPT supported CZA catalysts as integrated monolithic reactor for $CO_2$ hydrogenation into methanol at low-pressure (≤10 atm) conditions.

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2:00 PM ***KEYNOTE* Tue-555AB-1400 Copper-Based Catalysts for Selective Carbon Dioxide Activations: From Mechanistic Understanding to Catalyst Optimization. Ping Liu**, *Brookhaven National Laboratory, USA*.

**Short Summary:**
The present talk will rationalize the nature of diverse promoters in tuning the catalytic behaviors of Cu-based catalysts toward the $CO_2$ hydrogenation, using the combined density functional theory (DFT) calculations, kinetic Monte-Carlo (KMC) simulations and machine learning method and in strong interaction with the experimental studies.

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2:40 PM **Tue-555AB-1440** Kinetic and Mechanistic Study of $CO_2$ Conversion into Methanol over $Cu/TiO_2$ and $Cu/SiO^2$ Catalysts Promoted By $CeO_2$.
**Tomás Vergara Senociain**[1], Bruno Lacerda de Oliveira Campos[2], Karla Herrera-Delgado[2], Romel Jiménez[1] and Alejandro Karelovic[1], *(1)Universidad de Concepción, Chile, (2)Karlsruhe Institute of Technology (KIT), Germany*.

**Short Summary:**
$Cu/TiO_2$ and $Cu/SiO_2$ catalysts promoted by different concentrations of $CeO_2$ were studied for the synthesis of methanol. A promotion in the methanol rate was observed as $CeO_2$ concentration increased. By means of characterization techniques, the active site was determined, and a reaction mechanism and a kinetic model were derived.

3:00 PM **Tue-555AB-1500** Mechanistic Investigation of Selective Cu-Ga-Zr Catalysts for the Hydrogenation of $CO_2$ to Methanol.
**Abdullah J. Al Abdulghani**[1], Edgar E. Turizo-Pinilla[2], Ryan H. Hagmann[1], Theodore O. Agbi[1], Maria J. Fabregas-Angulo[2], Miguel A. Sepulveda Pagan[2], Diana M. Aponte-Claudio[2], Paola N. Fargas-Lopez[2], Faysal Ibrahim[1], Morgan Kraimer[1], Yomaira Pagan Torres[2] and Ive Hermans[1], *(1)University of Wisconsin-Madison, USA, (2)University of Puerto Rico-Mayaguez, USA*.

**Short Summary:**
We have identified CuGaZr-based $CO_2$ hydrogenation catalysts that are more selective to methanol than the industrial CuZnAl catalyst. Our characterization and *operando* modulation excitation infrared spectroscopy show $CO_2$ hydrogenation on the CuGaZr occurs via a formate-based, GaH-assisted pathway whereas the reaction on the CuZnAl proceeds via a direct CO cleavage.

## Methane Combustion or Partial Oxidation

Session Chairs: Felipe Polo-Garzon, *Oak Ridge National laboratory, USA* and Partha Nandi, *ExxonMobil, USA*.

3:45 PM **Tue-555AB-1545** Effect of Pd Speciation on $CH_4$ Oxidation and Passive NOx Adsorption/Desorption Performance over Zeolite-Based Catalysts.
Tala Mon, Junjie Chen and **Eleni Kyriakidou**, *University at Buffalo (SUNY), USA*.

**Short Summary:**
Pd speciation is essential to the investigation of Pd/zeolite catalysts for passive NOx adsorbers (PNAs) and methane ($CH_4$) oxidation catalysts. $H_2O$ exposure at ambient conditions can alter Pd species in Pd/BEA compared to Pd/MFI and Pd/CHA to significantly affect the catalyst performance in PNA and $CH_4$ oxidation.

4:05 PM **Tue-555AB-1605** Improving the Activity of Pd Single Atoms by Tuning Their Local Environment on Ceria for Methane Combustion.
**Yuanyuan Li**, Weiwei Yang, Felipe Polo-Garzon and Zili Wu, *Oak Ridge National Laboratory, USA*.

**Short Summary:**
Pd single atoms can take different structure on ceria support. By a simple thermal pretreatment to ceria prior to Pd deposition, a unique anchoring site is created. Anchored at this site, Pd4+ can be activated to $Pd^{\delta}$+ ($0 < \delta < 2$) which shows enhanced activity for methane oxidation.

4:25 PM **Tue-555AB-1625** Effect of Support on Pd-Catalyzed $CH_4$ Combustion in the Wet Feed.
Jing Shen[1], William Barrett[2], Somaye Nasr[1], Yongfeng Hu[3], Robert E. Hayes[1], Robert W. J. Scott[2] and **Natalia Semagina**[1], *(1)University of Alberta, Canada, (2)University of Saskatchewan, Canada, (3)Canadian Light Source, Canada*.

**Short Summary:**
Oxygen-donor ability of the support and water presence in the feed affect Pd-catalyzed methane combustion and methane steam reforming. The work compares $Co_3O_4$, $SnO_2$ and $Al_2O_3$ as supports and includes *in situ* XAS characterization of Pd species.

4:45 PM **Tue-555AB-1645** Effect of $Co_3O_4$ Promoter in Pd-Pt/$SnO_2$ Catalysts on the Kinetics of Wet Low-Temperature Methane Combustion.
**Roshni Sajiv Kumar**, Robert E. Hayes and Natalia Semagina, *University of Alberta, Canada*.

**Short Summary:**
Presence of water vapour (15 vol%) in the exhaust of NGVs causes Pd catalyst deactivation. Adding Pt to the catalyst formulation and appropriately choosing the support material, significantly improves the catalytic performance. This work attempts to understand the promoting effect of $Co_3O_4$on the Pd-Pt/$SnO_2$catalysts under wet feed conditions.

5:05 PM **Tue-555AB-1705** Breaking the Selectivity-Conversion Shackles in the Platinum Catalyzed Methane Oxidation to Formaldehyde.
Eric van Steen, **Sinqobile Mahlaba**, Nasseela Hytoolakhan Lal Mahomed, Alisa Govender and Gerard Leteba, *University of Cape Town, South Africa*.

**Short Summary:**
The selective oxidation of methane often suffers from the conversion-selectivity limitation. Here, we report on the high selectivity for the formation of formaldehyde in the aerobic oxidation of methane over platinum in the presence of liquid water showing a selectivity higher than 95% at a methane conversion of ca. 3-4%.

# 556 AB

### TUESDAY MORNING

## Alkene Epoxidation

Session Chairs: Jun Wang, *SABIC, USA* and Junhee Jang, *National Renewable Energy Laboratory, USA*.

9:30 AM **Tue-556AB-0930** Effects of Ti-Zeolite Framework and Hydrophilicity on Vapor-Phase Propylene Epoxidation Kinetics with Gaseous $H_2O_2$.
**Ohsung Kwon**, Zeynep Ayla and David Flaherty, *University of Illinois Urbana-Champaign, USA*.

**Short Summary:**
Rates and selectivities for oxidation pathways among $C_3H6$ and gaseous $H_2O_2$ differ with Ti-zeolite topology, (SiOH)*x* density, and intrapore solvent density. Rate measurements utilize a vapor-phase reactor which eliminates obfuscations by bulk solvents. Differences in kinetics reflect noncovalent interactions that stabilize transition states for epoxidation, epoxide ring-opening, and other steps.

9:50 AM **Tue-556AB-0950** Niobium-Modified Hierarchical Zeolites As Effective Catalysts for Cyclohexene Epoxidation.
Agnieszka Feliczak-Guzik, Paulina Szczyglewska and **Izabela Nowak**, *Adam Mickiewicz University, Poznan, Poland*.

**Short Summary:**
Much attention is being paid to the development of new active amaterials that are used in the cyclohexene epoxidation. The results of the activity of the niobium-modified hierarchical catalyst show that the conversion of cyclohexene is about 70% with the main product of the reaction - 2-cyclohexanediol (selectivity > 80%).

10:10 AM **Tue-556AB-1010** Sensitivity of Ethylene Epoxidation Rates to Ag Particle Size Distributions and Chlorine Content.
**Krishna Iyer** and Aditya Bhan, *University of Minnesota, Twin Cities, USA*.

**Short Summary:**
We probe particle size effects in Ag-catalyzed ethylene epoxidation by developing a model that correlates the Ag particle size distribution to changes in ethylene oxide rates. A narrow Ag particle size distribution centered around ~130-150 nm would enable operation of ethylene epoxidation with high EO rates and EO selectivity.

10:30 AM **Tue-556AB-1030** Combined First-Principles, Spectroscopic, and Data Science Studies of Ethylene Epoxidation on Non-Model $Ag/\alpha\text{-}Al_2O_3$ Catalysts.
**Shawn Lu**[1], Jinxun Liu[1,2], Shiuan-Bai Ann[1] and Suljo Linic[1], *(1)University of Michigan - Ann Arbor, USA, (2)University of Science Technology China, China*.

**Short Summary:**
*In operando* SERS characterization of $Ag/Al_2O_3$ catalysts coupled with machine-learning augmented DFT modelling shows that a mixture of atomic oxygen, surface oxide, and molecular oxygen motifs exist under reaction conditions. Data science-aided analysis of large amounts of data allowed us to correlate specific oxygen species to EO selectivity.

10:50 AM **Tue-556AB-1050** Silver Particle Size Effects on Unpromoted $Ag/\alpha\text{-}Al_2O_3$ during Ethylene Epoxidation with Molecular Oxygen.
**Hashim Alzahrani** and Juan Bravo Suárez, *The University of Kansas, USA*.

**Short Summary:**
Silver particle size effects on unpromoted $Ag/\alpha\text{-}Al_2O_3$ during ethylene epoxidation with molecular oxygen was studied by Operando Raman spectroscopy. Active and selective oxygen species at reaction conditions on unpromoted $Ag/\alpha\text{-}Al_2O_3$ with large Ag particles were identified which can help in the understanding of intermediate species in complex industrial $Ag/\alpha\text{-}Al_2O_3$ catalysts.

11:10 AM ***KEYNOTE*** **Tue-556AB-1110 The Shell Ethylene Oxide Catalyst Journey.**
**John R. Lockemeyer**, *Shell Global Solutions US, USA*.

**Short Summary:**
This presentation will offer an overview of some of the significant contributions by Shell scientists, engineers, and technical staff to the field of ethylene oxide (EO) production. The presentation will focus on the long history of catalyst development, with emphasis on the major breakthroughs that have shaped the EO industry.

## TUESDAY AFTERNOON

### Catalysis for Functionalization II

Session Chairs: Liheng Wu, *SABIC, USA* and Tracy Lohr, *Shell, USA*.

1:20 PM **Tue-556AB-1320** Kinetic Requirements and Solvent Effects in Polyoxymethylene Dimethyl Ether Synthesis on Brønsted Acid Catalysts.
**Junfeng Guo** and Cathy Chin, *University of Toronto, Canada*.

**Short Summary:**
We decoupled the three factors controlling the Brønsted acid catalyzed synthesis of Polyoxymethylene dimethyl ethers (OMEs) from methanol and trioxane, solvent dependent rate limiting C-O scission, $H^+$ site occupation by methanol and solvents, and quasi-equilibrated C-O formation leading to OMEs, then established their kinetic and thermodynamic requirements.

1:40 PM WITHDRAWN: Ionic Liquid-Intensified Bimetallic Catalysts for Anthraquinone Hydrogenation.

2:00 PM **Tue-556AB-1400** Production of Delta-Valerolactone from Furfural for Biobased Polyesters – Combined DFT and Experimental Study.
**Raka Ghosh Dastidar**, Javier E. Chavarrio, Zhen Jiang, Manos Mavrikakis and George Huber, *University of Wisconsin Madison, USA*.

**Short Summary:**
Delta-valerolactone synthesis from dehydrogenation of furfural-derived 2-hydroxytetrahydropyran is demonstrated. DVL ring opens to yield biocompatible, recyclable polyesters that rival HDPE.

2:20 PM **Tue-556AB-1420** Design of Au-Based Selective Oxidation Catalysts with Unique Mixed-Oxide and Metal-Oxide Interfaces.
**Francisco Zaera**, *University of California, Riverside, USA*.

**Short Summary:**
Prototypical surface sites comprised of silica supports (mainly well-structured mesoporous materials such as SBA-15), titania thin films deposited using atomic layer deposition (ALD), and Au or Pt nanoparticles have been developed, as that combination has proven to offer some unique and useful surface chemistry for low-temperature molecular-oxygen-based oxidation catalysis.

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2:40 PM **Tue-556AB-1440** Kinetics of Selective Hydrogen Combustion on Bismuth Oxide.
**Matthew Jacob** and Aditya Bhan, *University of Minnesota, USA*.

**Short Summary:**
This study examines the kinetics of hydrogen combustion on bismuth oxide in binary mixtures with various $C_1$-$C_3$ hydrocarbons, demonstrating that molecular descriptors related to bond strength cannot explain the high selectivity to hydrogen. We present methods to analyze combustion kinetics free from transport limitations by solid state oxygen diffusion.

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3:00 PM **Tue-556AB-1500** Heteropoly Acid Catalysts for Limonene Oxide Isomerization: The Relationship between Catalyst Acid Strength and Activity and Selectivity.
**Hyunju Lee**[1] and Brent H. Shanks[1,2], *(1)Iowa State University, USA, (2)Center for Biorenewable Chemicals (CBiRC), USA*.

**Short Summary:**
Dihydrocarvone has been widely used in the food, cosmetics, agrochemicals, and pharmaceutical industries. Limonene oxide isomerization was studied over a wide range of bulk and supported heteropoly acids. It was found that the high acid strength of heteropoly acid catalysts led to a high reaction rate and high dihydrocarvone selectivity.

## Thermocatalytic Conversion of $CO_2$ I

Session Chairs: Matthias Waegele, *Boston College, USA* and Yuxin Wang, *West Virginia University, USA*.

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3:45 PM **Tue-556AB-1545** Development of Catalytically Active Zeolite ZSM-5 Membranes and Demonstrating Their Performance in the Conversion of $CO_2$ to $CH_4$.
**Romy Riemersma**[1], Thijs Timmers[1], Liliana Baron[2], Anne-Eva Nieuwelink[1], Eelco T.C. Vogt[1] and Bert M. Weckhuysen[1], *(1)Utrecht University, Netherlands, (2)TU Delft, Netherlands*.

**Short Summary:**
We have developed catalytically active *b*-oriented zeolite ZSM-5 membranes for $CO_2$ methanation. We show the development of a reactor that supports a catalytically active zeolite ZSM-5 membrane and demonstrates its separation and catalytic performance. The reactor could be used at point sources of $CO_2$, mitigating its release into the atmosphere.

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4:05 PM **Tue-556AB-1605** Nucleation of Rhodium Clusters in Metal Oxide Frameworks and Their Influence on $CO_2$ Hydrogenation.
**Shuting Xiang**[1], Juan Jimenez[2], Luisa Posada[3], Samantha Rubio[3], Steven Suib[3], Anatoly Frenkel[1,2] and Sanjaya D. Senanayake[2], *(1)Stony Brook University, USA, (2)Brookhaven National Laboratory, USA, (3)University of Connecticut, USA*.

**Short Summary:**
By leveraging structural information from in-situ XAFS and the surface species evidenced via in-situ DRIFTS at reaction conditions, we are poised to gain a strong understanding of the structure/function relationship for Rh catalysts with controlled nuclearity and discern the kinetic and mechanistic influence of secondary metal addition for $CO_2$ hydrogenation.

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4:25 PM **Tue-556AB-1625** Enhancement of Ni-Ce Interface Generation Using Surfactant-Assisted Melt-Infiltration Method: Application for $CO_2$ Hydrogenation.
**Byung Sun Yoon**, Eui Hyun Cho, Yeon Jeong Yu, Sung June Cho and Chang Hyun Ko, *Chonnam National University, Korea, Republic of (South)*.

**Short Summary:**
Melt-infiltration method using surfactant was used to prepare high loading of nickel (40 wt%) and ceria (Ce/Ni = 0.5) on mesoporous silica SBA-15 with higher dispersion. This catalysts showed higher catalytic activity at low temperature (~ 493 K) compared to other catalysts without using surfactant.

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4:45 PM **Tue-556AB-1645** Ru-Promoted Perovskites for $CO_2$-Splitting and Syngas Generation in a Chemical Looping Scheme.
**Sherafghan Iftikhar**[1], William Martin[1], Xijun Wang[2], Junchen Liu[1], Yunfei Gao[3] and Fanxing Li[1], *(1)North Carolina State University, USA, (2)Northwestern University, USA, (3)East China University of Science and Technology, China*.

**Short Summary:**
This study is significant since(a) it validated a DFT guided mixed oxide design strategy, which can be effective in further optimizing the redox catalysts for $CO_2$ utilization;(b) it unveils the deactivation mechanism for a mixed redox catalyst and reports an effective approach to reverse the deactivation and ensures long-term stability.

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5:05 PM **Tue-556AB-1705** Ethylene and Carbon Monoxide Production through Coupled $CO_2$ Reduction and Ethane Dehydrogenation over Chromium Sites Stabilized By Highly Siliceous MFI Zeolite.
**Wenqi Zhou**, Noah Felvey, Coleman Kronawitter and Ron Runnebaum, *University of California, Davis, USA*.

**Short Summary:**
Catalytic packed-bed reactor experiments, combined with *in-situ* spectroscopic characterization, enable elucidation of the catalytic cycle of $CO_2$-ethane dehydrogenation by dispersed Cr cations supported on the crystalline silicate Si-MFI. It was found that Cr/Si-MFI exhibits high stability and selectivity towards ethylene and carbon monoxide.

## Ballroom A

### TUESDAY MORNING

### Catalytic Upcycling of Oxygenated Polymers

Session Chairs: Ali Hussain Motagamwala, *Shell, USA* and Eleni Kyriakidou, *University at Buffalo (SUNY), USA*.

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9:30 AM **Tue-BLRMA-0930** Depolymerization of Chitosan By Supported Bimetallic Catalysts - Towards Waterborn Plastic Alternatives.
**Kordula Schnabl**, Florian Zand, Ina Vollmer, Mies van Steenbrgen and Bert M. Weckhuysen, *Utrecht University, Netherlands*.

**Short Summary:**
A novel strategy for the biopolymer chitosan depolymerization with supported bimetallic catalysts is explored which is able to depolymerize at relatively low temperatures and atmospheric pressure. The effect of changing catalyst properties are investigated on the depolymerization mechanism and final size and size distribution of the chitosan oligomer.

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9:50 AM **Tue-BLRMA-0950** Catalytic Upcycling of Micro/Nanoplastics from Clothes Washing.
**Silvia Parrilla-Lahoz**[1] and Melis Duyar[2], *(1)University of Surrey, United Kingdom, (2)University of Surrey, United Kingdom*.

**Short Summary:**
Microplastics' widespread environmental presence has drawn attention in recent years. Currently, several approaches are under development in order to upcycle microplastics. A bimetallic Ni-Fe catalyst was tested in a catalytic pyrolysis reaction for textile microfibres, demonstrating the ability of this process to produce hydrogen, valuable hydrocarbons, and carbon.

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10:10 AM **Tue-BLRMA-1010** Mechanochemical Conversion of Different Carbon-Based Polymers to Light Hydrocarbons.
**Linfeng LI** and Ferdi Schüth, *Max-Planck-Institut für Kohlenforschung, Germany*.

**Short Summary:**
A mechanochemical method by ball milling was developed to convert biomass, plastics and coal into light hydrocarbons. A radical mechanism was conceived based on radical trapping experiments. This proves that ball milling could be a promising method to convert those polymers into small molecules without external heating.

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10:30 AM ***KEYNOTE*** **Tue-BLRMA-1030 Developing Strategies for Polymer Redesign and Recycling Using Reaction Pathway Analysis.**
**Linda Broadbelt**[1], Gorugantu SriBala[1], Rebecca Harmon[1], Eugene Chen[2], Changxia Shi[2], Matthew Coile[1], Sai Phani Kumar Vangala[1] and Alexander Shaw[1], *(1)Northwestern University, USA, (2)Colorado State University, USA*.

**Short Summary:**
It is imperative that approaches are developed to address the reuse, recycling, and upcycling of plastics. In this contribution, we outline two promising approaches and the role that kinetic modeling and reaction pathway analysis can play in process and catalyst design.

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11:10 AM **Tue-BLRMA-1110** Tuning Catalyst Design for Selective Conversion of Polar Polymers in Multilayer Films.
Dai-Phat Bui, Han Chau, Luis Trevisi, Quy Nguyen, Bin Wang, Lance Lobban and **Steven Crossley**, *University of Oklahoma, USA*.

**Short Summary:**
Multicomponent polymer films present numerous challenges upon recycling and upcycling. Here we report catalytic strategies for selective conversion of EVOH polymers to polyolefins. We highlight the role of the metal-reducible oxide interface on promotion of this chemistry, as well as strategies to understand and mitigate the complex local solvating environment.

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11:30 AM **Tue-BLRMA-1130** Formation of Long Chain PET Oligomers Via Microwave Induced Swelling and Depolymerization.
**Sean Najmi**, Dylan Huang, Brandon Vance, Esun Selvam and Dionysios Vlachos, *University of Delaware, USA*.

**Short Summary:**
The formation of long chain PET oligomers during depolymerization are studied and characterized. The oligomers formed demonstrate characteristics similar to starting PET. They can undergo self-condensation and reform to PET demonstrating a new recycling method. The oligomers can be coblended with other materials for development of new polymers.

### TUESDAY AFTERNOON

### Polyolefins Waste Conversion I

Session Chairs: Lucas Dorazio, *BASF Corporation, USA* and Yixiao Wang, *Idaho National Laboratory, USA*.

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1:20 PM **Tue-BLRMA-1320** Chemical Recycling of Polyethylene By Tandem Catalytic Conversion to Propylene.
**Garrett Strong**[1], Vanessa DaSilva[2], Lijun Gao[3], Saam Farzam[1], Damien Guirronet[2] and Susannah Scott[4], *(1)UCSB, USA, (2)UIUC, USA, (3)University of California, Santa Barbara, USA, (4)UC Santa Barbara, USA*.

**Short Summary:**
We provide experimental demonstrations of our tandem catalysis strategy, which uses ethylene to convert PE to propylene, the commodity monomer used to make PP. The approach combines rapid olefin metathesis with rate-limiting isomerization. Monounsaturated PE is progressively disassembled at modest temperatures via many consecutive ethenolysis events, resulting selectively in propylene.

1:40 PM **Tue-BLRMA-1340** Identifying Active Species in Low-Temperature Polyolefin Upcycling Via Cracking and Alkylation.
**Boda Yang**[1], Wei Zhang[2], Sungmin Kim[1], Oliver Y. Gutierrez[1] and Johannes A. Lercher[1,2], *(1)Pacific Northwest National Laboratory, USA, (2)Technical University of Munich, Germany*.

**Short Summary:**
We investigate the reaction pathways in a new polyolefin upcycling process (tandem cracking-alkylation) and the actives species formed within reactive chloroaluminate ionic liquids. Kinetic experiments and *in-situ* $^{27}$Al-NMR indicate that tuning the anion size can shift the equilibria to increase the concentration of active Al species and, therefore, reaction rates.

2:00 PM **Tue-BLRMA-1400** Kinetic Phenomena in Mechanocatalytic Polyolefin Depolymerization.
**George Y. Chang**[1], Van Son Nguyen[2] and Carsten Sievers[1], *(1)Georgia Institute of Technology, USA, (2)Technical University of Munich, Germany*.

**Short Summary:**
Novel chemical approaches for processing solid plastic waste are growing in relevance. Here, solid-state depolymerization of poly(styrene) and poly(ethylene) in a ball mill reactor was investigated to reveal the importance of continuous monomer removal from the reactor during depolymerization, particle-scale dilution effects involving chemical additives, and a shared oxidation-cleavage mechanism.

2:20 PM **Tue-BLRMA-1420** Catalytic Upcycling of Real-World Contaminated Polyolefin Plastic Waste Using Hydroconversion.
**Pavel Kots** and Dionysios Vlachos, *University of Delaware, USA*.

**Short Summary:**
We outline two basic strategies to convert severely contaminated plastic waste over heterogeneous catalysts using hydroconversion. The first approach involves polyethylene mixed with various antioxidants and stabilizers over a bifunctional hydrocracking catalyst. The second strategy proposes a time and energy-efficient chlorine removal step enabling hydrogenolysis of PVC-contaminated polypropylene.

2:40 PM **Tue-BLRMA-1440** Reaction Mechanisms of Acid-Catalyzed Cracking and Alkylation in the Upcycling of Polyethylene: AIMD Study.
**Mal-Soon Lee**[1], Debmalya Ray[1], Rachit Khare[2], Wei Zhang[2], Donald M. Camaioni[1], Oliver Y. Gutierrez[1] and Johannes A. Lercher[1,2], *(1)Pacific Northwest National Laboratory, USA, (2)Technical University of Munich, Germany*.

**Short Summary:**
Reaction mechanisms of acid-catalyzed cracking and alkylation of polyolefins with isoalkanes and a Lewis acidic chloroaluminate ionic liquid from AIMD simulations combined with a Blue Moon ensemble method will be presented to understand experimentally observed low-temperature conversion of polyethylene to liquid isoalkanes ($C_6$-$C_{10}$) at $T \leq 70$ °C.

3:00 PM **Tue-BLRMA-1500** Catalytic Hydrogenolysis and Hydrocracking of Polyethylene to Gaseous Hydrocarbons on MFI-Based Zeolites.
**Jun Zhi Tan**, Cole Hullfish, Yiteng Zheng, Bruce E. Koel and Michele Sarazen, *Princeton University, USA*.

**Short Summary:**
In this study, we utilized catalytic hydrogenolysis and hydrocracking reactions to convert polyethylene to gaseous hydrocarbons on metal-loaded (Ru, Pt, Ni) zeolites to elucidate the reaction mechanism for C-C bond cleavage of long-chain polymers into desired products.

## Polyolefins Waste Conversion II

Session Chairs: Karl Krueger, *Shell, USA* and Kerry Dooley, *Louisiana State University, USA*.

3:45 PM **Tue-BLRMA-1545** Support Effects on the Hydroconversion of Polyolefin Plastics over Highly Dispersed Ru Catalysts.
**Linxiao Chen**[1], Julia B. Moreira[1], Libor Kovarik[1], Jorge Perez-Aguilar[2], Adam Hoffman[3], Simon Bare[3], Oliver Y. Gutierrez[1] and Janos Szanyi[1], *(1)Pacific Northwest National Laboratory, USA, (2)University of California, Davis, USA, (3)SLAC National Accelerator Laboratory, USA*.

**Short Summary:**
The catalyst support can regulate the structural properties of ultra-small Ru species, thus altering their performances in polyolefin hydrogenolysis, and/or add Brønsted acidity, thus allowing polyolefin hydrocracking. This work facilitates the development of more efficient and selectivity plastic upcycling catalysts, while enhancing the understanding of structure-function relationships and reaction mechanisms.

4:05 PM **Tue-BLRMA-1605** The Effects of $CeO_2$ Morphology for Polyethylene Hydrogenolysis on Ru/$CeO_2$ Catalysts Under Mild Conditions.
Achmad Buhori[1,2], Jae-Wook Choi[2], Dong Jin Suh[2], Jeong-Myeong Ha[1,2] and **Chun-Jae Yoo**[2], *(1)Korea University of Science and Technology, Korea, Republic of (South), (2)Korea Institute of Science and Technology, Korea, Republic of (South)*.

**Short Summary:**
Maximizing liquid yield is critical for converting waste plastics into naphtha cracker feed and liquid fuel. In this study, the effects of $CeO_2$ morphology on the hydrolysis of polyethylene over Ru/$CeO_2$ was investigated. The smaller Ru particle size and the higher $H_2$ spillover capacity effectively inhibited the formation of methane.

4:25 PM **Tue-BLRMA-1625** Deconvoluting the Contributions of Polyolefin Branching and Unsaturation for Upcycling Reaction Rates.
**Ana Carolina Jerdy**[1], Miguel Gonzalez Borja[2], Masud Monwar[2], Ron Abbott[2], Lance Lobban[1] and Steven Crossley[1], *(1)University of Oklahoma, USA, (2)Chevron Phillips Chemical Company LP, USA*.

**Short Summary:**
We decompose different polyethylene samples over acid catalysts to assess the importance of branching and unsaturation to the reaction rate and product distribution. We contrast these results with alkane cracking chemistry and assess the role of diffusion by removing acid sites from the external surface of an industrially relevant zeolite.

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4:45 PM **Tue-BLRMA-1645** Hydrogenolysis of Polyethylene and Polypropylene into Propane over Cobalt-Based Catalysts.
Guido Zichittella[1], Amani Ebrahim[2], Jie Zhu[1], **Anna Brenner**[1], Griffin Drake[1], Gregg T. Beckham3, Simon Bare[2], Julie Rorrer[1] and Yuriy Roman[1], *(1)Massachusetts Institute of Technology, USA, (2)SLAC National Accelerator Laboratory, USA, (3)National Renewable Energy Laboratory, USA*.

**Short Summary:**
We found that 5 wt.% cobalt supported on ZSM-5 catalyzes the hydrogenolysis of PE and PP into propane with impressive selectivity (80 wt.% gas phase) when compared to bulk cobalt where the formation of methane is favored. Furthermore, zeolite topology was demonstrated as a handle to tune gas-phase selectivity.

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5:05 PM **Tue-BLRMA-1705** Active Ni/$Al_2O_3$ Catalysts with Reduced Methane in Polyolefin Hydrogenolysis.
**Brandon Vance**, Sean Najmi, Pavel Kots, Cong Wang and Dionysios Vlachos, *University of Delaware, USA*.

**Short Summary:**
Polyolefin hydrogenolysis is promising for deconstructing polyolefin waste to valuable products. Hydrogenolysis is prone to producing undesired methane and limited strategies exist to reduce methane generation. This work establishes a simple method for reducing the methane selectivity to <5% over cheap Ni-based catalysts with high yields to liquid products.

## Ballroom BC

### TUESDAY MORNING

### New Modeling Approaches for Electrocatalysis and Photocatalysis

Session Chairs: Aaron Deskins, *Worcester Polytechnic Institute, USA* and Jingjie Wu, *University of Cincinnati, USA*.

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9:30 AM ***KEYNOTE*** **Tue-BLRMBC-0930 First-Principles Based Modelling of Electrocatalysis Beyond the Potential of Zero Charge.**
**Karsten Reuter**, *Fritz-Haber-Institut der MPG, Germany*.

**Short Summary:**
The fusion of first-principles multiscale modeling methodology with modern concepts from machine learning (ML) opens a roadmap to interfacial electrocatalysis at applied potential conditions and concomitant operando evolution of the electrode surface.

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10:10 AM **Tue-BLRMBC-1010** First Step of the Oxygen Reduction Reaction on Au(111): An *Ab Initio* Molecular Dynamics Study of the O2 Adsorption at the Electrified Metal/Water Interface.
**Alexandra M. Dudzinski**, Elias Diesen, Hendrik H. Heenen, Vanessa J. Bukas and Karsten Reuter, *Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany*.

**Short Summary:**
Going beyond simplified charge-neutral simulation cells shows that O2 adsorption on Au(111) is strongly enhanced (~0.9 eV) under reducing conditions. We elucidate the role of electrostatic potential, suggesting that its effects cannot be neglected in corresponding DFT models and may explain the experimental pH-dependent ORR activity on weak-binding catalysts.

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10:30 AM **Tue-BLRMBC-1030** Modeling Specific Alkali Cation Adsorption and Electrochemical Double-Layers with DFT and Classical MD.
**Andrew Wong**, Bolton Tran, Scott Milner and Michael Janik, *The Pennsylvania State University, USA*.

**Short Summary:**
We present a combined DFT and Classical MD approach that provides insight into electrochemical double layer structure at the electrode-electrolyte interface, specifically during alkali cation adsorption. Our investigation suggests that specific cation adsorption is possible and these cation-adsorbate interactions can affect the rates and selectivity of electrocatalytic processes.

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10:50 AM **Tue-BLRMBC-1050** Impact of Structure and Applied Potential on Proton-Coupled Electron Transfer.
**Phillips Hutchison**[1], Robert Warburton[2] and Sharon Hammes-Schiffer[1], *(1)Yale University, USA, (2)Case Western Reserve University, USA*.

**Short Summary:**
This work demonstrates the importance of accounting for applied potential and local structure in modeling electrocatalysis. Fe-N-C models agree better with experimental findings when an axial water ligand is included on the active site. With graphite-conjugated catalysts, an electronic structure feature describes doping-induced changes to proton-coupled redox potentials.

11:10 AM **Tue-BLRMBC-1110** Discovery of Stable and Active Iridium-Molybdenum Oxide Electrocatalyst for the Oxygen Evolution Reaction Using Bayesian Optimization.
**Aarti Mathur**[1], Jacques Esterhuizen[1], Bryan Goldsmith[1] and Suljo Linic[2], *(1)University of Michigan, USA, (2)University of Michigan - Ann Arbor, USA*.

**Short Summary:**
We used machine-learning-aided Bayesian optimization paired with density functional theory calculations to assess the stability and activity of Ir-doped mixed oxide materials for the oxygen evolution reaction. We electrochemically tested IrMo, which emerged from this study, and found that it demonstrated low overpotentials and maintained high stability under reaction conditions.

11:30 AM **Tue-BLRMBC-1130** Transfer Learning Aided High-Throughput Computational Design and Experimental Validation of Oxygen Evolution Reaction Catalysts in Acid Condition.
**Siwen Wang**, Honghong Lin, Yui Wakabayashi, Li Qin Zhou and Chen Ling, *Toyota Research Institute - North America, USA*.

**Short Summary:**
We presented a machine learning-aided high-throughput screening protocol incorporating MP database, DFT calculations and machine learning models. Screening ~7,000 pyrochlores, 39 candidates were suggested meeting requirements. Experimental synthesis and OER performance evaluation have also been carried out to demonstrate the effective tuning of catalytic performance through appropriate selection of compositions.

## TUESDAY AFTERNOON

## Development of $CO_2$ Conversion Catalysts by Machine Learning and Theory

Session Chairs: Alyssa Hensley, *Stevens Institute of Technology, USA* and Matteo Maestri, *Politecnico di Milano, Italy*.

1:20 PM **Tue-BLRMBC-1320** Innate Dynamics and Identity Crisis of a Metal Surface Unveiled By Machine Learning of Atomic Environments.
**Matteo Cioni**[1], Daniela Polino[2], Daniele Rapetti[1], Massimo Delle Piane[1] and Giovanni Maria Pavan[1,2], *(1)Politecnico di Torino, Italy, (2)University of applied sciences and arts of southern Switzerland - SUPSI, Switzerland*.

**Short Summary:**
Metal surfaces are mobile at the *operando* conditions of thermal catalysis. Insight in their structural dynamics is fundamental to understand their properties and improve their performance. Here we show how deep-potential molecular dynamics simulations combined with high-dimensional structural descriptors allow the atomistic-resolution characterization of the dynamics of various copper surfaces.

1:40 PM **Tue-BLRMBC-1340** Machine Learning-Driven High Entropy Alloy Catalyst Discovery to Circumvent the Scaling Relation for $CO_2$ Reduction Reaction.
**Zachary Gariepy**, *University of Toronto, Canada*.

**Short Summary:**
Using machine learning and DFT, FeCoNiCuMo HEA electrocatalysts that circumvent the linear scaling relation between CO* and COOH*/CHO* are designed with some of the lowest reported overpotentials in literature. The mechanism used to achieve these low overpotentials were further elucidated through neural network decomposition

2:00 PM **Tue-BLRMBC-1400** Designing High Entropy Catalysts Via AI-Accelerated First-Principles Calculations: Catalyst Structure, Active Sites & Mechanisms.
**Teck Leong Tan**, *Institute of High Performance Computing, A*STAR, Singapore*.

**Short Summary:**
With 5 or more principal-component elements, high entropy alloys (HEA) exists as solid-solution phases. A nascent development, HEA nanoparticles (HEA-NP) are currently explored as catalysts. We investigate the active sites and reaction mechanisms on AgAuCuPdPt HEA-NP for $CO_2$ reduction to $CH_4$ via first-principles calculations using a 55-atom and 147-atom icosahedron.

2:20 PM **Tue-BLRMBC-1420** Kinetic Model, Process Design and LCA of a $CO_2$ Valorization Plant to Produce Light Hydrocarbon Using a Pdzn/$ZrO_2$ + SAPO-34 Catalyst.
**Tomas Cordero-Lanzac**[1], Adiran Ramirez[2], Marta Cruz-Fernandez[3], Hans-Jörg Zander[4], Finn Joensen[5], Andreas Meiswinkel[4], Jorge Gascon[2] and Unni Olsbye[1], *(1)University of Oslo, Norway, (2)King Abdullah University of Science and Technology (KAUST), Saudi Arabia, (3)TataSteel, United Kingdom, (4)Linde GmbH, Germany, (5)TOPSOE A/S, Denmark*.

**Short Summary:**
A tandem catalytic system is proposed for the one-step hydrogenation of $CO_2$ to hydrocarbons. From lab-scale experiments, kinetic parameters were extracted and a plant for larger-scale valorization of $CO_2$ is proposed. Our results show that $CO_2$-based propane by this route can have lower environmental impact than fossil-based propane

2:40 PM **Tue-BLRMBC-1440** Enhanced $CO_2$RR-to-$C_3$+ Liquid Fuels over Bimetallic Systems.
**Yuting Xu**, Fanglin Che and Michael Ross, *University of Massachusetts Lowell, USA*.

**Short Summary:**
This work is able to directly synthesize liquid fuels from $CO_2$, reducing logistics required to transport fuels and increasing local resiliency to power outages and fuel consumption. While this is a net-zero carbon process because it actively removes $CO_2$ from the atmosphere to generate liquid hydrocarbon fuels, mitigating emissions.

3:00 PM **Tue-BLRMBC-1500** Identifying the Role of Coordination in the Catalysis of Single Atom Co-Carbon Nitride Materials.
**Qian Qian** and Aaron Deskins, *Worcester Polytechnic Institute, USA*.

**Short Summary:**
The coordination number of single metal atoms plays a crucial role in $CO_2$ photoreduction. This work focuses on modeling Co-carbon nitride catalysts and explains how their properties (coordination number, metal charge, support structure) affect $CO_2$ photoreduction.

## Modeling of Catalytic Reactions and Materials

Session Chairs: Joaquin Resasco, *The University of Texas at Austin, USA* and Luke Roling, *Iowa State University, USA*.

3:45 PM **Tue-BLRMBC-1545** Effective Modeling of Diffusion Limitations inside a Catalytic Filter Wall and Their Impact on the Catalyst Light-Off.
**Petr Koci**, Jan Nemec and Marie Placha, *University of Chemistry and Technology, Czech Republic*.

**Short Summary:**
A new 1D mathematical model describing diffusion limitations in a catalytic filter wall is proposed. CO oxidation is investigated both at low and high concentrations. The computed 1D concentration profiles are compared to detailed 3D pore-scale simulations using X-ray tomography reconstruction, and measured light-off curves for clean and soot-loaded filters.

4:05 PM **Tue-BLRMBC-1605** Modelling of Cyclic $CO_2$ Adsorption and in Situ Methanation over Dual Function Materials: A Parametric Study.
**Alessio Tauro**[1], Fabio Salomone[1], Emanuele Giglio[2], Samir Bensaid[1] and Raffaele Pirone[1], *(1)Polytechnic of Turin, Italy, (2)University of Calabria, Italy*.

**Short Summary:**
The work aims to create a model that describes the atmospheric methanation of $CO_2$ by using a DFM catalyst made of Ru and an alkaline-based adsorbent. A study of the kinetic parameters allows to select the optimal characteristics of the materials for cyclic $CO_2$ adsorption and methanation.

4:25 PM **Tue-BLRMBC-1625** DFT Study of Heterogeneous Catalysts for Direct Coupling of $CO_2$ and $C_2H_4$.
**Quy Nguyen** and Bin Wang, *University of Oklahoma, USA*.

**Short Summary:**
We computationally design heterogeneous catalysts for the direct coupling of $CO_2$ and $C_2H_4$ using nitrogen-doped metal atom-decorated graphene. We discuss the dependence of the energy profile on the nature of the metal and its local coordination. Furthermore, we propose approaches to reduce the activation barrier of the rate-determining step.

4:45 PM **Tue-BLRMBC-1645** Microkinetic Modeling with Accurately Predicted Pathways Involving Bidentate Adsorbates: An Ethane Hydrogenolysis Study with RMG.
Katrín Blöndal[1], **Bjarne Kreitz**[1], Richard West[2] and Franklin Goldsmith[1], *(1)Brown University, USA, (2)Northeastern University, USA*.

**Short Summary:**
The RMG catalysis database now includes training data for reactions involving bidentate H/C/O-containing adsorbates. This addition, along with the software's use of linear scaling relations for multidentate species, enhances microkinetic mechanisms for important catalytic processes on a range of metals. The improvement is demonstrated with an ethane hydrogenolysis modeling study.

5:05 PM **Tue-BLRMBC-1705** Descriptors for Oxygen Ion Transport in Metal Oxides.
Daniele Vivona[1], Kiarash Gordiz[1], Jaclyn Lunger[1], Yang Shao-Horn[1], Sumathy Raman[2] and **Randall Meyer**[2], *(1)Massachusetts Institute of Technology, USA, (2)ExxonMobil Technology and Engineering Corporation, USA*.

**Short Summary:**
Different descriptors involving crystal geometry, electronic structure and phonon modes of the solid have been examined for prediction of oxygen ion migration barriers in metal oxides using density functional theory. A multi-descriptor non-linear model has been developed which shows charge transfer to play a dominant role in oxygen ion migration.

# Ballroom DE

### TUESDAY MORNING

## Plasma-Enhanced Catalysis for $N_2$ Activation

Session Chairs: Christopher Keturakis, *Honeywell UOP, USA* and Krishna Gunugunuri, *Cummins Technical Center*.

9:30 AM **Tue-BLRMDE-0930** Plasma-Enhanced Chemical Looping Ammonia Synthesis over Bifunctional Catalysts.
**Sean Brown**[1], Brandon Robinson[1], Saleh Ahmat Ibrahim[2], Fanglin Che[2] and Jianli Hu[1], *(1)West Virginia University, USA, (2)University of Massachusetts Lowell, USA*.

**Short Summary:**
Chemical looping ammonia synthesis low pressure synthesis of ammonia is a cyclic nitrogen-fixation-ammonia-synthesis set of reactions. The combination of $N_2$ pre-activation by a microwave-plasma-enhanced catalytic process and a nitrogen storage material with low loadings of an $H_2$ catalyst. Density function theory modelling is used with experiment to guide catalyst design.

9:50 AM **Tue-BLRMDE-0950** Accessing and Stabilizing Metastable Nitrogen Species By Coupling Plasma and Metal Surface Chemistry: Evidence for Surface-Adsorbed Azide (N3).
Garam Lee, Chang Yan, William Schneider, David Go and **Casey O'Brien**, *University of Notre Dame, USA*.

**Short Summary:**
In this work, I will demonstrate that $N_2$ plasmas coupled to metal (Ni, Pd, Ag, Au, Cu) surfaces can access and stabilize metastable azide, or N3, species that are not accessible through thermal catalysis or plasma alone.

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10:10 AM **Tue-BLRMDE-1010** DFT Analysis of Speciation and Stability of Surface-Bound Nitrogen Species Under $N_2$ Plasma Exposure.
**Chang Yan**, Garam Lee, David Go, Casey O'Brien and William Schneider, *University of Notre Dame, USA*.

**Short Summary:**
Coupling $N_2$ plasma and catalyst can produce metastable species N3 at room temperature and DFT-computed vibrational frequencies align with experimental observations.

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10:30 AM **Tue-BLRMDE-1030** Reaction Mechanisms for Plasma-Catalytic Ammonia Synthesis.
**Leon Lefferts**, *University of Twente, Netherlands*.

**Short Summary:**
A rigorous experimental kinetic study reveals that Eley-Rideal reactions of plasma radicals with adsorbed species on the metal surface are dominant, in agreement with previous theoretical studies. True plasma-catalysis, dissociating excited $N_2$ molecules on the surface, may be relevant only at low SEI.

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10:50 AM **Tue-BLRMDE-1050** On the Potential Role of $N_2(v)$ in Plasma Catalysis.
**Brian Bayer**, Peter Bruggeman and Aditya Bhan, *University of Minnesota, Twin Cities, USA*.

**Short Summary:**
This work combines experimental measurement of vibrationally excited $N_2$ ($N_2(v)$) densities with kinetic modeling to assess formation and loss pathways for $N_2(v)$ during $NH_3$ formation by plasma catalysis. Results show that $N_2(v)$) undergoes vibrational relaxation faster than dissociative adsorption, which limits the ability of $N_2(v)$ to contribute to $NH_3$ formation.

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11:10 AM **Tue-BLRMDE-1110** Towards Understanding Plasma-Catalysts Interactions through Plasma -Temperature Programmed Reactions.
**Hope Otor**, Patrick Barboun, Hanyu Ma, Anshuman Goswami, William Schneider and Jason C. Hicks, *University of Notre Dame, USA*.

**Short Summary:**
This presentation focuses on our recent findings in elucidating plasma activation of dinitrogen and its reactivity over metal catalyst surfaces. Through carefully designed sequential experiments and microkinetic modeling, we show that the hydrogenation ability of metal catalysts is critical in determining reactivity trends in plasma-assisted ammonia synthesis.

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11:30 AM **Tue-BLRMDE-1130** Effect of Nickel Nitride on Plasma-Assisted Ammonia Synthesis over Nickel Catalysts.
**Yiteng Zheng**, Christopher Kondratowicz, Ari Gilman, Sonia Arumuganainar and Bruce E. Koel, *Princeton University, USA*.

**Short Summary:**
The effect of Ni nitride on plasma-assisted ammonia synthesis was systematically studied by temperature programmed reaction in a DBD plasma reactor. The catalysts were characterized ex situ to probe the extend of Ni nitride formation.

## TUESDAY AFTERNOON

## Low-Temperature Passive NOx Adsorption

Session Chairs: Do Heui Kim, *Seoul National University, Korea, Republic of (South)* and Leon Lefferts, *University of Twente, Netherlands*.

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1:20 PM ***KEYNOTE* Tue-BLRMDE-1320 Insight into CO Influence on Passive NOx Adsorption over Pd/SSZ-13.**
**Louise Olsson**[1], Dawei Yao[1], Johann Wurzenberger[2], Thomas Glatz[2] and Derek Creaser[1], *(1)Chalmers University of Technology, Sweden, (2)AVL List GmbH, Austria*.

**Short Summary:**
Passive NOx absorbers (PNA) can be used to reduce the emissions of NOx from vehicles. We have developed a model that describes the PNA behavior, including the mechanism of CO induced degradation. Furthermore, we developed the synthesis for a novel PNA sample that shows a better CO resistance.

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2:00 PM **Tue-BLRMDE-1400** Effects of Pretreatment on the Modes of NO Adsorption in Pd/H-CHA.
Paul Kim[1], Jeroen Van der Mynsbrugge[1], Hassan Aljama[1], Martin Head-Gordon[2] and **Alexis Bell**[1], *(1)University of California, Berkeley, USA, (2)Lawrence Berkeley National Laboratory, USA*.

**Short Summary:**
We show that $Pd^{2+}$ in Pd/H-CHA PNAs must be reduced to Pd+ to form strongly-bound NO that desorbs > 550 K, temperatures at which three-way catalytic convertors can reduce NO. Water vapor plus CO or NO are required to reduce $Pd^{2+}$ to $Pd^{+}/H^{+}$ pairs associated with neighboring charge-exchange sites.

2:20 PM **Tue-BLRMDE-1420** Mechanistic Roles of $H_2O$, CO, and $O_2$ during Passive $NO_x$ Adsorption on Atomically Dispersed Pd-CHA.
Surya Pratap S. Solanki[1], Mugdha Ambast[1], Chris Paolucci[2], Michael Harold[1] and **Lars Grabow**[1], *(1)University of Houston, USA, (2)University of Virginia, USA*.

**Short Summary:**
From a combination of density functional theory calculations and reaction experiments, we propose a complete mechanism for passive $NO_x$ adsorption (PNA) on atomically dispersed Pd-CHA. The presence of $H_2O$, CO and $O_2$ is explicitly considered, and mechanistic roles are assigned. Steps leading to deactivation are also included.

2:40 PM **Tue-BLRMDE-1440** Assessing Pd-Exchanged CHA Sites for Passive NOx Adsorption with the Aid of a High Throughput Workflow.
**Hassan Aljama**[1], Martin Head-Gordon[2] and Alexis Bell[3], *(1)Aramco, Saudi Arabia, (2)Lawrence Berkeley National Laboratory, USA, (3)University of California, Berkeley, USA*.

**Short Summary:**
Cation exchanged-zeolites present a challenge for computational studies using DFT due to the numerous possible active sites. We attempt to tackle this by implementing a workflow for a high throughput screening. The screening results shed light on critical active sites for NOx capture that were not previously studied.

3:00 PM **Tue-BLRMDE-1500** Effect of Zeolite Framework on the Operating Cycle of NO in Passive NOx Adsorbers.
**Marvi Kaushik**[1], Tuhin S. Khan[2], M. Ali Haider[1] and Divesh Bhatia[1], *(1)Indian Institute of Technology Delhi, India, (2)CSIR-Indian Institute of Petroleum, India*.

**Short Summary:**
DFT calculations for various zeolite frameworks on Pd-based passive NOx adsorbers are performed to study their effect on the NO binding strength and the energetics of inter-conversion between different Pd sites. The insights obtained are used to propose unique NOx adsorption-desorption operating cycles for various Pd/zeolites.

## Electrocatalytic $N_2$ Conversion

Session Chairs: Andrew Medford, *Georgia Institute of Technology, USA* and Craig Plaisance, *Louisiana State University, USA*.

3:45 PM **Tue-BLRMDE-1545** Investigation of Double Perovskite-Type Mixed Anion (oxynitride) Cathodes for High-Temperature Electrocatalytic $NH_3$ Production.
Seval Gunduz, Matthew Ferree, Jaesung Kim, Anne Co and **Umit Ozkan**, *The Ohio State University, USA*.

**Short Summary:**
High-temperature electrocatalytic nitrogen reduction reaction (NRR) has the potential to enable on-site, sustainable, scalable, and energy-efficient ammonia production. Double perovskite oxynitride-type materials are promising cathodes for electrocatalytic-NRR process due to their stability and endless possibilities to modify their structure to optimize their ionic/electrical conductivity and nitrogen activation ability.

4:05 PM **Tue-BLRMDE-1605** Understanding the Mechanism of Li-Mediated Nitrogen Reduction Reaction.
**Yuanyuan Zhou** and Jens K. Nørskov, *Technical University of Denmark, Denmark*.

**Short Summary:**
Lithium-mediated nitrogen reduction (LiNR) is the validated method for e-$NH_3$ synthesis at ambient temperature. However, the mechanism of LiNR is yet not fully understood. Herein, we investigate the mechanism of the LiNR fromthe *ab initio* atomistic reaction process, mean-field microkinetics, to the mass-transport simulations, explicitly considering the solid-electrolyte interphase.

4:25 PM **Tue-BLRMDE-1625** The Role of Competitive Water Adsorption in Controlling Anodic Dinitrogen Activation.
**Samuel Olusegun** and Joseph Gauthier, *Texas Tech University, USA*.

**Short Summary:**
Understanding the effects of competitive adsorption of water and $N_2$ on anodic $N_2$ activation for various catalyst material is important for investigating the possible reaction pathways for electrocatalytic $N_2$ oxidation and identifying catalyst materials that can best be used for this process.

4:45 PM **Tue-BLRMDE-1645** Design Principles for Transition Metal Nitride Stability and Ammonia Generation in Acid.
**Jiayu Peng**[1], Juan Giner-Sanz[1,2], Livia Giordano[1],[3], William Mounfield[1], Graham Leverick[1], Yang Yu[1], Yuriy Roman[1] and Yang Shao-Horn[1], *(1)Massachusetts Institute of Technology, USA, (2)Universitat Politècnica de València, Spain, (3)Università di Milano-Bicocca, Italy*.

**Short Summary:**
Transition metal nitride electrocatalysts suffer from severe dissolution in acidic electrolytes, causing degradation for ORR and false positives for N2RR. In this work, we established design principles governing the kinetics of nitride dissolution and ammonia generation in acid, offering a blueprint to design and optimize nitrides for acidic electrocatalytic applications.

5:05 PM **Tue-BLRMDE-1705** Photoelectrocatalytic Urea Oxidation at Silicon Photoanodes.
**Joudi Dabboussi**, *University of Rennes*[1], *France*.

**Short Summary:**
Our work present the synthesis of amorphous Ni-Mo-O(NMO) catalyst onto metal-insulator-semiconductor Silicon junctions by a hydrothermal method. These photoanodes exhibit high performance for the urea oxidation reaction(UOR), a promising half-reaction used for coupling water-depollution to $H_2$-production using urine-contaminated effluents, and presents an optically-adaptive-nature that promotes a maximum photocurrent with urea.

# Rotunda

## TUESDAY MORNING

### In Situ Vibrational Spectroscopy

Session Chairs: Kimber Stamm, *Toyota Research Institute - North America, USA* and Matteo Monai, *Utrecht University, Netherlands*.

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9:30 AM **Tue-RTND-0930** Coupling Operando Raman Methodology with Isotopic Experiments to Address the Redox Cycle of Molecularly Controlled MoOx Sites.
Thu Nguyen and **George Tsilomelekis**, *Rutgers, The State University of New Jersey, USA*.

**Short Summary:**
In this study, MoOx sites supported on $TiO_2$ and $CeO_2$-$TiO_2$, synthesized by equilibrium deposition filtration (EDF) method, were investigated. The structure and redox behavior of these materials were studied by isotopic labeling coupled with operando transient Raman spectroscopy - Mass Spectrometry with the goal to develop mechanistic understanding.

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9:50 AM **Tue-RTND-0950** Unravelling the Role of Oxygen Vacancy of $CeO_2$ in the Water-Gas-Shift Reaction by In Situ Spectroscopy Studies on Well-Defined Nanostructures.
**Gengnan Li**[1], Cameron J. Owen[2], Boris Kozinsky[2] and Jorge Boscoboinik[3], *(1)Brookhaven National Lab, USA, (2)Harvard University, USA, (3)Stony Brook University, USA*.

**Short Summary:**
Fundamental understanding of the atomic level structure-activity relationship allows rational design of effective metal oxide catalysts with tailored compositions for achieving optimum selectivity and activity in chemical reactions, such as water-gas-shift reaction, which will have an important impact in $H_2$ production process in industry.

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10:10 AM **Tue-RTND-1010** IR Nanospectroscopy Mapping of Reactivity Variations and Cooperative Communication within Oxide-Supported Nanoparticles.
**Elad Gross**, *The Hebrew University of Jerusalem, Israel*.

**Short Summary:**
The performance of heterogeneous catalysts is dictated by their nanoscale properties and local variations in structure and composition can have a dramatic impact on the catalytic reactivity. Structure-reactivity correlations were identified by conducting infrared nanospectroscopy measurements and provided molecular insights to the reactivity pattern of oxide-supported Au and Pt nanoparticles

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10:30 AM **Tue-RTND-1030** Beating Abbe's Diffraction Limit via Near-Field Nano-FTIR Spectroscopy: Vibrational Spectroscopic Investigation of Catalytic Sulfur Poisoning with Nanometer-Level Spatial Resolution.
**Emrah Ozensoy**, *Bilkent University, Turkey*.

**Short Summary:**
Current work provides fundamental insights on the design and synthesis of sulfur-tolerant and highly-durable catalytic metal/metal-oxide nanomaterials by unraveling nanometer-scale vibrational spectroscopic knowledge on the adsorption geometries, adsorption sites, and bonding configurations of poisons/inhibitors adsorbed on catalytic nanoparticles with high chemical contrast, which have not been available in the literature.

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10:50 AM **Tue-RTND-1050** Identifying the Active Sites and Their Kinetics for Butadiene Synthesis from Ethanol for $ZnO/SiO_2$, $ZrO_2/SiO_2$, and $ZnO$-$ZrO_2/SiO_2$ Catalysts By Modulation Excitation Infrared Spectroscopy.
Benjamin M. Moskowitz and **Israel Wachs**, *Lehigh University, USA*.

**Short Summary:**
Ethanol dehydrogenation and 1,3-butadiene synthesis were studied for $ZnO/SiO_2$, $ZrO_2/SiO_2$, and $ZnO$-$ZrO_2/SiO_2$ catalysts by *in situ* DR UV-vis spectroscopy and *operando* concentration modulation excitation infrared spectroscopy. The results reveal that surface ZrO4 sites are the active sites for BD synthesis.

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11:10 AM **Tue-RTND-1110** Tracking Surface Changes on hBN during the Oxidative Dehydrogenation of Propane Using Operando X-Ray Raman Spectroscopy.
**Melissa Cendejas**[1], Oscar Paredes[1], Dimosthenis Sokaras[1], Unni Kurumbail[2], Jacob Jansen[3], Simon Bare[1] and Ive Hermans[2,3], *(1)SLAC National Accelerator Laboratory, USA, (2)University of Wisconsin–Madison, USA, (3)University of Wisconsin-Madison, USA*.

**Short Summary:**
Boron-based materials are promising catalysts for the oxidative dehydrogenation (ODH) of light alkanes. The origin of activity on these materials has been difficult to identify. Here, we use *operando* X-Ray Raman Spectroscopy to probe the changes that occur on hBN during the catalyst induction period and water cofeed experiments.

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11:30 AM WITHDRAWN: Bifunctional Metal Films As an Electrocatalyst and a Surface-Enhanced Infrared Absorption Spectroscopy Amplifier for Dynamic Mechanistic Study of Interfacial Electrochemical Reactions.

## Electrocatalytic Hydrogen Evolution and Oxidation

Session Chairs: Nitish Govindarajan, *Lawrence Livermore National Laboratory,* and Marcel Schreier, *University of Wisconsin-Madison, USA*.

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1:20 PM **Tue-RTND-1320** Understanding Cation Effects for the Hydrogen Evolution Reaction.
**Jay Bender**[1], Amanda Petersen[2], Frederik Østergaard[2], Mikayla Wood[1], Sean Heffernan[1], Delia Milliron[1], Jan Rossmeisl[2] and Joaquin Resasco[1], *(1)The University of Texas at Austin, USA, (2)University of Copenhagen, Denmark*.

**Short Summary:**
We investigate alkali metal cations on hydrogen evolution reaction (HER) rates in acidic and alkaline electrolytes. Cations do not systematically affect HER rates in acid. In base, HER rates decreased with increasing cation size over Ir, Pd, Pt ($Li^+>Na^+>K^+>Cs^+$) while the trend was reversed for Cu, Ag, Au ($Li^+<Na^+<K^+<Cs^+$).

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1:40 PM **Tue-RTND-1340** The Role of Cations and Hydroxyl on HER Kinetics of Gold Electrode Under Alkaline Conditions.
**Hyeonjung Jung**[1], Michael Tang[2], Jeong Woo Han[1] and Frank Abild-Pedersen[3], *(1)Pohang University of Science and Technology (POSTECH), Korea, Republic of (South), (2)SUNCAT Center for Interface Science and Catalysis, SLAC National Accelerator Laboratory, USA, (3)SLAC National Accelerator Laboratory, USA*.

**Short Summary:**
Activity trends of alkaline HER underscore the potential role of electrolytes in altering catalytic performance. In this study, we show the role of cation sizes in stabilizing nearby hydroxyl molecules, forming a neutral-charged solvated pair close to the surface with decoupled potential energy surfaces and DFT-based kinetic simulations.

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2:00 PM **Tue-RTND-1400** Competitive Adsorption of Electrolytes Inhibits High-Current Hydrogen Oxidation in Non-Aqueous Media.
**Wei Lun Toh**, Andy Fong, Hai-Xu Wang, Bryan Tang and Yogesh Surendranath, *Massachusetts Institute of Technology, USA*.

**Short Summary:**
We investigate the hydrogen oxidation reaction (HOR) as a potential sustainable anode reaction in non-aqueous media in general. We find that at high current densities, HOR is not limited by $H_2$-transport but by competitive adsorption of the proton acceptor. We demonstrate strategies for mitigating this inhibition.

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2:20 PM **Tue-RTND-1420** Understanding Effects of Combined Applied Potential and $H_2$ Pressure on Hydrogenation on Pd in Aqueous Phase.
**Julia B. Moreira**, Laura C. Meyer, Thuy T. Le, Donald M. Camaioni, Oliver Y. Gutierrez and Johannes A. Lercher, *Pacific Northwest National Laboratory, USA*.

**Short Summary:**
We studied the hydrogenation of benzaldehyde on Palladium under applied potential (ECH), and/or $H_2$ pressure (i.e., open-circuit potential, OCP). We observed considerable higher rates for the combined operation mode than those observed for separate ECH and OCP, which we correlate with the dynamics of catalyst composition and reactants binding energies.

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2:40 PM **Tue-RTND-1440** CO-Tolerance of Supported PtRu Electrocatalysts Towards $H_2$ Oxidation.
Nelly M. Cantillo[1], Ernesto C. Zuleta[2], Gabriel A. Goenaga[2] and **Martha Cobo**[1], *(1)Universidad de La Sabana, Colombia, (2)The University of Tennessee, USA*.

**Short Summary:**
Modified carbon nanotubes-supported platinum (Pt)/ruthenium (Ru) catalysts were prepared by a modified chemical vapor deposition process. The 500 °C thermal treatment on graphitized samples (Pt80Ru20-g10/HT500) exhibited higher electroactivity towards the $H_2$ oxidation reaction in CO absence and presence. Performance was also evaluated in fuel cell setup with CO presence.

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3:00 PM **Tue-RTND-1500** Electrochemical Approaches to $C(sp^3)–H$ and $C(sp^3)–C(sp^3)$ Bond Activation.
**Christine Lucky** and Marcel Schreier, *University of Wisconsin-Madison, USA*.

**Short Summary:**
We present approaches to activate C–H and C–C bonds in small organic molecules, including a chloride-mediated pathway to enable $C(sp^3)–H$ bond activation for the valorization of ethanol to ethylene oxide and the real-time control of alkane reactivity through changes to the applied potential.

## Electrocatalytic Oxygen Reduction and Evolution

Session Chairs: Alexander Jenkins, *University of Colorado Boulder, USA* and Karsten Reuter, *Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany*.

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3:45 PM **Tue-RTND-1545** Microstructural Origin of Selective Water Oxidation to Hydrogen Peroxide at Low Overpotentials: A Study on Mn-Alloyed $TiO_2$.
**Devan Solanki**[1] and Shu Hu[2], *(1)Yale, USA, (2)Yale University, USA*.

**Short Summary:**
Electrochemical synthesis of $H_2O_2$ via 2e− water oxidation requires a +0.54 V more positive potential than 4e− $O_2$ evolution. Mn-alloyed $TiO_2$ coatings prepared by Atomic Layer Deposition are stable and selective electrocatalyst for 2e− WOR. Mid-gap states created within the $TiO_2$ forbidden band are energetically matched to peroxide generating intermediates.

4:05 PM **Tue-RTND-1605** Elucidating Structure Property Relationship in Metal-Metal Oxide Interface for Oxygen Reduction Reaction.
**Kaustubh Sawant**[1], Junxian Gao[1], Zhenhua Zeng[1], Dmitry Zemlyanov[1], Jeffrey T. Miller[2] and Jeffrey Greeley[1], *(1)Purdue University, USA, (2)Davidson School of Chemical Engineering, Purdue University, USA*.

**Short Summary:**
Although fuel cells have high theoretical efficiency, their performance is limited by slow kinetics at the cathode. Doping Pt alloys with group 6 elements increases both the stability and reactivity. We elucidate the exact nature of the active site and stabilization mechanism using DFT calculations with surface science experiments.

4:25 PM **Tue-RTND-1625** Supported Metal Catalysts Circumvent Limitations in Reactivity for Oxygen Electrocatalysis.
Kah Meng Yam[1,2], Asmee Prabhu[1], Lavie Rekhi[1], Luan Q. Le[1] and **Tej Choksi**[1,2], *(1)Nanyang Technological University, Singapore, (2)Cambridge Centre for Advanced Research and Education, Singapore*.

**Short Summary:**
Low-dimensional metal films supported on metal carbides/nitrides exhibit scaling relations for ORR that deviate from rigid bond order conservation rules. These deviations enhance the maximum attainable reactivity on a Sabatier volcano. This study reinforces the promise of using supported metal catalysts to transcend reactivity limitations imposed by scaling relations.

4:45 PM **Tue-RTND-1645** Enhancement in the ORR Activity of Nitrogen – Doped Carbon Nanostructures Via Electrochemical Bromine Doping.
**Dishari Basu**, Patrick McFarlane, Aravind Asthagiri, Anne Co and Umit Ozkan, *The Ohio State University, USA*.

**Short Summary:**
A facile, ambient electrochemical bromine doping strategy results in enhancement of ORR activity over CNx but degradation for Pt/C. CNx-Br exhibits lower tafel slopes than pristine CNx for ORR indicating faster kinetics. Characterization experiments support the activity data. The results reveal bifunctionality of CNx for ORR and bromine evolution reaction.

5:05 PM **Tue-RTND-1705** The Unique Electrocatalytic Properties of Polynitrogen Materials.
**Xianqin Wang**, *New Jersey Institute of Technology, USA*.

**Short Summary:**
A series of polynitrogens (PNs) were synthesized and approved to be an excellent cathode catalyst for fuel cells and batteries. A unique dissociative reaction mechanism with easy OH group removal is a major contract to the associative reaction mechanism on Pt, which highlights the higher current density on PNs.

# Wednesday, June 21, 2023

## Ballroom A-E

### WEDNESDAY MORNING

**2023 Michel Boudart Award Lecture: Johannes Lercher**
Session Chairs: Gary L. Haller, *Yale University, USA* and Yong Wang, *Washington State University, USA*

8:05 AM Towards Understanding Catalysis at Water-Solid Interfaces.
**Johannes Lercher**, *Technical University of Munich, Germany; Pacific Northwest National Laboratory, USA*.

## 551 AB

### Design and Synthesis of MOFs & Zeolites

Session Chairs: Emiel Hensen, *Eindhoven University of Technology, Netherlands* and Nick Brunelli, *The Ohio State University, USA*.

9:30 AM **Wed-551AB-0930** Flow Synthesis of Metal-Organic Frameworks.
**Suyong Han**, Sujay Bagi and Yuriy Román-Leshkov, *Massachusetts Institute of Technology, USA*.

**Short Summary:**
Utilizing accelerated flow synthesis of MOFs, we studied the kinetics of MOF crystallization and screened both intrinsic and operation parameters in a high-throughput manner. Furthermore, the optimized conditions and understanding of crystallization were expanded to a scale-out approach and solvent recycling strategy, promoting the sustainable production of MOFs.

9:50 AM **Wed-551AB-0950** Chemical Upgrading Reactions Facilitated By Metal-Organic Framework-Based Catalysts.
**Saumil Chheda**[1], Dong Yang[2], Katherine McCullough[3], Daniel King[4], J. Ilja Siepmann[1], Massimiliano Delferro[3], Bruce Gates[5] and Laura Gagliardi[4], *(1)University of Minnesota, Twin Cities, USA, (2)Nanjing Tech University, China, (3)Argonne National Laboratory, USA, (4)University of Chicago, USA, (5)University of California, Davis, USA*.

**Short Summary:**
Metal-organic frameworks can exhibit catalytic activity through their nodes and linkers, or can support catalytically active single-atom metals or nanoparticles. Using density functional theory with experimental catalytic measurements, we elucidated the active sites and reaction mechanisms in such MOF-based catalysts – illustrated for methanol dehydration and propyne dimerization.

10:10 AM **Wed-551AB-1010** Defect Modification on Metal-Organic Framework UiO-66 Via Modulated Synthesis for Aldol Condensation Reaction.
**Ruixue Zhao**[1], Ricardo Bermejo de Val[1], Yue Liu[1] and Johannes Lercher[1,2], *(1)Technical University of Munich, Germany, (2)Pacific Northwest National Laboratory, USA*.

**Short Summary:**
Defective UiO-66s with different concentrations of defect sites were prepared via modulated synthesis using formic acid as a modulator. The coordinational unsaturated Zr on the defect sites provides Lewis acidity catalyzing aldol condensation reaction between furfural and acetone showing high turn-over frequency.

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10:30 AM **Wed-551AB-1030** Encapsulated Au Nanoclusters in Ti-MFI Zeotypes for Enhancing the Direct Epoxidation of Propylene.
**Weixin Li** and Viktor Cybulskis, *Syracuse University, USA*.

**Short Summary:**
Encapsulated Au nanoclusters in Ti-MFI zeolties with isolated tetrahedral $Ti^{4+}$ species exhibit improved PO rates when accounting for product inhibition compared to conventional Au/Ti-MFI catalysts prepared by DP.

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10:50 AM **Wed-551AB-1050** Area-Selective Atomic Layer Deposition on Zeolite-Supported Metal Nanoparticles for Confined Catalysis.
Peng Zhai[1], Laibao Zhang[1], Divakar Reddy Aireddy[1], David Cullen[2] and **Kunlun Ding**[1], *(1)Louisiana State University, USA, (2)Oak Ridge National Laboratory, USA*.

**Short Summary:**
We demonstrate an inverse design of metal-zeolite interfaces which bypasses the intrinsic issues associated with metal encapsulation in microporous materials, offering a solution for the fabrication of task-specific metal-zeolite interfaces for desired catalytic applications. Infrared spectroscopy and several probe reactions confirmed the spatial confinement effects at the inverse metal-zeolite interfaces.

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11:10 AM **Wed-551AB-1110** Well-Defined Zeolite-Metal Nanoparticle Catalyst Synthesis and Kinetic Evaluation for Low-Temperature Natural Gas Upgrading.
**Cole Hullfish** and Michele Sarazen, *Princeton University, USA*.

**Short Summary:**
Energy-intensive natural gas processing necessitates alternate routes for methane upgrading. A controlled synthetic method yielded stable, bifunctional zeolite-metal nanoparticle catalysts. Both monometallic and bimetallic catalysts containing small, well-dispersed nanoparticles, the latter of which are primarily alloyed, were evaluated in preliminary methane partial oxidation to liquid products.

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11:30 AM **Wed-551AB-1130** Single-Walled Zeolite Nanotubes.
Akshay Korde[1], Byunghyun Min[1], Elina Kapaca[2], Omar Knio[1], Iman Nezam[1], Ziyuan Wang[1], Johannes Leisen[1], Xinyang Yin[3], Xueyi Zhang[3], David S. Sholl[1], Xiaodong Zou[2], Tom Willhammar[2], Sankar Nair[1] and **Christopher W. Jones**[1], *(1)Georgia Institute of Technology, USA, (2)Stockholm University, Sweden, (3)Penn State University, USA*.

**Short Summary:**
The first synthesis and structural characterization of a quasi-1D hierarchical zeolite, specifically a single-walled nanotube that has a microporous zeolitic wall enclosing a central mesoporous channel, is described. Opportunities for the material in catalysis and separations will be discussed.

## WEDNESDAY AFTERNOON

### Confinement and Solvation Effects

Session Chairs: David Hibbitts, *University of Florida, USA* and Ambarish Kulkarni, *University of California - Davis, USA*.

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1:20 PM **Wed-551AB-1320** Condensed Phase Effects in Metal Catalysis Under Sub- and Supercritical Conditions.
**Dia Sahsah** and Andreas Heyden, *University of South Carolina, USA*.

**Short Summary:**
We present a QM/MM-FEP framework employing classical and machine learning interaction potentials to compute the solvation effects on surface processes over metal surfaces. We investigated the adsorption and reaction of a collection of prototypical lignin-derived molecules under sub- and supercritical processing environments.

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1:40 PM **Wed-551AB-1340** Leveraging Machine Learning Interatomic Potentials to Probe the Kinetic Consequences of Solvation in Acid Zeolites.
Mingze Zheng and **Brandon Bukowski**, *Johns Hopkins University, USA*.

**Short Summary:**
We trained machine learning interatomic potentials on Density Functional Theory (DFT) molecular dynamics simulations to interrogate the effects of Al density and distribution on water structuring in Brønsted acid zeolites. These inform local solvent models for calculating transition state energies of dehydration reactions in different framework topologies.

2:00 PM ***KEYNOTE*** **Wed-551AB-1400 Theoretical Insights into Low-Temperature $NH_3$-SCR over Copper-Exchanged Small-Pore Zeolites. Donghai Mei**, *Tiangong University, China; Tiangong University, China*.

**Short Summary:**
Cu-exchanged small-pore zeolite catalysts have been successfully used in the ammonia selective catalytic reduction ($NH_3$-SCR) for NO*x* abatement. In this contribution, using DFT calculations and AIMD simulations, the key role of secondary ions, i.e., Sm, in enhancing the catalytic $NH_3$-SCR activity of Cu-SSZ-13 have been elucidated on the atomic level.

2:40 PM **Wed-551AB-1440** Development and Implementation of a Non-Linear Cavity-Free Implicit Electrolyte Model in the Vienna Ab-Initio Simulation Package.
**S M Rezwanul Islam**, Foroogh Khezeli and Craig Plaisance, *Louisiana State University, USA*.

**Short Summary:**
We have developed and implemented a non-linear cavity-free implicit electrolyte model in VASP that is able to reproduce the "double hump" capacitance curve of metals while excluding solvent in spaces smaller than a water molecule.

3:00 PM **Wed-551AB-1500** Forcefield-Assisted Transition-State Sampling of Complex Reactions in Confinement.
Shubham Malviya and **Peng Bai**, *University of Massachusetts Amherst, USA*.

**Short Summary:**
This work presents a computational method to model confinement effects in nanoporous catalysts involving large, flexible reactants. The method allows for the estimation of transition-state entropy and for the systematic calculation of site-dependent activation energies, which can then be used to derive rigorous ensemble-averaged barriers for comparison with experiments.

## Understanding Solvation and Diffusion

Session Chairs: Alex Mironenko, *University of Illinois Urbana-Champaign, USA* and Susannah Scott, *University of California, Santa Barbara*.

3:45 PM **Wed-551AB-1545** Selective Reduction of O2 for the Synthesis of $H_2O_2$ Via $H_2$ and Hydroxyquinone Mediators.
**Mayank Tanwar**[1], Jason Adams[2], David Flaherty[2] and Matthew Neurock[1], *(1)University of Minnesota, Twin Cities, USA, (2)University of Illinois Urbana-Champaign, USA*.

**Short Summary:**
Selective pathways for $H_2O_2$ synthesis by O2 reduction with $H_2$ are developed using hydroxyquinone mediators in water as opposed to organic solvents currently used in the industrial anthraquinone auto-oxidation. These aqueous quinone-mediated paths avoid high deactivation and significantly lower the costs associated with organic solvents while allowing for high yields.

4:05 PM **Wed-551AB-1605** Solvent Structure and Dynamics over Brønsted Acid MWW Zeolite Nanosheets.
**Woodrow Wilson**[1], Justin Whittington[1,2] and Neeraj Rai[1,2], *(1)Mississippi State University, USA, (2)Center for Advanced Vehicular Systems, USA*.

**Short Summary:**
MWW zeolite nanosheets with varying Brønsted acidity are simulated in the presence of water and methanol. Solvent molecules interact differently with the acid site depending on the location of the site itself and the type of solvent, and a Grotthuss mechanism may or may not be the proton transport mechanism.

4:25 PM **Wed-551AB-1625** Solvent and Framework Polarity Effects on Aldol Addition Rates in Hf-BEA Zeolites.
**Alexander Khechfe**[1], Thaïs Matha[2] and Yuriy Roman[1], *(1)Massachusetts Institute of Technology, USA, (2)École Polytechnique Fédérale de Lausanne (EPFL), Switzerland*.

**Short Summary:**
Liquid-phase aldol addition rates of ethyl pyruvate over Hf-BEA zeolites were found to vary by up to 100x by varying pore and solvent polarity. Using kinetic modeling, we build a framework for how aldol addition proceeds in the liquid-phase in microporous catalysts that may be extended to other reaction systems.

4:45 PM **Wed-551AB-1645** Spatial Proximity for Adsorption Thermodynamics in Zeolite.
**Ajibola Lawal** and Omar Abdelrahman, *University of Massachusetts Amherst, USA*.

**Short Summary:**
This work looks to establish differences in adsorption energetics for transition state like molecules to interpret and understand trends for zeolite catalyzed reactions. We also detail the effect of proximate sites, by showing that one can rationalize the decreased stabilization through van der Waals interaction.

5:05 PM **Wed-551AB-1705** Descriptors of Free Energies of Solvation of $C_1$-$C_3$ Oxygenates in Hydrophobic Versus Hydrophilic Pores in FAU Zeolite.
**Xiuting Chen** and Rachel Getman, *Clemson University, USA*.

**Short Summary:**
we elucidate the descriptors that determine solvation thermodynamics of catalytic intermediates in zeolites with liquid water solvent using computational simulation. Models comprising hydrophobic and hydrophilic pores are used to learn the influence of pore hydrophilicity on the descriptors.

# 552 AB

## WEDNESDAY MORNING

### Hydrotreating and Hydrodeoxygenation of Bio-Oils

Session Chairs: Julia Valla, *University of Connecticut, USA* and Tibor Szilvasi, *The University of Alabama, USA*.

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9:30 AM **Wed-552AB-0930** Oxygen Coverage Effect on Phenolic Hydrodeoxygenation over Ru(0001) Surface.
**Haider Ejaz** and Fuat Celik, *Rutgers, The State University of New Jersey, USA*.

**Short Summary:**
Phenol hydrodeoxygenation is studied computationally while taking into account the effect of oxygen coverage. The presence of oxygen is shown to reduce phenol deoxygenation and is able to show better agreement with experimental product distribution.

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9:50 AM **Wed-552AB-0950** Deactivation-Free Continuous Production of Bio-Aviation Fuel from Biomass Pyrolysis Oil Using La-Ti-Ce-Ni Perovskite-Derived Catalysts.
**Jong Hyun Lee**[1,2], Lien Thi Do[3], Jina Eun[1,2], Jae-Wook Choi[1], Dong Jin Suh[1], Choi Jungkyu[2], Chun-Jae Yoo[1] and Jeong-Myeong Ha[2], *(1)Korea Institute of Science and Technology, Korea, Republic of (South), (2)Korea University, Korea, Republic of (South), (3)Phenikaa University, Viet Nam*.

**Short Summary:**
Hydrodeoxygenation of biomass pyrolysis oil was performed to obtain bio-aviation fuels. While the deactivation of catalysts is a major problem to suppress the continuous flow process, the continuous reaction without significant deactivation was achieved using the combination of Pd/C and La-Ti-Ce-Ni catalysts.

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10:10 AM **Wed-552AB-1010** Towards Green Fuels and Chemicals – Feedstock-Catalyst-Product Interactions during Catalytic Cracking of Pyrolysis Oils.
**Lucas Dorazio**[1], James Fu[1], Marco J. Castaldi[2], Snehesh Shivanandra[2] and Golam Chowdhury[2], *(1)BASF Corporation, USA, (2)City College of New York, CUNY, USA*.

**Short Summary:**
This work explores the interaction between pyrolysis oil chemistry, catalyst design, and the yield of products during catalytic cracking. Catalytic cracking of pyrolysis oils derived from various biogenic and polymer based wastes was explored using different commercial FCC catalysts.

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10:30 AM **Wed-552AB-1030** Co-Processing Biomass Pyrolysis Oils and Wet Waste Hydrothermal Liquefaction Crudes with Petroleum Streams in Refinery Hydroprocessing.
**Huamin Wang**, Daniel Santosa, Igor Kutnyakov and Matthew Flake, *Pacific Northwest National Laboratory, USA*.

**Short Summary:**
Co-processing biomass-derived feedstocks with petroleum in a traditional refinery leverage the well-established technologies and existing infrastructure, which will enable a fast adoption of biofuel production technologies. We will present our recent work on the coprocessing of woody fast pyrolysis bio-oil and wastewater sludge with different petroleum streams in hydroprocessing.

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10:50 AM **Wed-552AB-1050** Nb2O5 Polymorphs As Catalyst Supports for Fast-Pyrolysis Oil Upgrading through Hydrodeoxygenation.
**Mariana Myriam Campos Fraga**, Jonas Vogt, Caroline Carriel Schmitt, Klaus Raffelt and Nicolaus Dahmen, *KIT, Germany*.

**Short Summary:**
High oxygen and water contents of fast-pyrolysis oil can be mitigated by catalytic hydrodeoxygenation (HDO), broadening its application possibilities. In this comprehensive study, the performance of Nb2O5 polymorphs as catalyst supports of noble and non-noble metals was investigated. Correlations between remarkable performances and physicochemical properties of the polymorphs were established.

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11:10 AM **Wed-552AB-1110** Production of Sustainable Aviation Fuel from Lignocellulosic Biomass Via Catalytic Pyrolysis and Hydrotreating.
Kristiina Iisa[1], Calvin Mukarakate[1], Cody J. Wrasman[1], Susan Habas[1], Frederick G. Baddour[1], Brittney E. Petel[1], Kinga A. Unocic[2], Biva Talukdar[2], Harry Meyer III[2], Mark R. Nimlos[1], Matthew M. Yung[1], Abhijit Dutta[1] and **Mike Griffin**[1], *(1)National Renewable Energy Laboratory, USA, (2)Oak Ridge National Laboratory, USA*.

**Short Summary:**
Integrated catalytic fast pyrolysis and hydrotreating experiments reveal the potential to produce a high quality SAF product from woody biomass and waste feedstocks. Detailed characterization of CFP catalysts informs deactivation mechanisms and mitigation strategies for industrially relevant technical formulations.

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11:30 AM **Wed-552AB-1130** Continuous Upgrading of Hydrothermal Liquefaction Food Waste Oil on $Mo_2C$ Based Catalysts.
**Andres Granados**[1], Yuriy Roman[2] and Michael Timko[3], *(1)MIT, USA, (2)Massachusetts Institute of Technology, USA, (3)Worcester Polytechnic Institute, USA*.

**Short Summary:**
Selective deoxygenation of food waste oil using $Mo_2C$ produces renewable diesel hydrocarbons. This highlights the necessity for testing promising wet waste upgrading catalysts using realistic feedstocks.

## Design and Synthesis of Metal & Bimetallic Single-Atom Catalysts

Session Chairs: George Tsilomelekis, *Rutgers, The State University of New Jersey, USA* and Vitaly Alexandrov, *University of Nebraska-Lincoln, USA*.

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1:20 PM **Wed-552AB-1320** Support Effects on the Reactivity of Atomically Dispersed Pt Catalysts for Reverse Water Gas Shift Reaction.
**Haodong Wang**[1], Anatoly Frenkel[2] and Yuanyuan Li[3], *(1)Stony Brook University, USA, (2)University of Connecticut, USA, (3)Oak Ridge National Laboratory, USA*.

**Short Summary:**
Two systems consisting of $CeO_2$ decorated either on $TiO_2$ nano-oxides or on $CeO_2$ nano-oxides were prepared to support Pt “single atom”. Results indicated that Pt-$CeO_2$-$TiO_2$ sample exhibit higher activity for RWGS at low temperature (below 300°C) while deactivate at elevated temperature due to the aggregation of Pt atoms.

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1:40 PM **Wed-552AB-1340** Single Site Catalysis within Second Coordination Sphere: Single Metal Atom-Support Interaction Create “Ensemble Reaction Pool”.
**JI SU**[1] and Gabor A. Somorjai[1,2,3,4], *(1)Lawrence Berkeley National Laboratory, USA, (2)University of California Berkeley, USA, (3)University of California, Berkeley, USA, (4)University of California, Berkeley and Lawrence Berkeley National Laboratory, USA*.

**Short Summary:**
In this presentation, we will introduce our recent achievements on the catalysis and surface chemistry of single site catalyst which designed by combining the single metal atom and surrounding metal species and functional groups on supports to construct "ensemble reaction pool”.

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2:00 PM **Wed-552AB-1400** Fundamental Insights into Enhanced Olefin Metathesis with Bimetallic Single Site Catalysts.
**Anoop Uchagawkar**, Anand Ramanathan, Justin Douglas and Bala Subramaniam, *The University of Kansas, USA*.

**Short Summary:**
The selective enhancement of metathesis activity of Mo-based catalysts upon addition of a second metal such as Zr or Nb is significant. It introduces a relatively simple technique for creating more active catalytic sites and tuning catalyst activity, most likely by varying the O=M=O bond angle with the added metal.

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2:20 PM **Wed-552AB-1420** Effects of Nanoparticle Size on Structural Stability and Catalytic Behavior of Dilute Bimetallic and Single Atom Alloy Catalysts.
**Sucharita Vijayaraghavan**, Tomas Ricciardulli, Jason Adams and David Flaherty, *University of Illinois Urbana-Champaign, USA*.

**Short Summary:**
We demonstrate the effects of decreasing $Pd_1Au_x$-$SiO_2$ nanoparticle size on alloy structure, stability, and catalytic performance. Small $Pd_1Au_x$ nanoparticles (< 2 nm) form single atom alloy motifs at lower Au to Pd ratios, undergo- surface restructuring upon adsorption, and demonstrate higher $H_2O_2$ selectivities and formation rates than large $Pd_1Au_x$-$SiO_2$ nanoparticles.

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2:40 PM ***KEYNOTE* Wed-552AB-1440 From Deposited Metal Precursors to Supported Atoms or Nanoparticles.** Abolfazl Shakouri, Christopher Williams and **John Regalbuto**, *University of South Carolina, USA*.

**Short Summary:**
We are working to achieve an understanding of the mechanism through which metal precursors deposited at carbon and oxide support surfaces evolve into nanoparticles, cluster and atoms. We have preliminary evidence of the ability to control the formation of the deposited metals into these forms.

## Lignin and Bio-Oil Conversion II

Session Chairs: Susan Habas, *National Renewable Energy Laboratory, USA* and Nelson Cardona-Martínez, *University of Puerto Rico at Mayagüez, USA*.

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3:45 PM **Wed-552AB-1545** Towards the Development of a Kinetic Model for Selective Hydrodeoxygenation of Lignin Derivatives to Petrochemical Intermediates Using $MoO_3$.
**Andrew J. Kohler**[1,2], Charles H. Walter[1,2] and Brent H. Shanks[2], *(1)Iowa State University, USA, (2)Center for Biorenewable Chemicals (CBiRC), USA*.

**Short Summary:**
We utilize a combination of kinetic and isotopic experiments to infer an HDO mechanism for various oxygenated aliphatics over $MoO_3$. This revealed that carbonyl bond cleavage is kinetically limited by being entirely hydrogenated to an alcohol, which is then facilely dehydrated.

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4:05 PM **Wed-552AB-1605** Catalytic Fast Pyrolysis on Zeolites : Activity and Stability of Different Structures and Acidic Catalysts for Anisole Transformation.
**Nathan Pichot**[1,2,3], Ludovic Pinard[2], Anthony Dufour[1] and Yannick Pouilloux[4], *(1)Université de Lorraine, France, (2)ENSICaen, France, (3)Université de Poitiers, France, (4)IC2MP-Université de Poitiers, France*.

**Short Summary:**
Anisole transformation is used as a model reaction for catalytic fast pyrolysis of biomass (for its methoxy group). The impact of the zeolite structure on TOF, deactivation and conversion is studied, as well as the importance of Si/Al ratio.

4:25 PM **Wed-552AB-1625** Enhanced Lignin Upgrading to Aromatic and Olefinic Hydrocarbons By Streamlining Reductive Catalytic Fractionation and Hydrodeoxygenation.
Daniel Vincent Sahayaraj, Lusi A, Andrew J. Kohler, Hamed Bateni, Harish Radhakrishnan, Alireza Saraeian, Brent H. Shanks, Xianglan Bai and **Jean-Philippe Tessonnier**, *Iowa State University, USA*.

**Short Summary:**
Char formation during lignin pyrolysis sequesters >50% of the carbon atoms, allowing only a portion of the lignin to be upgraded. This work addresses this challenge and unveils a strategy combining RCF and HDO that drastically reduces char formation and enhances the production of aromatic and olefinic platform hydrocarbons.

4:45 PM **Wed-552AB-1645** Understanding Facet Dependent Selectivity Trends in Catalytic Hydrogenation and Hydrodeoxygenation of Lignin-Derived Aromatic Compounds..
**Haseena K V**[1], M. Ali Haider[1], Govind Porwal[2] and Vinod C. Prabhakaran[2], *(1)Indian Institute of Technology Delhi, India, (2)CSIR-NCL Pune, India*.

**Short Summary:**
Hydrogenation reactions of cinnamaldehyde and guaiacol over synthesized spheres, octahedra Pd (111) and cubes Pd (100) are explored. Density functional theory (DFT) simulations suggests that the carbonyl hydrogenation to form alcohol product is primarily decided by the Pd(100) sites and the aldehyde product formation is catalyzed by the Pd(111) sites.

5:05 PM **Wed-552AB-1705** Mechanocatalytic Hydrogenolysis of the Lignin Model Compound Benzyl-Phenyl Ether over Supported Pd Catalysts.
**Erin Phillips**, Marta Hatzell and Carsten Sievers, *Georgia Institute of Technology, USA*.

**Short Summary:**
This study explores the hydrogenolysis of the lignin model dimer benzyl phenyl ether (BPE) using a mechanocatalytic approach. Heterogenous palladium catalysts supported on silica, alumina and carbon were chosen to facilitate this homolytic cleavage, with an emphasis on support effect on production, reaction rate and catalyst recyclability.

## 555 AB

### WEDNESDAY MORNING

### Carbon Dioxide Conversion to Methanol II

Session Chairs: Qiaowan Chang, *Columbia University, USA* and Vasile Parvulescu, *University of Bucharest, Romania*.

9:30 AM **Wed-555AB-0930** Rates, Reversibility, and Site Densities for $CO_2$ Hydrogenation on Cu-Based Catalysts.
**Ting Lin** and Aditya Bhan, *University of Minnesota, Twin Cities, USA*.

**Short Summary:**
$H_2$ reaction order indicates a dearth of H* species during catalysis. *In situ* titration and cofeed experiments show the invariance of site density with $H_2$ pressure, where methanol synthesis and RWGS share a common active site. Herein, reversibility and kinetic analyses are presented to elucidate the mechanism of $CO_2$ hydrogenation.

9:50 AM **Wed-555AB-0950** Enhancing the Activity of Cu Nanoparticles for $CO_2$ Hydrogenation to Methanol through Tuning the Anion Sites in a Perovskite Support.
Yang He[1], Yuanyuan Li[2] and **Zili Wu**[2], *(1)Oak Ridge National laboratory, USA, (2)Oak Ridge National Laboratory, USA*.

**Short Summary:**
We show how the anion tuning of a perovskite support ($BaTiO_3$), lattice hydride (H-) vs. oxide ($O^{2-}$), can significantly improve the catalytic activity of Cu nanoparticles in $CO_2$ hydrogenation to methanol. The lattice hydrides participate in the reaction through a pathway similar to the Mars van Krevelen mechanism.

10:10 AM **Wed-555AB-1010** Imaging the Evolution of an Inverse $CeO_2$/Cu Catalyst Under $CO_2$ Hydrogenation Conditions.
Jorge Moncada[1], Xiabo Chen[2], Kaixi Deng[1], Yuxi Wang[3], Nebojsa Marinkovic[1], Arturo Martinez-Arias[4] and **Jose Rodriguez**[1], *(1)Brookhaven National Laboratory, USA, (2)SUNY Binghamton, USA, (3)SUNY Stony Brook, USA, (4)Consejo Superior de Investigaciones Científicas, Spain*.

**Short Summary:**
The behavior of highly active inverse oxide/metal catalysts ($CeO_x$/Cu) for $CO_2$ hydrogenation was investigated using environmental transmission electron microscopy (E-TEM) and a combination of *in-situ* techniques (time-resolved XRD, XAFS and AP-XPS). Big changes in the morphology of the catalysts were observed depending on the reaction conditions.

10:30 AM **Wed-555AB-1030** Tailoring the Formate Binding Strength of Cu/$ZrO_x$ Clusters on MgO By Liquid-Phase ALD for Increased Methanol Selectivity in $CO_2$ Hydrogenation.
**Seongmin Jin**, Bartu Karakurt, Yu-Cheng Lin and Jeremy Luterbacher, *École Polytechnique Fédérale de Lausanne (EPFL), Switzerland*.

**Short Summary:**
Here, we designed a unique molecular cluster catalyst (Cu/$MgOZrO_2$) with a uniform interface via the liquid-phase atomic layer deposition (ALD). Cu/$ZrO_x$ cluster grown on the corner site of MgO exhibited moderate binding strength of monodentate formate, which is an essential reaction intermediate for methanol production, leading to highly enhanced activity.

10:50 AM **Wed-555AB-1050** Engineering Nanoscale H Supply Chain to Accelerate Methanol Synthesis on ZnZrOx.
**Ning Yan**, *National University of Singapore, Singapore*.

**Short Summary:**
We introduce a Pd/CNT-$ZnZrO_x$ methanol synthesis catalyst, in which CNT delivers hydrogen activated on Pd to a broad area on $ZnZrO_x$ surface, with an enhancement factor of 10 compared to the conventional Pd-promoted $ZnZrO_x$ catalyst, which only transfers hydrogen to Pd-adjacent sites.

11:10 AM **Wed-555AB-1110** NAP-XPS Studies of $CO_2$ Hydrogenation on Cu/$ZrO_2$/ZnO Model Catalysts.
**Luolin Shi**1, Jason Wang1 and Michael White[1,2], *(1)Stony Brook University, USA, (2)Brookhaven National Laboratory, USA*.

**Short Summary:**
This study confirms that the addition of $Cu_4$ and $ZrO_2$ clusters improves the reactivity of ZnO(0001) using NAP-XPS. The results also show that $CO_2$ hydrogenation leads primarily to formate for all Cu/$ZrO_2$/ZnO model catalysts studied, and temperature dependence is consistent with a formate pathway to form methoxy.

11:30 AM **Wed-555AB-1130** Aluminum in Cu-ZnO Catalysts: Would It be a Key Component for the Synthesis of Methanol from $CO_2$ and $H_2$?
Bruna J.S. Bronsato[1,2], **Guilherme G. Gonzalez**[2], Priscila C. Zonetti[2], Luciano H. Chagas[2], Roberto R. de Avillez[1] and Lucia Gorenstin Appel[2], *(1)Pontifícia Universidade Católica do Rio de Janeiro, Brazil, (2)Instituto Nacional de Tecnologia, Brazil*.

**Short Summary:**
The main role of Al in the CuZnAl catalyst is the generation of oxygen vacancies, which are defects that promote the methanol synthesis from $CO_2$ and $H_2$.

## WEDNESDAY AFTERNOON

### Thermocatalytic Conversion of $CO_2$ II

Session Chairs: Wes Thompson, *Evonik,* and Andreas Jentys, *Technical University of Munich, Germany*.

1:20 PM **Wed-555AB-1320** Effect of Isomorphous Substitution in ZSM-5 in Tandem with ZnO-$ZrO_2$ for Direct Conversion of $CO_2$ to Aromatics.
**Dhrumil Shah**, Iman Nezam and Christopher Jones, *Georgia Institute of Technology, USA*.

**Short Summary:**
H-[Al/Ga/Fe]-ZSM-5 samples with Si/T ratios = 80, 300 were synthesized and mixed with ZnO-$ZrO_2$ to test for the effect of isomorphous substitution of $CO_2$ hydrogenation. The catalytic results coupled with the acid characteristics suggest that weaker acid site strength improves aromatics selectivity.

1:40 PM **Wed-555AB-1340** Transformation of Various Amine Carbamates into Organic Urea Derivatives over $CeO_2$ Catalyst.
**Mizuho Yabushita**[1], Jie Peng[1], Yingai Li[1], Ryotaro Fujii[1,2], Masazumi Tamura[3], Yoshinao Nakagawa[1] and Keiichi Tomishige[1,4], *(1)Tohoku University, Japan, (2)Tosoh Corporation, Japan, (3)Osaka Metropolitan University, Japan, (4)Tohoku University, Graduate School of Engineering, Japan, Japan*.

**Short Summary:**
Amine carbamates, which are synthesized via chemical absorption of $CO_2$ into amines, were transformed into urea derivatives over $CeO_2$ catalyst in corresponding amine solvents. This systems offer a higher turnover frequency compared to previously reported catalytic systems due to the suppression of thermal decomposition of substrates.

2:00 PM **Wed-555AB-1400** Effect of Doping Agents on the Catalytic Activity of $in_2O_3$ for the Conversion of $CO_2$ to Hydrocarbons.
Camila P. Ferraz, Marlon Tavares, Luís F. Bordini, João M.A.R. de Almeida, Eduardo Falabella Sousa-Aguiar and **Pedro N. Romano**, *Universidade Federal do Rio de Janeiro, Brazil*.

**Short Summary:**
The presented work helps to elucidate the effects of promoting $in_2O_3$-based catalysts with 1 wt.% Ga, Nb, La and Mg on $CO_2$ hydrogenation. By suppressing this reaction's inherent low conversion and concurrent RWGS problem, it is possible to advance in the low carbon footprint fuel industry.

2:20 PM **Wed-555AB-1420** Synthesis and Characterization of Multifunctional Fe-Based Catalysts for Efficient Hydrogenation of $CO_2$ to Hydrocarbons.
**Elena Corrao**[1], Fabio Salomone[1], Emanuele Giglio[2], Micaela Castellino[1], Silvia Maria Ronchetti[1], Raffaele Pirone[1] and Samir Bensaid[1], *(1)Politecnico di Torino, Italy, (2)University of Calabria, Italy*.

**Short Summary:**
The aim of this work is the synthesis of innovative structures made of a Fe-based active phase as core and a zeolite as shell, in order to produce liquid hydrocarbons via a sustainable pathway involving carbon dioxide hydrogenation as an alternative to the conventional fossil-based route.

2:40 PM **Wed-555AB-1440** Syngas Production from $CO_2$ and Water over Highly Active, Stable and Selective Cubic Molybdenum Carbide Catalyst.
**Milad Ahmadi Khoshooei**, *University of Calgary, Canada*.

**Short Summary:**
Cubic molybdenum carbide nanocatalyst shows great activity and stability in production of hydrogen from water at 623 K. Raman and XRD shows minor oxidation to $MoO_2$. The catalyst also shows outstanding activity, 100% CO selectivity, and long stability that offers a tandem system to produce syngas from water and $CO_2$.

3:00 PM **Wed-555AB-1500** Co-Mn Interactions in Co1-XMnxo Nanoparticles during the $CO_2$ Hydrogenation Reaction.
**Anh To**[1], Nicole LiBretto[1], Kinga A. Unocic[2], A. Jeremy Kropf[3], Susan Habas[1] and Dan Ruddy[1], *(1)National Renewable Energy Laboratory, USA, (2)Oak Ridge National Laboratory, USA, (3)Argonne National Laboratory, USA*.

**Short Summary:**
Well-defined Co-Mn oxide systems were synthesized and insights to the interaction between Mn and Co atoms at different pretreatment temperatures were investigated and correlated to their activity in the $CO_2$ hydrogenation reaction.

## Thermocatalytic Conversion of $CO_2$ III

Session Chairs: James J. Spivey, *Louisiana State University, USA* and Yizhi Xiang, *Mississippi State University, USA*.

3:45 PM **Wed-555AB-1545** $CO_2$ Hydrogenation to Methanol over Cu.ZnO-Promoted Catalysts. Effect of Aging Conditions on the Activity and Selectivity.
**Claudio José de Araújo Mota**, *Universidade Federal do Rio de Janeiro, Brazil; Universidade Federal do Rio de Janeiro, Brazil; Federal University of Rio de Janeiro, Brazil*.

**Short Summary:**
Promoted Cu.ZnO catalysts were prepared for $CO_2$ hydrogenation to methanol. The catalytic performance was dependent on the aging conditions applied to the formulations in order to observe Malachite phases. The results point out for the importance of the proper aging conditions when metal oxide promotors are included in the formulation.

4:05 PM **Wed-555AB-1605** Conversion of $CO_2$ to Cyclic and Poly- Carbonates over Constrained Di-Nuclear Catalysts.
Sreenath Pappuru[1], Dina Shpasser[2], Pini Shechter[3], Raanan Carmeli[4], Friederike C. Jentoft[5] and **Oz Gazit**[2], *(1)Technion- Israel institute of Technology, Israel, (2)Israel Institute of Technology -Technion, Israel, (3)Tel Aviv University, Israel, (4)Weizmann institute, Israel, (5)University of Massachusetts Amherst, USA*.

**Short Summary:**
We show, for the first time, a grafted reduced di-iron Robson-type catalyst can effectively promote the $CO_2$ condensation with epoxides at 1atm to cyclic carbonates. We further report a new grafted catalyst that allows the post-grafting incorporation of the metal and demonstrate the production of polycarbonates even under an $O_2$.

4:25 PM **Wed-555AB-1625** Direct Syngas to Olefins Using Zinc Oxide Based Catalysts and SAPO-34.
Michael Nikolajsen[1], **Martin Høj**[1], Jakob M. Christensen[1], Niels Christian Schjødt[2], Jens Sehested[3] and Uffe V. Mentzel[2], *(1)Technical University of Denmark, Denmark, (2)Haldor Topsøe A/S, Denmark, (3)Haldor Topsoe A/S, Denmark*.

**Short Summary:**
Here we report a comprehensive comparison between $ZnAl_2O_4$, $ZnGa_2O_4$ and $ZnO$-$ZrO_2$ catalysts for methanol synthesis and for syngas to olefines when combined with SAPO-34. This includes fundamental characterization using BET, ICP and XRD and in-depth characterization using operando XAS and DRIFTS.

4:45 PM **Wed-555AB-1645** Direct $CO_2$ Hydrogenation to Light Olefins over Bifunctional Doped in2O3 and SAPO-34 Catalysts.
**Fabio Salomone**[1], Alberto Biasin[2], Pierdomenico Biasi[2] and Samir Bensaid[1], *(1)Polytechnic of Turin, Italy, (2)CASALE SA, Switzerland*.

**Short Summary:**
Light olefins are currently produced from non-renewable fossil resources. However, green olefins could be directly produced from captured $CO_2$ and renewable-based $H_2$ on a bifunctional catalyst, enhancing the $CO_2$ conversion and the productivity of light olefins with engineered structure of the catalytic particles.

5:05 PM **Wed-555AB-1705** Tandem Electrocatalytic-Thermocatalytic Processes for Sustainable $CO_2$ Valorization.
**Samay Garg**[1], Akash Biswas[1], Zhenhua Xie[2] and Jingguang Chen[1,2], *(1)Columbia University, USA, (2)Brookhaven National Laboratory, USA*.

**Short Summary:**
This work demonstrates a two-stage tandem electrocatalytic-thermocatalytic reaction scheme for $CO_2$ conversion to $C_3$oxygenates (1-propanol and propanal) wherein electrochemical $CO_2$ reduction using an oxide-derived Cu/C catalyst is followed by $Rh_1Co_3$/MCM-41-catalyzed thermochemical hydroformylation. The tandem process achieves a $C_3$ oxygenate selectivity of 18.6% at a 160 °C hydroformylation temperature.

# 556 AB

### WEDNESDAY MORNING

## Alkene Oligomerization and C-C Bond Formation

Session Chairs: Enrique Iglesia, *University of California, USA* and Sarah Specht, *Braskem America, USA*.

9:30 AM **Wed-556AB-0930** Influences of Zeolite Topology on Reaction and Diffusion Phenomena That Govern Brønsted Acid-Catalyzed Propene Oligomerization.
**Elizabeth Bickel** and Raj Gounder, *Purdue University, USA*.

**Short Summary:**
Zeolite topology influences kinetic rates and the composition of occluded hydrocarbon products that regulate intrazeolite diffusion during propene oligomerization catalysis, and thereby rates and selectivity. These insights into reaction-diffusion phenomenon during alkene oligomerization catalysis are revealed by interrogating different zeolite topologies synthesized with independently varied Al density and crystallite size.

9:50 AM **Wed-556AB-0950** Density Functional Theory and Microkinetic Interrogation of Ethylene Oligomerization By Transition Metal Ions Supported on Silica.
**Neha Mehra** and William Schneider, *University of Notre Dame, USA*.

**Short Summary:**
Mechanistic and kinetic investigations of silica supported metal ions (M) for ethylene coupling and sensitivity of rates and product distribution to the nature of metal ion, site environment and reaction conditions. The approach presented can guide catalyst design for optimal performance.

10:10 AM **Wed-556AB-1010** Ethylene Dimerization to *n*-Butene with Nickel Sulfate on Zirconia: Investigation of the Molecular Structure and Activity of Surface Nickel and Sulfate Species.
**Erin Sobchinsky**, Shiao-Chien Tsai and Israel Wachs, *Lehigh University, USA*.

**Short Summary:**
This work examines nickel sulfated zirconia as a heterogenous ethylene dimerization catalyst. Multiple *in-situ* characterization techniques have been utilized to investigation the molecular structure and the nature of the nickel-sulfate interactions that contribute to enhanced ethylene dimerization activity.

10:30 AM **Wed-556AB-1030** Propene Metathesis on MoO$_x$/MCM-41: Kinetics, Mechanism, and Catalytic Consequences of Chemical and Thermal Treatments.
**Jorge Quesada** and Enrique Iglesia, *University of California, Berkeley, USA*.

**Short Summary:**
This study proposes a plausible explanation for the metathesis rates increase at near-ambient temperatures upon treatments of Mo-based catalysts at elevated temperatures through dehydroxylation to form open Mo-centers responsible for the evolution of active sites. Metathesis elementary steps involved kinetically-relevant steps that occur on Mo-carbenes nearly-saturated with strongly-bound alkene-derived intermediates.

10:50 AM **Wed-556AB-1050** The Role of Carbonaceous Deposits during Butene Isomerization.
**Pawel Chmielniak**, Karoline Lena Hebisch, Risha Goel and Carsten Sievers, *Georgia Institute of Technology, USA*.

**Short Summary:**
The reaction mechanism of 1-butene isomerization is contested. While carbonaceous deposits likely contribute to reactivity, literature evidence for the active species and reaction location is scarce. A combination of probe molecules, spectroscopic analysis and kinetic data provides insights into the isomerization mechanism, laying the foundation for prolonging catalyst lifetime.

11:10 AM **Wed-556AB-1110** Preferential Removal of Ga in Ga Incorporated MFI Catalysts By HCl Treatment, and Its Application in Propane Aromatization.
**Yong Hyun Lim**, Hyungjoo Kim, Kihun Nam, Haewon Ryu and Do Heui Kim, *Seoul National University, Korea, Republic of (South)*.

**Short Summary:**
Facile HCl treatment of various Ga-zeolites preferentially removed the Ga species sharing weaker interaction with the zeolite, allowing for qualitative determination of the major Ga species. Through such tailoring of Ga species by HCl, the propane aromatization abilities of each Ga species in various Ga-zeolites were evaluated.

11:30 AM **Wed-556AB-1130** High-Yield Carbon Nanotube Synthesis on Lamellar Supports.
**Caleb Q. Bavlnka**, Tianhao E. Zhang, Brian Grady and Steven Crossley, *University of Oklahoma, USA*.

**Short Summary:**
High-yield carbon nanotubes were grown on lamellar supports exfoliated with various species. Monitoring hydrogen evolution during CNT synthesis provided insight into the impact of water on deactivation rates and the kinetics of nanotube growth on both lamellar supports and silicon wafers.

## WEDNESDAY AFTERNOON

### New Concepts in Electrocatalysis II

Session Chairs: Bin Wang, *University of Oklahoma, USA* and Tej Choksi, *Nanyang Technological University, Singapore*.

1:20 PM **Wed-556AB-1320** pH-Dependent Spontaneous Polarization of Metal Nanoparticles on Nonconductive Surfaces.
Thejas Wesley[1], Max Hulsey[1], **Karl Westendorff**[1], Noah Lewis[1], Ethan J. Crumlin[2], Yuriy Roman[1] and Yogesh Surendranath[1], *(1)Massachusetts Institute of Technology, USA, (2)Lawrence Berkeley National Laboratory, USA*.

**Short Summary:**
Conventional wired methods cannot measure the potential of electronically-remote catalytic sites, yet it has significant implications for heterogeneous catalysis. We employ IR and AP-XPS spectroscopies to qualitatively and quantitatively measure catalytic site potentials as a function of solution pH. Our results demonstrate that solution compositions predictably set catalytic sites' potential.

1:40 PM **Wed-556AB-1340** Electrochemical Stability and Activity of Thiolate Self-Assembled Monolayer Modified Metals.
**Nathanael Ramos**[1,2], J. Will Medlin[1] and Adam Holewinski[1,3], *(1)University of Colorado Boulder, USA, (2)Renewable and Sustainable Energy Institute, USA, (3)Renewable and Sustainable Energy Insitute, USA*.

**Short Summary:**
The stable electrochemical potential windows of different thiolate self-assembled monolayers on Au, Pt, and Cu were identified. Based on these results, low potential furfural oxidation on Cu was identified as a possible catalytic application. CuNi alloys were also shown to have an earlier peak potential for furfural oxidation than Cu.

2:00 PM **Wed-556AB-1400** Probing Solid-Solid Interfacial Catalysis for Efficient Development of Energy Storage Systems.
**Kunal Velinkar**[1], Alex Von Gunten[2], Jeffrey Greeley[2] and Eranda Nikolla[1], *(1)University of Michigan, USA, (2)Purdue University, USA*.

**Short Summary:**
Our studies emphasize the development of a framework for studying solid-solid interfacial catalysis at the electrode of energy storage systems that would aid in improving their performance by leading to the identification of effective electrocatalysts by desired product formation.

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2:20 PM **Wed-556AB-1420** A Versatile, Stable, $Li_xFePO_4$ Reference Electrode for Non-Aqueous Electrochemistry.
**Peter Benedek**, Eric McShane, Valerie Niemann, Adam Nielander, Matteo Cargnello and Thomas F. Jaramillo, *Stanford University, USA*.

**Short Summary:**
Disentangling counter electrode from working electrode and electrolyte effects, the reference electrode plays a crucial in electrocatalysis. While numerous reference electrodes exist for aqueous electrocatalysis, the harsh environment in non-aqueous electrochemistry poses challenges. Here, we present a versatile $Li_{0.5}FePO_4$ reference electrode and show its stability in Li-mediated $N_2$ reduction.

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2:40 PM **Wed-556AB-1440** Mechanistic Origin of Selective and Active Electrochemical Ozone Evolution Reaction over Ni-Sb-$SnO_2$ Electrode.
**Seokhyun Choung**, Seok Kim, Hayoung Jeong, Yoojin Lee, Kangwoo Cho and Jeong Woo Han, *Pohang University of Science and Technology (POSTECH), Korea, Republic of (South)*.

**Short Summary:**
The ozone evolution reaction (OZER) mechanism and active site configurations are revealed for Ni-Sb-$SnO_2$ as a model system, through density functional theory (DFT) calculations corroborated by ex-situ and in-situ X-ray absorption spectroscopy (XAS) and electrochemical measurements, which is believed to provide mechanistic insights to design efficient Sn-based OZER catalysts.

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3:00 PM **Wed-556AB-1500** Mechanistic Studies of Water Oxidation to Ozone on Rutile SnO2 (110) with Computational Chemistry and Experiments.
**Lingyan Zhao**[1], Rayan Alaufey[2], Maureen Tang[2] and John Keith[1], *(1)University of Pittsburgh, USA, (2)Drexel University, USA*.

**Short Summary:**
We will present a thorough assessment of complex electrochemical ozone pathways on doped tin oxide using Kohn-Sham density functional theory. This work highlights the critical role of hydrogenated species on the surface that stabilize these structures and reflect on our prior work of solvated reaction intermediates.

## Synthesis of Clusters and Supported Complexes

Session Chairs: Justin Notestein, *Northwestern University, USA* and Yuanyuan Li, *Oak Ridge National Laboratory, USA*.

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3:45 PM **Wed-556AB-1545** Design of Supported Scandium Complexes and Fundamental Investigation of Catalyst Structure.
**Yuting Li**[1], Long Qi[2], Aaron Sadow[3], Frederic Perras[4] and Scott Southern[1], *(1)Ames Laboratory, USA, (2)University of California, Santa Barbara, USA, (3)Ames Laboratory and Iowa State University, USA, (4)Iowa State University, USA*.

**Short Summary:**
A new type of heterogeneous catalyst with Brønsted acid sites (in supports) grafting rare earth borohydride complexes was designed and studied, presenting decent catalytic performance of CH borylation. It is promising to develop catalysts for efficient activation or functionalization of hydrocarbons by optimizing supported rare-earth element catalysts.

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4:05 PM **Wed-556AB-1605** Rh Clusters Dispersion at Low Temperature and the Consequences for CO Oxidation Kinetics.
Malik Albrahim[1], **Ayman M. Karim**[1], Abhijit Shrotri[2], Raymond R. UnociC$_3$, Adam Hoffman[4] and Simon Bare[4], *(1)Virginia Polytechnic Institute and State University, USA, (2)Hokkaido University, Japan, (3)Oak Ridge National Laboratory, USA, (4)SLAC National Accelerator Laboratory, USA*.

**Short Summary:**
This work shows the importance of following the dynamics of supported metal nanoparticles and the effect on interpretation of the reaction kinetics and correctly building structure-activity relations. The Rh single atoms resulting from clusters dispersion exhibit much higher activity at room temperature.

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4:25 PM **Wed-556AB-1625** Effects of Domain Size and Support Composition on the Reactivity and Reducibility of Oxide-Supported Tungsten Oxide Clusters.
**Anukriti Shrestha**, Konstantin Mamedov, Robert Davis and Chris Paolucci, *University of Virginia, USA*.

**Short Summary:**
We explore the speciation of Pd-promoted, oxide supported WO*x* tandem catalysts. Combined modeling and experimental analyses determined that at <600 K Brønsted acid sites form on titania supported tungsten oxide clusters without significantly affecting their oxidation state. These acid sites may catalyze steps in the reduction of carboxylic acids.

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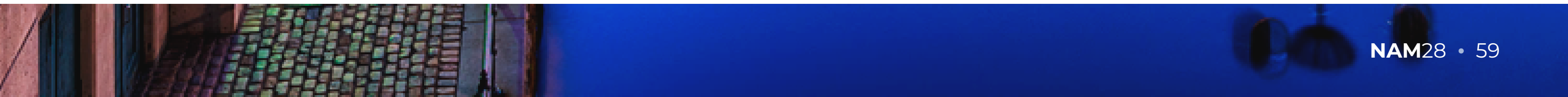
4:45 PM **Wed-556AB-1645** Highly Accessible and Electronically Tunable Sites on Ligand-Protected Gold Nanoparticles for Oxidation and Reduction Catalysis.
**Sayed Abu Sufyan**, Brian van Devener, Paulo Perez and Michael Nigra, *University of Utah, USA*.

**Short Summary:**
In this work, highly accessible and reactive Au nanoparticles are synthesized using similarly structured bulky phosphine and thiol ligands. Results show the significant impact of the electronic state of the Au surface on reduction catalysis, while showing a less significant effect for oxidation reactions catalyzed by the same Au nanoparticles.



5:05 PM **Wed-556AB-1705** Modification of Single Atom Catalysts with Amine-Functionalized Organic Monolayers to Promote $CO_2$ Hydrogenation.
**Alexander Jenkins**, Charles Musgrave and Will Medlin, *University of Colorado, USA*.

**Short Summary:**
Monolayers of alkyl and amine-functionalized organophosphonic acids were deposited onto $Rh_1/TiO_2$ single-atom catalysts. It was found that the amine groups in close proximity to Rh1 single-atom sites improved per-site turnover frequencies for $CO_2$ hydrogenation. In addition, these organic monolayers reduced the degree of metal sintering at reaction conditions.

## Ballroom A

### WEDNESDAY MORNING

### Polyolefins and Polymer Waste Conversion

Session Chairs: Joe Bergmeister, *Research Chemist at Chevron Phillips Chemical Company, USA* and Jesse Bond, *Syracuse University, USA*.

9:30 AM **Wed-BLRMA-0930** Pyrolysis Oil Catalytic Upgrading of Plastics and Biomass.
Snehesh Shivanandra[1], Golam Chowdhury[1], **Marco J. Castaldi**[1,2], Lucas Dorazio[3] and James Fu[3], *(1)City College of New York, CUNY, USA, (2)City University of New York, City College, USA, (3)BASF Corporation, USA*.

**Short Summary:**
This presentation will discuss the details of using FCC catalysts to upgrade pyrolysis oils from waste plastics, MSW and biomass to olefins. Main findings demonstrate that nearly 50% of the hydrocarbons in the pyoils can be converted to precursors to make products, therefore ensuring that carbon remains in the economy.

9:50 AM **Wed-BLRMA-0950** Hydroformylation of Plastic Pyrolysis Oils: A New Route to Create Chemicals from Plastic Wastes.
**Houqian Li**[1], Jiayang Wu[1], Zhen Jiang[1], Manos Mavrikakis[1], Clark Landis[2] and George Huber[1], *(1)University of Wisconsin Madison, USA, (2)UW-Madison, USA*.

**Short Summary:**
Pyrolysis of waste plastics produces pyrolysis oils with high concentrations of olefins. We demonstrated the olefins in the pyrolysis oil can undergo hydroformylation to create aldehydes followed by reduction into mono-/di-alcohols using thermal depolymerization, homogeneous catalysis, and heterogeneous catalysis. This route produces high-value oxygenates from low-value post-consumer recycled polyethylene.

10:10 AM ***KEYNOTE* Wed-BLRMA-1010 Catalytic Polyolefin Depolymerization to Value-Added Products.**
**Susannah Scott**, *UC Santa Barbara, USA*.

**Short Summary:**
The conversion of polyolefins using a variety of catalytic approaches leads to desirable small-molecule products. The talk will describe our efforts to accelerate the reaction and target specific classes of products, using tandem strategies and bifunctional catalysts to achieve selective depolymerization.

10:50 AM **Wed-BLRMA-1050** Water Enhances the Activity of Chloroaluminate Ionic Liquid for Tandem Polyethylene Conversion.
**Jiande Mai**[1], Wei Zhang[2], Oliver Y. Gutierrez[1] and Johannes A. Lercher[1], *(1)Pacific Northwest National Laboratory, USA, (2)Technical University of Munich, Germany*.

**Short Summary:**
We study the promoting effect of water on polyethylene conversion in a tandem cracking-alkylation process, enabled by acidic chloroaluminate ionic liquids. Our work shows that the effect is due to synergies between Brønsted and Lewis acid sites, which provide an effective way to enhance and control reaction performance.

11:10 AM **Wed-BLRMA-1110** C–H Functionalization in Light Alkanes and Polyolefins Using Ozone at Ambient Temperature.
**Hongda Zhu**, Timothy Jackson and Bala Subramaniam, *The University of Kansas, USA*.

**Short Summary:**
A facile method to safely activate C–H bonds in light alkanes and plastics with ozone, minimizing C1 formation, is demonstrated. This novel process has potential applications to other substrates, such as long chain alkanes and those of interest in pharmaceuticals and specialty chemicals.

11:30 AM **Wed-BLRMA-1130** Computational Solvent Screening for Extraction of Additives in Polymer Upcycling.
**Pooja Bhalode**, Sean Najmi, Pavel Kots, Christine Oberhausen, Zachary R. Hinton, Montgomery Baker-Fales and Dionysios Vlachos, *University of Delaware, USA*.

**Short Summary:**
To upcycle end-of-use commodity polymers, it is important to separate the additives. This work presents a computationally devised framework for high-throughput screening of green solvents to isolate additives for polymer upcycling. This framework is applied to multi-layer plastics and waste rubber tires and the extracted additives converted to valuable chemicals.

# WEDNESDAY AFTERNOON

## Alkane Dehydrogenation I (Oxidative)

Session Chairs: Linda Broadbelt, *Northwestern University, USA* and Stuart Soled, *ExxonMobil Research and Engineering, USA*.

1:20 PM **Wed-BLRMA-1320** Chemical Looping Oxidative Dehydrogenation of *n*-Hexane Using CuMgAlOx: Towards Structure-Reactivity Relationship.
Yi Du[1], Jonathan Mitchell[1], Bradley Wooler[2], Chris Kliewer[1] and **Kun Wang**[1], *(1)ExxonMobil Technology and Engineering Company, USA, (2)ExxonMobil, USA.*

**Short Summary:**
High surface area mixed oxides CuMgAlOx with atomic-level dispersion of Cu were prepared and evaluated for the stoichiometric oxidation of n-hexane to hexenes. Presence of Na significantly improves n-hexene selectivity and compresses the d-d gap in Cu($^{2+}$) (UV/Vis). The d-d band pre-edge could be a potential olefin selectivity descriptor.

1:40 PM **Wed-BLRMA-1340** Multifunctional Redox Catalysts for Chemical Looping Oxidative Dehydrogenation of Diisopropylbenzene.
**Junchen Liu**, Xijun Wang, Jacob Stana, Tyler Stana and Fanxing Li, *North Carolina State University, USA.*

**Short Summary:**
This work presents the chemical looping oxidative dehydrogenation of meta-diisopropylbenzene to meta-diisopropenylbenzene (DIPEB). 75% single-pass yield is achieved with La-Ca-Mn-O@K-Fe-O as the multifunctional catalyst. DFT indicates the rate limiting step is α-H abstraction on the isopropyl chain. It is determined that 72% energy saving could be achieved via Aspen Plus.

2:00 PM **Wed-BLRMA-1400** Ethylbenzene Production By Consecutive Oxidative Dehydrogenation of Ethane and Benzene Alkylation.
**Eric Steinman** and Marat Orazov, *University of Delaware, USA.*

**Short Summary:**
Ethane cracking is the predominant industrial process for ethylene production, but it suffers from equilibrium limitations, coking, high temperatures, and expensive separations. We mitigate these drawbacks using catalyst selection and reaction engineering to enable a consecutive oxidative dehydrogenation of ethane and benzene alkylation process for the production of ethylbenzene.

2:20 PM **Wed-BLRMA-1420** Selective Propane Oxidative Dehydrogenation By Using Platinum-Metal Oxides Based Tandem Catalysts..
**Geun-Ho Han** and Justin Notestein, *Northwestern University, USA.*

**Short Summary:**
This study develops tandem catalysts for selective propylene production from propane oxidative dehydrogenation. Despite the reaction's advantages, it suffers from low selectivity due to a highly spontaneous side reaction, propane combustion to $CO_2$. Thus, we developed $Pt/Al_2O_3$ catalyst by coating metal oxides with ALD, which improved the selectivity.

2:40 PM **Wed-BLRMA-1440** Probing a Proposed Mechanism for the Oxidative Dehydrogenation of Propane over Boron Nitride Using a Radical Initiator.
**Unni Kurumbail**[1], Will McDermott[2], Edgard Lebron Rodriguez[3] and Ive Hermans[3,4], *(1)UW-Madison, USA, (2)Proctor & Gamble, USA, (3)University of Wisconsin-Madison, USA, (4)University of Wisconsin–Madison, USA.*

**Short Summary:**
Boron-containing materials catalyze the oxidative dehydrogenation of propane to propylene (ODHP) with high selectivity. To validate the mechanistic hypothesis that these catalysts owe their unique performance to gas-phase reactivity, we use ozone to initiate a gas-phase ODHP reaction and show it mimics the selectivity-conversion distribution over boron-containing materials.

3:00 PM **Wed-BLRMA-1500** Multiple Promotional Effects of Vanadium Oxide on Boron Nitride for Oxidative Dehydrogenation of Propane.
**Xiao Jiang**[1], Xuanyu Zhang[2], Stephen Purdy[3], Yang He[4], Zhennan Huang[3], Rui You[2], Zeyue Wei[2], Harry Meyer III[3], Miaofang Chi[3], Katharine Page[3], Weixin Huang[2] and Zili Wu[3], *(1)Aramco Americas: Aramco Research Center - Boston, USA, (2)University of Science and Technology of China, China, (3)Oak Ridge National Laboratory, USA, (4)Oak Ridge National laboratory, USA.*

**Short Summary:**
The presence of vanadia facilitates the surface oxyfunctionalization of boron nitride during $O^{2-}$assisted oxidative dehydrogenation of propane, leading to activity enhancement. Released nitric oxide, through oxyfunctionalization, might further improve the activity by mediating the gas-phase chemistry.

## Alkane Dehydrogenation II

Session Chairs: Steven Lim, *Research Engineer at Chevron Phillips Chemical Company, USA* and Raj Gounder, *Purdue University, USA.*

3:45 PM ***KEYNOTE* Wed-BLRMA-1545 Gallium, Zinc, and Indium Speciation in Zeolite Catalysts for Light Alkane Dehydrogenation. Raul Lobo** and Yong Yuan, *University of Delaware, USA.*

**Short Summary:**
We have conducted a investigation of Ga-, In- and Zn-containing zeolites for ethane and propane dehydrogenation spanning a wide range of zeolite structures (MFI, CHA and SZR), Si/Al ratios, and metal loadings, and characterizing the materials using classical kinetic studies, FTIR spectroscopy, pulse-reaction studies. This talk will summarize these investigations.

4:25 PM **Wed-BLRMA-1625** Enhancing the Tandem Reactions of $CO_2$-Assisted Ethane Dehydrogenation and Aromatization.
**Elaine Gomez**[1], Xiaowa Nie[2], Ji Hoon Lee[1], Zhenhua Xie[1] and Jingguang Chen[3], *(1)Columbia University, USA, (2)Dalian University of Technology, China, (3)University of Delaware, USA*.

**Short Summary:**
The addition of phosphorous at an optimal loading improved the hydrothermal stability of Ga/ZSM-5, reduced coke formation on the catalyst surface, and allowed for the formation of more liquid aromatics through the $CO_2$-assisted oxidative dehydrogenation and aromatization reaction pathway compared to the direct dehydrogenation and aromatization reaction.

4:45 PM **Wed-BLRMA-1645** Taming the Energetics of the Transition State By Leveraging the Water-Catalyst Interactions during Alkane Dehydrogenation.
**Jord Haven**, Jimmy Faria and Leon Lefferts, *University of Twente, Netherlands*.

**Short Summary:**
The role of $H_2O$ on the reaction kinetics of non-oxidative ethane dehydrogenation on a $Pt/ZnAl_2O_4$ catalyst is investigated. Interestingly, $H_2O$ is found to substantially reduce the enthalpy of the transition state, indicating stabilization of the transition state at the Pt active sites by $H_2O$.

5:05 PM **Wed-BLRMA-1705** Mechanism of Methylcyclohexane Dehydrogenation on Dispersed Pd Nanoparticles and Kinetic Consequences of Lewis Acid-Base Pairs on Oxide Supports.
**Zhongyao Zhang**[1], Sai Chen[1], Trenton Otto[2] and Enrique Iglesia[1], *(1)University of California, Berkeley, USA, (2)Chevron Energy Technology Co., USA*.

**Short Summary:**
This work reveals mechanism of MCH dehydrogenation on dispersed Pd nanoparticles and demonstrates the promotive effect of using supports with Lewis acid-base pairs. The findings help design catalysts for methylcyclohexane-toluene cycle that provides a practical way of using $H_2$ as an energy carrier.

## Ballroom BC

### WEDNESDAY MORNING

### Accelerated Chemical Space Exploration

Session Chairs: Chris Paolucci, *University of Virginia, USA* and Diego Gomez-Gualdron, *Colorado School of Mines, USA*.

9:30 AM **Wed-BLRMBC-0930** Autonomous Multiobjective Computational Discovery of NRR Electrocatalysts.
**Lance Kavalsky**[1], Vinay I. Hegde[2] and Venkatasubramanian Viswanathan[1], *(1)Carnegie Mellon University, USA, (2)Citrine Informatics, USA*.

**Short Summary:**
Electrocatalyst discovery is an inherently multiobjective problem. In this work we demonstrate an autonomous discovery framework that efficiently balances multiple target criteria as it explores the SAA design space. We will highlight identified NRR candidates and show how they can be ranked considering all target metrics.

9:50 AM **Wed-BLRMBC-0950** Machine Learning Accelerated Discovery of Single-Atom Catalysts for Nitrogen Reduction Reaction.
Zhi Wen Chen and **Chandra Veer Veer Singh**, *University of Toronto, Canada*.

**Short Summary:**
We investigate structure-activity relationships of single atom catalysts for nitrogen reduction reaction by combining high-throughput DFT data with machine learning. A new bidirectional activation mechanism is proposed for activation of $N_2$ and model predictions are verified with available experimental data. The new descriptor has potential to accelerate data-driven catalyst design.

10:10 AM **Wed-BLRMBC-1010** Catlas: An Automated Framework for Catalyst Discovery Demonstrated for Direct Syngas Conversion.
**Brook Wander**, Zachary Ulissi and Kirby Broderick, *Carnegie Mellon University, USA*.

**Short Summary:**
We present an open source framework for high-throughput catalyst screenings using off-the-shelf pretrained machine learning models. To demonstrate its efficacy, we use it to screen 947 binary, transition metal intermetallics for the direct conversion of syngas to multi-carbon oxygenates.

10:30 AM **Wed-BLRMBC-1030** An Extensible and FAIR Datahub for Multiscale Modeling in Heterogeneous Catalysis.
**Siddhant Lambor**, Sashank Kasiraju and Dionysios Vlachos, *University of Delaware, USA*.

**Short Summary:**
We introduce CKineticsDB™, a state-of-the-art datahub for multiscale modeling in heterogeneous catalysis. It provides curated files from simulations at multiple scales, metadata extracted from files and obtained from researchers, and sufficient provenance to reproduce publication results. CKineticsDB resolves research challenges in computational catalysis stemming from unorganized, incomplete, and barricaded data.

10:50 AM ***KEYNOTE*** **Wed-BLRMBC-1050 Discovering Stable and Active Catalysts with Machine Learning and Community Knowledge. Heather Kulik**, Aditya Nandy and Husain Adamji, *Massachusetts Institute of Technology, USA*.

**Short Summary:**
We develop machine learning models and employ efficient global optimization to accelerate the discovery of new homogeneous and MOF catalysts for direct methane-to-methanol conversion. We identify catalysts that simultaneously optimize for multiple reaction steps and use data-driven models of stability to maximize the stability of the designed catalyst.

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11:30 AM WITHDRAWN: Obtaining Catalyst Design Rules for $CO_2$ Hydrogenation Via Machine Learning Tools.
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## WEDNESDAY AFTERNOON

### Homogeneous and Molecular Catalysis I

Session Chairs: Heine Anton Hansen, *Technical University of Denmark, Denmark* and Xu Jason, *Argonne National Laboratory, USA*.

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1:20 PM ***KEYNOTE*** **Wed-BLRMBC-1320 Molecular Transition Metal Catalysts for Arene Alkylation and Alkenylation: Progress on Improved Catalysts and Mechanistic Understanding.**
**T. Brent Gunnoe**[1], William Goddard III[2], Weihao Zhu[1], Xiaofan Jia[1], Marc Bennett[1], Charles Musgrave III[2], Kwanwoo Park[1], Diane Dickie[1], Lucas Frye[1] and Jeffrey Ellena[1], *(1)University of Virginia, USA, (2)California Institute of Technology, USA*.

**Short Summary:**
This presentation will focus on progress toward the development and understanding of molecular catalysts based on Ru, Pd, Pt and Rh for arene alkylation and alkenylation with a primary focus on new Rh-based catalysts that provide long-lived and highly selective reactivity.

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2:00 PM **Wed-BLRMBC-1400** Adventures in Cross-Coupling Chemistry with Sulfones As Electrophiles.
**Cathleen Crudden**, *Queen's University, Canada*.

**Short Summary:**
The development of a new class of electrophile for use in Suzuki-Miyaura cross coupling reactions that create stereochemistry.

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2:20 PM **Wed-BLRMBC-1420** Homogeneous Catalyst Design with Schrödinger's Digital Chemistry Platform.
**Pavel Dub**[1,2], Thomas Mustard[2], Thomas Hughes[2] and Mathew Halls[2], *(1)Schrödinger Inc., USA, (2)Schrödinger, Inc, USA*.

**Short Summary:**
High-Throughput ab initio Automated Homogeneous Catalyst Design with Schrödinger's AutoReaction Workflow Module will be Presented.

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2:40 PM **Wed-BLRMBC-1440** Computational Screening of Improved Catalysts for the Buchwald-Hartwig Amination Reaction.
**Roberto Schimmenti**[1], Megha Anand[2] and Jens K. Nørskov[1], *(1)Technical University of Denmark, Denmark, (2)Data Science and Modeling, Pharmaceutical Sciences, R&D, AstraZeneca, United Kingdom*.

**Short Summary:**
We have engaged in high-throughput computational screening of catalytic materials for the Buchwald-Hartwig Amination reaction. In particular, we have tested more than 70 new candidates containing a wide range of electron-withdrawing groups. Furthermore, we have developed new insights on the transferability of scaling relations across different catalysts/substrates combinations.

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3:00 PM **Wed-BLRMBC-1500** Carboxylic Acid-Based Ligands to Improve Ceria-Supported Ligand-Dispersed Pt Catalysts for Hydrosilylation.
Iyad Ali[1], Linxiao Chen[2], Fereshteh Rezvani[1], Xuemei Zhou[1] and **Steven Tait**[1], *(1)Indiana University Bloomington, USA, (2)Pacific Northwest National Laboratory, USA*.

**Short Summary:**
We tuned ligand-coordinated supported catalysts (LCSCs) of highly-dispersed Pt with carboxylic acid-based ligands as anchoring ligands with bidentate N-based ligand or as coordination ligand. Using trimesic acid as the anchoring ligand reduced Pt leaching from 34% after only 1 batch to ~25% after 4 batches of hydrosilylation of 1-octene.

### Homogeneous and Molecular Catalysis II

Session Chairs: Cong Liu, *Argonne National Laboratory, USA* and Pavel Dub, *Schrödinger Inc., USA*.

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3:45 PM **Wed-BLRMBC-1545** Improvements to the Bond Energy/Bond Order and Population Method.
**Barbaro Zulueta**[1], John Keith[1] and George Petersson[2], *(1)University of Pittsburgh, USA, (2)Temple University, USA*.

**Short Summary:**
We have developed the Bond Energy/Bond Orders and Populations (BEBOP) model for improved accuracy of intramolecular energy decomposition analyses and ab initio molecular energies of molecules involving first row atoms. Outlook for future directions in development and applications of BEBOP as a computational quantum chemistry tool will be discussed.

4:05 PM **Wed-BLRMBC-1605** Surfactant and Ligand-Free Synthesis of Platinum Nanoparticles in Aqueous Solution for Catalytic Applications.
Rashmi Charde, Brian van Devener and **Michael Nigra**, *University of Utah, USA*.

**Short Summary:**
In this work, we demonstrate the synthesis of platinum nanoparticles without the use of additional stabilizing agents beyond the borohydride that is used for the reduction of the platinum precursor. These Pt nanoparticles show enhanced activity for $H_2O_2$ decomposition and the electron transfer reaction between hexacyanoferrate(III) ions and thiosulfate ions.

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4:25 PM **Wed-BLRMBC-1625** On Route to Molecular Control over Aluminosilicate-Supported Cationic Molecular Catalysts.
Yifan Wu[1], Michael Boreen[1], John Arnold[1], Christopher Lew[2], Stacey I. Zones[2] and **Alexander Katz**[1], *(1)University of California, Berkeley, USA, (2)Chevron Energy Technology Company, USA*.

**Short Summary:**
We demonstrate control of inner- and outer-sphere effects in stabilizing cationic supported molecular catalysts on anionic aluminosilicate surfaces. Overall, our results demonstrate that the retention of molecular-scale control in this class of catalysts remains a grand challenge, with active-site isolation being key to achieving this degree of control.

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4:45 PM **Wed-BLRMBC-1645** Catalytic Activity Tunning Via Li Intercalation for Hydrogenation of Cyclohexene over Atomic Ni Supported By Redox Non-Innocent $LiMn_2O_4$ and $Li_2Mn_2O_4$ Catalyst Support.
**Xu Jason**, David Kaphan, A. Jeremy Kropf, Cong Liu and Massimiliano Delferro, *Argonne National Laboratory, USA*.

**Short Summary:**
The hydrogenation reactivity of atomic Ni catalyst supported by $LiMn_2O_4$ was tuned by Li intercalation into the catalyst support. Upon lithiation, the oxidation state of Ni was reduced and hydrogenation activity was improved. This work demonstrated the catalytic activity tuning via modulating the electronic structure of redox non-innocent catalyst support.

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5:05 PM **Wed-BLRMBC-1705** At-Line Monitoring of Diphenhydramine Synthesis Via Low-Field NMR Spectroscopy As Process Analytical Technology.
**Jakub Konkol** and George Tsilomelekis, *Rutgers, The State University of New Jersey, USA*.

**Short Summary:**
Low-field flow NMR enables PAT analysis of microfluidic reaction mixtures and determination of kinetics in the synthesis of active pharmaceutical ingredients. This is shown using diphenhydramine, a pharmaceutical ingredient that has some interest in the literature for continuous manufacturing, but kinetics has not yet been shown.

## Ballroom DE

### WEDNESDAY MORNING

### Novel Approaches in Catalysis

Session Chairs: Cathy Chin, *University of Toronto, Canada* and Abhaya Datye, *University of New Mexico, USA*.

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9:30 AM ***KEYNOTE*** **Wed-BLRMDE-0930 Fundamentals and Applications of Mechanocatalytic Processes.** Andrew Tricker, George Y. Chang, Anuoluwatobi Osibo, Karoline Lena Hebisch, Erin Phillips, Jacob DeWitt and **Carsten Sievers**, *Georgia Institute of Technology, USA*.

**Short Summary:**
Collisions in ball mills create unique transient reaction environments and can shear solids to induce reactions between two surfaces. This contribution provides insight into these phenomena and shows the application of mechanocatalytic processes for ammonia synthesis and polymer upcycling.

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10:10 AM **Wed-BLRMDE-1010** Catalytic Condensers for Programmable Surface Chemistry.
**Paul Dauenhauer**, *University of Minnesota, USA*.

**Short Summary:**
An alternative approach to catalyst design tunes the electron density of the active site by stabilizing charge in the exposed catalytic surface by the method of a ‘catalytic condenser’ that uses a high-k dielectric $HfO_2$ layer to separate an electrode and conductive active layer of ultrathin alumina on graphene.

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10:30 AM **Wed-BLRMDE-1030** Intensification of Catalytic $NH_3$ Cracking Using Thermally and Electrically Conductive Packed Cellular Internals.
Federico Sascha Franchi[1], Nicola Usberti[1], Matteo Ambrosetti[1], **Alessandra Beretta**[1], Gianpiero Groppi[1], Robert W. Gallen[2] and Enrico Tronconi[1], *(1)Politecnico di Milano, Italy, (2)Johnson Matthey, United Kingdom*.

**Short Summary:**
Two innovative reactor designs based on an aluminium packed-POCS and on an electrified SiC packed-foam were tested in view of intensifying the catalytic cracking of ammonia via enhanced heat management. In comparison with a conventional packed-bed reactor configuration, both packed structures showed significantly better performances.

10:50 AM **Wed-BLRMDE-1050** Relating Kinetic and Mechanistic Features to Dynamic Rate Enhancement in Catalytic Oxidation Reactions..
**Austin Morales**, Praveen Bollini and Michael Harold, *University of Houston, USA*.

**Short Summary:**
Degrees of rate enhancement during periodic operation can be derived from mechanistic features and kinetic parameters. Multi-reactant modulation may improve cyclic average rates beyond that of single reactant modulation. The effects of dynamic parameters on rates during catalytic oxidation reactions are dictated by surface coverages and competitive adsorption.

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11:10 AM **Wed-BLRMDE-1110** Decarbonizing Dry Reforming of Methane Using Rapid Pulse Joule Heating.
**Kewei Yu**, Cong Wang, Weiqing Zheng and Dionysios Vlachos, *University of Delaware, USA*.

**Short Summary:**
We develop a rapid pulse Joule heating (RPH) reactor for Methane dry reforming reaction. With carbon fiber paper as the heating element, the reactor can reach a heating rate of ~14000 °C/s. RPH showed better catalyst stability, higher reaction rate, and improved energy efficiency compared with steady-state operation.

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11:30 AM **Wed-BLRMDE-1130** Multicavity CuO Nanostructures for Sonocatalytic Glucose Oxidation.
**Zhangyue Xie** and Wen Liu, *Nanyang Technological University, Singapore*.

**Short Summary:**
Multicavity CuO nanoparticles present effective sonocatalysts enabling the oxidation of glucose in water at ambient conditions in the presence of low intensity high frequency pulsed ultrasound. The said approach enables the production of value-added products in the absence of other chemical additive or homogeneous catalysts in an energy-efficient manner.

## WEDNESDAY AFTERNOON

## Ammonia Synthesis and Decomposition

Session Chairs: Todd Toops, *Oak Ridge National Laboratory, USA* and William Tarpeh, *SLAC National Accelerator Laboratory, USA*.

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1:20 PM **Wed-BLRMDE-1320** Intrinsic Catalytic Activity of Carbon Nanotubes for Electrocatalytic Nitrate Reduction to Ammonia.
**Nia Harmon** and Hailiang Wang, *Yale University, USA*.

**Short Summary:**
We discover that pristine carbon nanotubes are active and selective electrocatalysts for nitrate ($NO_3$-) reduction to ammonia ($NH_3$). Heteroatom doping decreases catalytic performance and indicates that C is the active site for this reaction. These results provide evidence for a new type of active site for $NO_3$- reduction.

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1:40 PM **Wed-BLRMDE-1340** Electrosynthesis of Ammonia with High Selectivity and High Rates Via Engineering of the Solid-Electrolyte Interphase.
**Shaofeng Li** and Ib Chorkendorff, *Technical University of Denmark, Denmark*.

**Short Summary:**
In this work, we demonstrate that record selectivity and $NH_3$ production rate at a current density of -1.0 A cmgeo-2 under 20 bar $N_2$ are achieved by combining a highly porous copper electrode with LiF-enriched solid-electrolyte interphase layer.

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2:00 PM **Wed-BLRMDE-1400** Understanding the Selectivity of Single Atom Alloys in Complex Reaction Pathways through Spill-over Effects: Examining the Electrochemical Nitrate Reduction Reaction through Ab-Initio Calculations.
Srishti Gupta, Daniel Rivera, Matthew Shaffer, Adam Chismar and **Christopher Muhich**, *Arizona State University, USA*.

**Short Summary:**
The activity and selectivity of single atom alloys for $N_2$ or $NH_3$ electrochemical nitrate reduction depends on the relative energy of N on the single atom site or bulk metal. Performance and activity are assessed by density functional theory calculations.

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2:20 PM **Wed-BLRMDE-1420** Assessing the Activity of Electrochemical $N_2$ Oxidation to $NO_x$ on Transition Metal Oxides.
**Haldrian Iriawan**[1], Livia Giordano[1], Ifan Stephens[2] and Yang Shao-Horn[1], *(1)Massachusetts Institute of Technology, USA, (2)Imperial College London, United Kingdom*.

**Short Summary:**
We performed DFT calculations to investigate possible reaction mechanisms electrochemical $N_2$ oxidation to NOx on rutile (110) and perovskite surfaces to quantify fundamental constraints from binding energetics point of view. We performed electrochemical testing for the reaction using perovskites and assess the ability of the catalysts to oxidise $N_2$.

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2:40 PM **Wed-BLRMDE-1440** Effect of Pt Particle Size on Ammonia Oxidation Selectivity Using Microkinetic Modeling.
**Amish Chovatiya**[1], Brandon K. Bolton[2], Hanyu Ma[1], Rohil Daya[3], Dylan Trandal[3], Rajat Ghosh[3], Krishna Gunugunuri[4], Krishna Kamasamudram[3], Raj Gounder[2] and William Schneider[1], *(1)University of Notre Dame, USA, (2)Purdue University, USA, (3)Cummins Inc., USA, (4)Cummins Technical Center, USA*.

**Short Summary:**
We combine the Wulff construction for Platinum nanoparticles with site specific catalytic ammonia oxidation microkinetic models to build a particle size dependent model. We show the dependence of activity and selectivity on Pt particle size using this model and use our results to explain experimental rate order observations.

3:00 PM **Wed-BLRMDE-1500** Influence of Host Structure and Synthesis Technique on the Formation of Active Fe, Co and Ni Catalysts for Ammonia Decomposition.
Baris Alkan[1,2], Clara Patricia Marshall[1], Gregor Koch[1], Anh Binh Ngo[1], Abdulrhman Moshantaf[1], Pierre Kube[1], Kassiogé Dembélé[1], Thomas Lunkenbein[1], Shan Jiang[1], Nils Pfister[1], Frank Girgsdies[1], Holger Ruland[2] and **Annette Trunschke**[1], *(1)Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany, (2)Max Planck Institute for Chemical Energy Conversion, Germany*.

**Short Summary:**
Co and Ni catalysts can achieve performance in ammonia decomposition comparable to that of Ru catalysts if the properties of the interface between the metal and the embedding matrix are tuned in a controlled manner by the choice of crystal structure and synthesis method of the oxide host.

## Active Sites and Reaction Mechanisms for $CO_2$ Conversion

Session Chairs: Emma Lovell, *University of New South Wales, Australia* and Wen Liu, *Nanyang Technological University, Singapore*.

3:45 PM **Wed-BLRMDE-1545** Catalytic $CO_2$ Hydrogenation Using Cobalt Ferrite Nanoparticles for Selective Production of Light Olefins.
**Kwangjin An**, *Ulsan National Institute of Science and Technology (UNIST), Korea, Republic of (South)*.

**Short Summary:**
Research on $CO_2$ hydrogenation using well-defined nanoparticless for producing high value-added chemicals can provide valuable insights into the design of high-performance catalysts, which can contribute to slowing climate change by recycling $CO_2$ to produce fuels and chemicals.

4:05 PM **Wed-BLRMDE-1605** Ceria Shell Formation on Cu Nanoparticles By Promoting Surface Oxygen Transfer for Highly Active and Durable $CO_2$ Hydrogenation.
**Gunjoo Kim** and Hyunjoo Lee, *Korea Advanced Institute of Science and Technology, Korea, Republic of (South)*.

**Short Summary:**
Amorphous ceria shell was formed over small Cu nanoparticles as surface oxygen species were activated by Cu doping on $CeO_2$. From facile $CO_2$ activation and $H_2$ spillover, this catalyst showed high activity and durability in $CO_2$ hydrogenation. It was successfully scaled up to bench scale reactor, showing record-high CO productivity.

4:25 PM **Wed-BLRMDE-1625** Elementary Steps on Crowded Metal Surfaces and Assessments of the Prevalence and Binding Properties of Uncovered Site Ensembles.
**Wenshuo Hu** and Enrique Iglesia, *University of California, Berkeley, USA*.

**Short Summary:**
We describe a probabilistic method that systematically assesses the energy required to create an ensemble of vicinal uncovered sites via desorbing contiguous bound-species to determine the probability of finding such ensembles; then, it considers binding properties of each ensemble for the kinetically-relevant transition states ($CO_2$ dissocaition as the illustrative case).

4:45 PM **Wed-BLRMDE-1645** Breaking Structure Sensitivity in $CO_2$ Hydrogenation: On the Role of the Interface between Metallic Co Clusters and a Reducible Oxide Support.
**Emiel Hensen**, *Eindhoven University of Technology, Netherlands*.

**Short Summary:**
We demonstrate the possibility to design a structure-insensitive $CO_2$ hydrogenation catalyst by engineering the metal-oxide interface in Co on $CeO_2$-$ZrO_2$ catalysts. By using a low Co loading and partially reducing Co, much higher activity is achieved than conventional Co metal nanoparticle catalysts.

5:05 PM **Wed-BLRMDE-1705** In Situ FTIR Investigation of Cerium Oxide Catalysts for Direct Conversion of Carbon Dioxide into Diethyl Carbonate.
**Mara Arduino**, Enrico Sartoretti, Samir Bensaid and Fabio Alessandro Deorsola, *Politecnico di Torino, Italy*.

**Short Summary:**
In situ FTIR technique was performed to study the DEC synthesis mechanism. Active species were identified through the interaction of the catalyst with carbon dioxide, ethanol and diethyl carbonate. The preferential exposure of the (1 1 0) crystal plane in rod-shaped $CeO_2$ is crucial in the activation of the reagents.

# Rotunda

### WEDNESDAY MORNING

## Fischer-Tropsch Synthesis

Session Chairs: Lars Grabow, *University of Houston, USA* and Phil Christopher, *University of California Santa Barbara, USA*.

9:30 AM **Wed-RTND-0930** Synthesis of Carbon Nanotubes Supported Iron Catalysts for Light Olefins via Fischer-Tropsch Synthesis.
**Ajay Dalai**, Arash Yahyazadeh and Lifeng Zhang, *University of Saskatchewan, Canada*.

**Short Summary:**
In this study, techno-economic analysis (TEA) and life cycle assessment (LCA) of light olefin production in Fischer-Tropsch synthesis reaction were investigated. Data from a lab-scale experiment using the optimum bimetallic promoted catalyst (0.5K5Mo10Fe/CNTs) were used to simulate a plant to produce 1 kg of ethylene/h.

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9:50 AM **Wed-RTND-0950** Oxidation of Hägg Carbide during High Temperature Fischer-Tropsch Synthesis: In-Situ Observations.
**Michael Claeys**[1], Eric van Steen[2], Thys Botha[3], Renier Crous[4], Alta Ferreira[4], Avinash Harilal[4], Denzil Moodley[5], Prabashini Moodley[4], Esna du Plessis[4] and Kobus Visagie[4], *(1)Catalysis Institute and c*change (DSI-NRF Centre of Excellence in Catalysis), University of Cape Town, South Africa, (2)University of Cape Town, South Africa, (3)Sasol Technology, South Africa, (4)Sasol Technology R&D, South Africa, (5)Sasol Research & Technology, South Africa*.

**Short Summary:**
In this study the oxidation threshold of a fused iron catalyst was studied at industrially relevant high temperature Fischer-Tropsch synthesis conditions using an in-situ magnetometer. No oxidation was observed at $CO_2$ levels up to 8 bar, while, in agreement with thermodynamic calculations conducted in this study, $H_2O$ induced oxidation.

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10:10 AM **Wed-RTND-1010** Role of Titania in Cobalt-Based FT Catalysts- an Inverse Catalyst Approach.
**Yatheshth Ragoo**[1], Melissa Petersen[1], Glenn Jones[2], Hellen Chuma[2] and Eric van Steen[1], *(1)University of Cape Town, South Africa, (2)Johnson Matthey Technology Center, United Kingdom*.

**Short Summary:**
The term “strong-metal support interactions” encapsulates different effect affecting the performance of the catalytically active phase. Here, we use TiOx(OH)y clusters adsorbed on Co(111) to study SMSI in cobalt-based Fischer-Tropsch catalysts. These clusters affect the strength of adsorption of CO as well as the activation barrier for the CO dissociation.

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10:30 AM **Wed-RTND-1030** DFT Insights into the Platinum Promotion of Cobalt-Based Fischer-Tropsch Catalysts.
Tracey van Heerden, Yatheshth Ragoo and **Eric van Steen**, *University of Cape Town, South Africa*.

**Short Summary:**
DFT calculations demonstrate that the presence of platinum has a marked effect on the direct dissociation of CO on cobalt. Platinum promotion reduces the barrier of CO dissociation on the Co(100) surface by up to 0.5 eV, opening up an additional reaction channel for CO-dissociation.

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10:50 AM **Wed-RTND-1050** Sorption-Enhanced Fischer-Tropsch Synthesis – Effect of Water Removal.
**Ljubisa Gavrilovic**[1], Saima Sultana Kazi[1], Mogahid Osman[2], Oscar Luis Ivanez Encinas[3] and Edd A. Blekkan[3], *(1)Institute for Energy Technology, Norway, (2)ZEG POWER AS, Norway, (3)Norwegian University of Science and Technology, Norway*.

**Short Summary:**
The present paper presents the development of a innovative technology that reshapes Fischer-Tropsch synthesis via sorption enhanced approach where the water is systematically removed by solid water adsorbents. *In-situ* removal of the water can lead to significant conversion enhancement of equilibrium-limited reactions, while also protecting catalysts from steam-induced deactivation.

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11:10 AM **Wed-RTND-1110** Construction of Efficient Ni and K Modified Molybdenum Carbides Based on Lignin Carbon for Higher Alcohols Synthesis.
Shihang Meng[1], Yujing Weng[2], Qi Sun[2] and **Yulong Zhang**[1], *(1)Henan Polytechnical University, China, (2)Henan Polytechnic university, China*.

**Short Summary:**
Lignin was found to be a good carbon source and support for $Mo_2C$ based catalyst. Ni and K promoters showed synergistic promotion effects for higher alcohol selectivity and yield by tuning the active surfaces to enhance the adsorption of both dissociative and non-dissociative adsorption of CO.

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11:30 AM **Wed-RTND-1130** Low Oxygen Surface Coverage Drives the Activity of Two-Dimensional Molybdenum Carbide in the Fischer-Tropsch Synthesis (FTS).
**Evgenia Kountoupi**[1], Alan Barrios[2], Zixuan Chen[1], Christoph Müller[1], Vitaly Ordomsky[2], Aleix Comas Vives[3,4] and Alexey Fedorov[1], *(1)ETH Zürich, Switzerland, (2)Université Lille, France, (3)TU Wien, Austria, (4)Universitat Autònoma de Barcelona, Spain*.

**Short Summary:**
Two-dimensional $Mo_2C$ catalyzes the Fischer-Tropsch Synthesis to higher alkanes. High activity correlates with the absence of surface O* sites. DFT analysis explains the absence of olefins and oxygenates in products. This work shows how catalytic properties of transition metal carbides depend on the surface oxygen coverage.

## WEDNESDAY AFTERNOON

## Catalytic Oxidation of Emissions I

Session Chairs: Fabio Ribeiro, *Purdue University, USA* and Fudong Liu, *University of Central Florida, USA*.

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1:20 PM **Wed-RTND-1320** Spectroscopic Determination of Metal Redox and Segregation Effects during CO and CO/NO Oxidation over Pd and PdCu Catalysts.
**Stephen Kristy**[1], Kostas Goulas[1] and Simon Bare[2], *(1)Oregon State University, USA, (2)SLAC National Accelerator Laboratory, USA*.

**Short Summary:**
Under LTC Diesel Exhaust Conditions PdCu shows lower temperature activity for CO oxidation than Pd. Cu eliminates NO inhibition and CO poisoning, and enables binding of dissociated oxygen. PdCu remains metallic over the course of CO oxidation, Pd undergoes a transformation to form undercoordinated Pd sites (a PdO surface layer).

1:40 PM **Wed-RTND-1340** Highly Active and Stable Single Atom Rh1/$CeO_2$ Catalyst for CO Oxidation during Redox Cycling.
**Shiva Murali**[1], Carlos Eduardo Garcia Vargas[1,2], Xavier Isidro Pereira Hernandez[1,2], Dong Jiang[2], Ryan Alcala[3], Andrew De La Riva[3], Abhaya Datye[3] and Yong Wang[1,2], *(1)Pacific Northwest National Laboratory, USA, (2)Washington State University, USA, (3)University of New Mexico, USA*.

**Short Summary:**
The single atom Rh1/$CeO_2$ catalysts synthesized by the high temperature calcination (Atom Trapping) method do not exhibit activity (CO oxidation) and/or structural changes during redox cycling hence are promising catalysts for emission control where redox cycling is encountered, and severe oxidation (fuel cut) leads to loss of performance.

2:00 PM **Wed-RTND-1400** A Versatile Microkinetic Model of CO Oxidation over Rh/$Al_2O_3$.
Nawaf M. Alghamdi[1], **Dionysios Vlachos**[2] and S. Mani Sarathy[1], *(1)King Abdullah University of Science and Technology (KAUST), Saudi Arabia, (2)University of Delaware, USA*.

**Short Summary:**
We present a thermodynamically consistent, DFT-based parametrized microkinetic model that predicts low and high temperature CO oxidation on Rh/$Al_2O_3$. We demonstrate the model's versatility by accurately simulating our experimental data as well as data from the literature at different temperatures, flow rates, and inlet compositions.

2:20 PM **Wed-RTND-1420** Surface Embedded Pt Atomic Single-Layer Catalyst on Ceria Achieving High Efficiency for CO Oxidation.
**Shaohua Xie**[1], Liping Liu[2], Yue Lu[3], Hongliang Xin[2] and Fudong Liu[1], *(1)University of Central Florida, USA, (2)Virginia Polytechnic Institute and State University, USA, (3)Beijing University of Technology, China*.

**Short Summary:**
Local coordination environment of metal sites essentially determines their catalytic performance. On the surface defect-enriched $CeO_2$, the lattice embedded Pt atomic single-layer structure derived from embedded Pt single-atoms significantly outperforms the surface adsorbed Pt atomic single-layer structure derived from adsorbed Pt single-atoms on the conventional $CeO_2$ for CO oxidation.

2:40 PM **Wed-RTND-1440** Deactivation of Real-World Aged Diesel Oxidation Catalysts.
**Krishna Gunugunuri**, Rama Krishna Dadi and Hongmei An, *Cummins Inc., USA*.

**Short Summary:**
The understanding of the real-world aged diesel oxidation catalyst deactivation at various stages of useful life will help to develop accelerated lab-based aging protocols and kinetic models which are capable of correctly capturing DOC performance deterioration during vehicle use.

3:00 PM **Wed-RTND-1500** Impact of Potential Net-Zero Carbon Fuels on Oxidation Catalyst Reactivity for Emissions Control.
**Sreshtha Sinha Majumdar** and Josh Pihl, *Oak Ridge National Laboratory, USA*.

**Short Summary:**
Net-zero carbon fuels are critical to decarbonization of the hard-to-electrify transportation sectors. As fuel composition has significant impacts on catalyst efficiency, evaluation of reactivity of net-zero carbon fuels on emissions control catalysts under engine-exhaust relevant conditions will inform selection of future fuels while ensuring compliance with the stringent emissions regulations.

## Catalytic Oxidation of Emissions II

Session Chairs: Kunlun Ding, *Louisiana State University, USA* and Sreshtha Sinha Majumdar, *Oak Ridge National Laboratory, USA*.

3:45 PM **Wed-RTND-1545** Enhanced Stability and Low Temperature Performance of Pd-Based CHA Zeolite Catalysts for Complete Methane Oxidation.
**Jingzhi Liu**[1], Tala Mon[2], Eleni Kyriakidou[2] and Viktor Cybulskis[1], *(1)Syracuse University, USA, (2)University at Buffalo (SUNY), USA*.

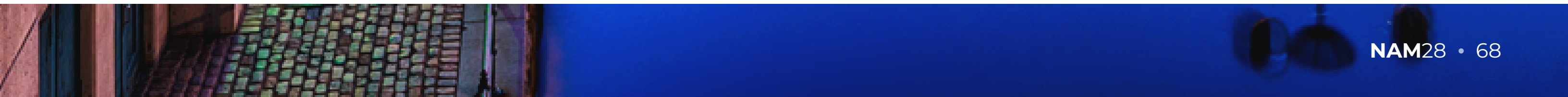
**Short Summary:**
Increasing the support Si/Al ratio of Pd/CHA catalysts leads to greater hydrophobicity and improved catalyst stability in presence of $H_2O$ during complete $CH_4$ oxidation by decreasing the mobility of active Pd species and reducing the effect of $H_2O$ inhibition on $CH_4$ oxidation rates.

4:05 PM **Wed-RTND-1605** Deactivation Mechanisms of Pd/γ-$Al_2O_3$ Catalysts for Lean Methane Oxidation.
Haiying Chen[1], **Yuliana Lugo-Jose**[2], Joseph Fedeyko[2], Todd Toops[1] and Jacqueline Fidler[3], *(1)Oak Ridge National Laboratory, USA, (2)Johnson Matthey Inc., USA, (3)CONSOL Energy Inc., USA*.

**Short Summary:**
This study reveals, for the first time, that PdO becomes less reducible after methane oxidation, suggesting reconstruction of PdO surface layer could be one of the fundamental deactivation mechanisms of Pd/γ-$Al_2O_3$ catalyst for lean methane oxidation.

4:25 PM **Wed-RTND-1625** Optimizing Regeneration Conditions after SO2 Poisoning of Spinel-Containing $CH_4$ Oxidation Catalysts.
**Natalia Diaz Montenegro** and William Epling, *University of Virginia, USA*.

**Short Summary:**
This work examines the optimization of the regeneration conditions (temperature, feed composition, modulation parameters) after $SO_2$ exposure of a new $CH_4$ oxidation catalyst formulation that incorporates spinel-structured materials with precious metal-based catalysts for the abatement of pollutants in stoichiometric natural gas engines.



4:45 PM **Wed-RTND-1645** 2D-Platinum As a Palladium Substitute for Hydrocarbon Oxidation.
**Andrew De La Riva**[1], Abhaya Datye[1], Dong Jiang[2], Weixin Huang[3], Yong Wang[4], Hien Pham[1], Yipeng Sun[5] and Homayoun Ahari[6], *(1)University of New Mexico, USA, (2)Washington State University, USA, (3)Stanford University, USA, (4)Pacific Northwest National Laboratory, USA, (5)BASF Corporation, USA, (6)Stellantis, USA*.

**Short Summary:**
The use of Pt in lieu of Pd to completely oxidize hydrocarbons such as propane and propylene can yield significant cost savings. Pt catalysts can be stable during 800°C accelerated ageing and highly active for HC oxidation if the Pt is synthesized to produce a particular morphology.

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5:05 PM **Wed-RTND-1705** Trace Amounts of Atomic Layer Deposition Alumina Prevent Pt Sintering.
**Gennaro Liccardo**[1,2], Michael L. Stone[1], Bang T. Nhan[1], Melissa Cendejas[2], Jacob Smith[3], Abinash Kumar[4], Shyama Charan Mandal[2], Simon Bare[2], Miaofang Chi[4], Frank Abild-Pedersen[2], Matteo Cargnello[1] and Stacey Bent[1,2], *(1)Stanford University, USA, (2)SLAC National Accelerator Laboratory, USA, (3)North Carolina State University, USA, (4)Oak Ridge National Laboratory, USA*.

**Short Summary:**
Herein we find that trace amounts of alumina ALD are able to stabilize Pt nanoparticles from sintering at 800 °C in $C_3H_6$ oxidation conditions. We performed rates measurements, XRF, and TEM analysis to study our materials before and after aging in reaction conditions at 800 °C.

# Thursday, June 22, 2023

## Ballroom A-E

### THURSDAY MORNING

**2023 Eugene J. Houdry Award Lecture: Stephen Schmidt**
Session Chairs: Christopher W. Jones, *Georgia Institute of Technology, USA* and Bala Subramaniam, *The University of Kansas, USA*

8:05 AM The Evolution of Raney® Catalysts.
**Steve Schmidt**, *WR Grace, USA*.

## 551 AB

### Design and Synthesis of Zeolites

Session Chairs: Francielle Candian Firmino Marcos, *Clemson University, USA* and Michael Smith, *Villanova University, USA*.

9:30 AM **Thu-551AB-0930** Synthesis and Structure Elucidation of SCM-25: A Zeolite with Ordered Meso-Cavities.
Yi Luo[1], **Wenhua Fu**[2], Bin Wang[1], Zhiqing Yuan[2], Junliang Sun[1,3], Xiaodong Zou[1] and Weimin Yang[2], *(1)Stockholm University, Sweden, (2)Sinopec Shanghai Research Institute of Petrochemical Technology, China, (3)Peking University, China*.

**Short Summary:**
The synthesis and structure elucidation of a novel germanosilicate SCM-25 is presented. The zeolite structure contains ordered meso-cavities (29.9 × 7.6 × 6.0 Å$^3$) interconnected by 12 × 12 × 10-ring channels.

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9:50 AM **Thu-551AB-0950** Investigating the Influences of Different Si and Al Sources on Accelerating the Kinetics of Interzeolite Conversion of FAU to CHA.
**Ricem Diaz Arroyo**[1], Raj Gounder[1] and Stacey I. Zones[2], *(1)Purdue University, USA, (2)Chevron Energy Technology Company, USA*.

**Short Summary:**
CBV720 (FAU) has demonstrated to have the fastest rate of conversion to CHA compared to other FAU reagents, but the underlying reasons are not well understood. The kinetics of interzeolite conversion can be assessed by using different locally organized starting materials that can influence the nucleation step.

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10:10 AM **Thu-551AB-1010** Effect of Cis/Trans OSDA Content on SSZ-39 Formation Kinetics.
**Zheng Cui**, Jeewan Pokhrel and Daniel F. Shantz, *Tulane University, USA*.

**Short Summary:**
The pronounced effect of the OSDA isomer on the growth kinetics of SSZ-39 is a unique finding in zeolite syntheses. Understanding why this is will provide the community new insights on how to control material synthesis kinetics, and potentially the discovery of new materials.

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10:30 AM **Thu-551AB-1030** Controlling Defects and Si/Al of High-Silica LTA Zeolites Using Charge Balancing Approach.
**Wei Fan**, *University of Massachusetts Amherst, USA*.

**Short Summary:**
LTA zeolite was selected as a model system to study the effects of charge balance between OSDA, F-, and defects. Our studies suggest, a charge balance can be achieved with two BULKY cations, one TMA cation, and three F- anions in one unit cell of LTA zeolite.

10:50 AM **Thu-551AB-1050** Dimethyl Ether Conversion into Light Olefins over MFI-Type Zeolites: The Effect of Acidity and Superficial Passivation on Catalytic Performance and Stability.

**Emanuele Giglio**[1], Giorgia Ferrarelli[1,2], Fabio Salomone[3], Elena Corrao[3], Massimo Migliori[1], Samir Bensaid[3], Raffaele Pirone[3] and Girolamo Giordano[1], *(1)University of Calabria, Italy, (2)University of Messina, Italy, (3)Politecnico di Torino, Italy*.

**Short Summary:**

MFI-type zeolite catalysts were synthesized, characterized and tested in dimethyl ether conversion into olefins (DTO). The effect of superficial passivation of MFI structures with Silicalite-1 on catalytic performance has been evaluated. Passivated catalyst showed improved stability, especially above 350 °C. A sustainable route to produce olefins can be carried out.

11:10 AM **Thu-551AB-1110** Design of Lewis Acid Zeolites for the Epoxide Ring Opening with Alcohols.

**Nick Brunelli**[1], Alexander Spanos[1], Nitish Deshpande[1], Leah Ford[1], Aamena Parulkar[1], Ambarish Kulkarni[2], Medha Kasula[1] and Rutuja Joshi[1], *(1)The Ohio State University, USA, (2)University of California, Davis, USA*.

**Short Summary:**

We tune the synthesis of Lewis acid zeolites to create highly active and selective catalysts for the alcohol ring opening of epoxides. We control the hydrophobicity and hydrophilicity of nanozeolite Beta and use alkyltin precursors to control the fraction of open and closed sites to create highly active catalysts.

11:30 AM **Thu-551AB-1130** Low Temperature $CH_4$ Oxidation for High Silica Pd/LTA Catalysts.

**Tala Mon**[1], Jingzhi Liu[2], Viktor Cybulskis[2] and Eleni Kyriakidou[1], *(1)University at Buffalo (SUNY), USA, (2)Syracuse University, USA*.

**Short Summary:**

Small-pore LTA zeolites were synthesized at Si/Al > 1 with 1 wt.% Pd and $CH_4$ oxidation performances were compared to 1 wt.% Pd/$Al_2O_3$. The results indicated that an improved $CH_4$ oxidation performance in the presence of $H_2O$ can be achieved by increasing the hydrophobicity of Pd/LTA.

## THURSDAY AFTERNOON

## Zeolite Characterization and Adsorption Thermodynamics

Session Chairs: Brian Frederick, *University of Maine, USA* and Zili Wu, *Oak Ridge National Laboratory, USA*.

1:20 PM **Thu-551AB-1320** Correlation of Structural Properties Determined via Gas Sorption and Catalytic Properties of Micro- and Mesoporous Zeolites.

**Katie Cychosz**[1] and Matthias Thommes[2], *(1)Anton Paar Quantatec, USA, (2)University of Erlangen-Nuremburg, Germany*.

**Short Summary:**

To advance application of the next generation of micro- and mesoporous zeolite catalysts, one must understand structural properties such as pore size and volume, and especially, pore connectivity and correlate them to catalytic activity. Gas sorption is the ideal tool for determining these properties for different catalytically active zeolites.

1:40 PM **Thu-551AB-1340** Probing Active Sites in the ZSM-5 Based Working FCC Catalyst.

**Udayshankar Singh**, *W.R. Grace & Co.-Conn., USA*.

**Short Summary:**

Technique based on unit cell volume (UCV) measurement has been developed to monitor the deactivation of ZSM-5 in FCC catalyst. UCV is measured by combining X-ray diffraction with Rietveld analysis. Measured UCV correlates well with acidity and catalytic performance of ZSM-5 catalysts, which has significance in development of new products.

2:00 PM **Thu-551AB-1400** Characterization of the Structural Changes of Tin Sites throughout the Life Cycle of Sn-β Prepared By Solid-State Ion Exchange.

**Edgard Lebron Rodriguez**[1], Faysal Ibrahim[1], Isabel Hortal-Sánchez[2], Angela Montano-Herazo[2], Chenyao Huang[3], Lillian Mostek[3], Nelson Cardona-Martínez[2] and Ive Hermans[1], *(1)University of Wisconsin-Madison, USA, (2)University of Puerto Rico at Mayagüez, USA, (3)University of Wisconsin–Madison, USA*.

**Short Summary:**

Material characterization and kinetic measurements are employed to offer insights into structure-activity relationships for Sn-β materials that contain sites that undergo structural changes throughout their life cycle (synthesis preparation, storage, reaction, and regeneration). Findings from this work will provide design principles for the synthesis of more defined solid acid catalysts.

2:20 PM **Thu-551AB-1420** Adsorption and Desorption of Decalin, Water and Cyclohexanol in Zeolites by in Situ 2H MAS NMR and Computational Modeling.

**Wenda Hu**[1,2], Nicholas Jaegers[1], Sungmin Kim[1], Giovannimaria Piccini[1], Feng Chen[1], Oliver Y. Gutierrez[1], Yue Liu[3], Qiang Liu[3], Donald M. Camaioni[1], Yong Wang[1,2], Johannes A. Lercher[1],[3] and Jian Zhi Hu[1,2], *(1)Pacific Northwest National Laboratory, USA, (2)Washington State University, USA, (3)Technical University of Munich, Germany*.

**Short Summary:**

$^2$H NMR indicates decalin in HMFI fills micropores followed by forming bulk phase. Adding cyclohexanol displaces decalin from micropores. More decalin retaining in HFAU leads to different pore environment. Adding cyclohexanol does not displace the hydronium ions. This work unraveled the adsorption/desorption of solvent in zeolites for understanding solvent-meditated dehydration.

2:40 PM **Thu-551AB-1440** Dehydroxylation: The Mechanism for Deactivation of Lewis Acid Y-BEA Zeolite in High-Temperature Steam.
**Fan Lin**[1], Meijun Li[2], Andrew Sutton[2], Junyan Zhang[2], Sungmin Kim[1], Zhenglong Li[2] and Huamin Wang[1], *(1)Pacific Northwest National Laboratory, USA, (2)Oak Ridge National Laboratory, USA*.

**Short Summary:**
We demonstrated that dehydroxylation is the mechanism for hydrothermal deactivation of the yttrium-modified zeolite (Y-BEA) in high-temperature steam. Steaming causes the surface of Y-BEA to undergo hydration-rearrangement-condensation, which eventually leads to the loss of OH groups, turning the Lewis acidic open site $(SiO)_2YOH$ into the non-acidic closed site $(SiO)_3Y$.

3:00 PM **Thu-551AB-1500** Hierarchical Zeolites by Desilication: The Reaction Details Revealed by *In-Situ* MAS NMR.
**Nina Tsereshko**, Sang-Ho Chung, Teng Li and Javier Ruiz-Martinez, *King Abdullah University of Science and Technology (KAUST), Saudi Arabia*.

**Short Summary:**
Zeolite desilication provides a highly interconnected hierarchical structure that enhances catalytic performance. However, the molecular understanding of desilication is still unclear. This study aims to reveal the role of framework and extra-framework aluminum throughout desilication by *in-situ* $^{29}Si$ and $^{27}Al$ MAS NMR.

## Structure-Activity Relationships

Session Chairs: Nat Eagan, *Tufts University, USA* and Nicholas Jaegers, *University of California, Berkeley, USA*.

3:45 PM **Thu-551AB-1545** Atomic Control of Active Site Structure Uncovers Long-Range Effects in Olefin Hydrogenation.
**Griffin Canning**[1], Angela Nguyen[1], Kathryn MacIntosh[1], Haoran He[1,2], Anish Dasgupta[1], Michael Janik3 and Rob Rioux[1], *(1)Pennsylvania State University, USA, (2)BASF Corporation, USA, (3)The Pennsylvania State University, USA*.

**Short Summary:**
The Pd-Zn γ-brass system exposes isolated active sites with precisely tunable composition enabling fully coverage enumerated, experimentally verifiable mechanistic predictions. Low-nuclearity sites regulate the ethylene hydrogenation reaction mechanism via long-range effects despite C-H bond formation taking place only at high-nuclearity sites.

4:05 PM **Thu-551AB-1605** Interfacial Sites Determine Paths of O2 and $H_2$ Activation on Au Nanoparticles: Effects of Nanoparticle Size and Support Identity on O2 Reduction.
**Jason Adams**[1], Tomas Ricciardulli[2], Sucharita Vijayaraghavan[2], Abinaya Sampath3, Haoyu Chen[2] and David Flaherty[2], *(1)California Institute of Technology, USA, (2)University of Illinois Urbana-Champaign, USA, (3)University of Illinois at Urbana-Champaign, USA*.

**Short Summary:**
Supported Au nanoparticles determine the transformation of H-H, O-O, and O-H bonds during heterolytic reactions of $H_2$, $O_2$, and $H_2O$ at liquid-metal-support interfaces during the formation of $H_2O$ and $H_2O_2$. Basic and reducible supports favor the activation of O-O and H-H bonds, while acid and inert supports stabilize these bonds.

4:25 PM **Thu-551AB-1625** Effect of $H_2$ and Temperature on Shape and Reactivity of Supported Pt Nanoparticles.
Ricardo Pool Mazun[1], **Hung-Ling Yu**[1], Vinson Liao[2], Mi Yoo[1], Md Raian Yousuf[1], Salman A. Khan[2], Abhijit Shrotri[3], Adam Hoffman[4], Simon Bare[4], Dionysios Vlachos[2] and Ayman M. Karim[1], *(1)Virginia Polytechnic Institute and State University, USA, (2)University of Delaware, USA, (3)Hokkaido University, Japan, (4)SLAC National Accelerator Laboratory, USA*.

**Short Summary:**
The Effect of hydrogen and temperature on structure of supported Pt nanoparticles were investigated by spectroscopy and theoretical calculations. Reversible change in shape from hemispherical to a flat structure was demonstrated by spectroscopy. Additionally, the dependence of catalytic properties on cluster shape and size are further supported by DFT calculations.

4:45 PM **Thu-551AB-1645** Highly Active Geometry of Single Sn Atom Catalysts for $CO_2$ Activation.
**Jeongjin Kim**[1], Yi Tian[2], Sanjaya D. Senanayake[1] and Jose Rodriguez[1,2], *(1)Brookhaven National Laboratory, USA, (2)Stony Brook University, USA*.

**Short Summary:**
Scanning tunneling microscopy (STM) observations reveal the highly active geometry of atomically-dispersed single tin (Sn) model catalysts for carbon dioxide ($CO_2$) activation. Statistical analysis for the atom-resolved STM images of single Sn model systems supports evidence for the Sn-O geometries caused by $CO_2$ dissociation at 1 Torr $CO_2(g)$.

5:05 PM **Thu-551AB-1705** Propane Dehydrogenation on Pt Facets and Effect of $Al_2O_3$ Atomic Layer Deposition (ALD).
**Hoan Nguyen**, Sumandeep Kaur, Stuart Helikson and Líney Árnadóttir, *Oregon State University, USA*.

**Short Summary:**
Propane dehydrogenation is a promising pathway for the production of propylene. Herein we use DFT to explore propane dehydrogenation on $Al_2O_3$-supported Pt nanoparticles and effect of atomic layer deposition of alumina on the selectivity and productivity of propylene.

5:25 PM **Thu-551AB-1725** Dynamic Evolution of Pd Single Atoms on Anatase $TiO_2$ Support Determines the Reverse Water-Gas Shift Reaction Activity.
Linxiao Chen[1], Sarah Allec[1], Libor Kovarik[1], Deborah Meira[2], Adam Hoffman[3], Simon Bare[3], Roger Rousseau[1] and **Janos Szanyi**[1], *(1)Pacific Northwest National Laboratory, USA, (2)Argonne National Laboratory, USA, (3)SLAC National Accelerator Laboratory, USA*.

**Short Summary:**
The dynamic changes in single Pd atoms on anatase $TiO_2$ and its consequences on its RWGSR activity was investigated by detailed kinetic studies and comprehensive *in situ* characterization and theoretical modeling. The reduction of the $TiO_2$ support leads to Pd sites with unique electronic structure, thus, high reactivity in WGRSR.

# 552 AB

## THURSDAY MORNING

### Polymetallic Catalysts

Session Chairs: Praveen Bollini, *University of Houston, USA* and Alexis T. Bell, *University of California - Berkeley, USA*.

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9:30 AM ***KEYNOTE* Thu-552AB-0930 Computationally-Led Design and Experimental Realization of Catalysts of Ethylene Epoxidation. Anders Hellman**, *Chalmers University of Technology, Sweden*.

**Short Summary:**
We identified several novel catalyst formulations for ethylene epoxidation using computational methods and confirmed them via experiments. The formulations can be easily produced and scaled up, affordable and stable.

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10:10 AM **Thu-552AB-1010** Mechanistic Relationship between CO and $CO_2$ Hydrogenation on Co, Ni and Ni-Co Bimetallic Catalysts.
**Francisco Villagra**, Sebastián Godoy, Alejandro Karelovic and Romel Jiménez, *Universidad de Concepción, Chile*.

**Short Summary:**
The mechanistic relationship for the hydrogenation of CO and $CO_2$ over Ni, Co and Ni-Co catalysts was studied by kinetic, isotopic and operando-FTIR measurements. It is suggested that these share the rate-determining step and their activity depends on the nature of the sites involved and the adsorption strength of CO*.

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10:30 AM **Thu-552AB-1030** A Kinetic Analysis of CO Electro-Oxidation on Bimetallics: Understanding the Interplay of Bifunctional and Electronic Effects.
**Todd Whittaker**, Adam Baz, Taylor Spivey, Lindsey Hamblin and Adam Holewinski, *University of Colorado Boulder, USA*.

**Short Summary:**
In this talk we will discuss kinetic signatures of bifunctional mechanisms. We then experimentally investigate a series of $Ag_xPd_{1-x}$ alloy catalysts and compare their activities in CO electro-oxidation under a range of conditions to assess the extent to which enhancements may be attributed to bifunctional vs. electronic effects.

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10:50 AM **Thu-552AB-1050** Activity Enhancement in Au-Pd Bimetallic Systems As a Result of Co-Operation between Individual Redox Reactions.
**Isaac Daniel**, *Cardiff University, United Kingdom*.

**Short Summary:**
Spatial separation of supported Au and Pd results in heightened catalytic activity for the oxidative dehydrogenation of alcohols due to Co-Operative Redox Enhancement effects between metallic sites. Kinetic, thermochemical, and electrochemical evaluation shows that electrons produced during oxidation are consumed in an oxygen reduction reaction over a separate metallic site.

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11:10 AM **Thu-552AB-1110** Compositional Effects in the Direct Formation of $H_2O_2$ over AuPd Nanoparticles.
**Rasmus Svensson** and Henrik Grönbeck, *Chalmers University of Technology, Sweden*.

**Short Summary:**
This work highlights the importance of nanoparticle composition, and the importance of modeling multiple active sites, in the direct formation of $H_2O_2$ over AuPd alloys. Kinetic Monte Carlo simulations, based on first-principle calculations, are used to describe the kinetics over nanoparticles, and to compare with extended surfaces.

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11:30 AM WITHDRAWN: Active Site Requirements for Chemoselective Hydrogenation with Binary and Ternary Intermetallics.
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## THURSDAY AFTERNOON

### Catalyst Development for Conversion of Biomass-Derived Oxygenates

Session Chairs: Canan Sener, *University of Wisconsin Madison, USA* and Jean-Phillippe Tessonnier, *Iowa State University, USA*.

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1:20 PM **Thu-552AB-1320** Applied Potential Impacts the Cu Catalyst Fouling Mechanism during Electrochemical Reduction of Furfural.
**Andrew S. May** and Elizabeth Biddinger, *The City College of New York, CUNY, USA*.

**Short Summary:**
The fouling of Cu catalyst during the electrochemical reduction of furfural can lead to catalyst deactivation. We operated in conditions to intentionally promote fouling to investigate the mechanisms of fouling, and showed the applied potential impacts the mechanism of fouling and type of carbonaceous material formed on the Cu catalyst.

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1:40 PM **Thu-552AB-1340** Controlling C–O, C–C, and C–H Bond Scission Pathways on Metal-Modified Molybdenum Nitride Catalysts.
**William Porter**, Zhexi Lin and Jingguang Chen, *Columbia University, USA*.

**Short Summary:**
Tunable selectivity of Fe-, Cu-, and Pt-modified $Mo_2N$ is shown using isopropanol as a probe molecule, suggesting the potential of these catalysts for sustainable upgrading of biomass-derived oxygenates. Comparing results between model surfaces and powder catalysts demonstrates how model surface studies can inform the design of supported catalysts.

2:00 PM **Thu-552AB-1400** Insights into the Activity of Edge-Hosted Fe-N$_3$-C Catalysts for Catalytic Transfer Hydrogenation of Furfural.
**Piaoping Yang**, Stavros Caratzoulas and Dionysios Vlachos, *University of Delaware, USA*.

**Short Summary:**
We unraveled the structure-activity relationship of edge-hosted Fe-N$_3$ sites for the CTH reaction and established a relationship between the geometric structure and activity of Fe-N$_3$ sites. Moreover, we revealed the origin of the best active Fe-N$_3$ site by investigating the frontier orbitals of the Fe atom and the transition state.

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2:20 PM **Thu-552AB-1420** Spectroscopic Characterization of Inverse Catalysts.
**Sagar Sourav**[1], Yurong Wu[1], Jiahua Zhou[1], Alfred Worrad[1], Stavros Caratzoulas[1], Weiqing Zheng[1], George Tsilomelekis[2] and Dionysios Vlachos[1], *(1)University of Delaware, USA, (2)Rutgers, The State University of New Jersey, USA*.

**Short Summary:**
*In-situ/operando* spectroscopic characterization techniques, DFT calculations and probe reaction chemistry were engaged to understand the structure, activity and acidity of supported Pt-WOx inverse catalysts in controlled environmental conditions.

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2:40 PM **Thu-552AB-1440** The Role of Metal Cores on WOx/M Inverse Catalysts.
Jiahua Zhou, Siddharth Deshpande, **Weiqing Zheng** and Dionysios Vlachos, *University of Delaware, USA*.

**Short Summary:**
In this work, we demonstrate that Bronsted acidity on inverse catalysts can be tuned by orders of magnitude by catalyst pretreatment and judicious choice of the reaction conditions. Metal cores plays an improtant role and for the first time we elucidate the synergy between the metal and the overlayer oxide.

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3:00 PM **Thu-552AB-1500** Role of Phosphorous in Transition Metal Phosphides for Selective Hydrogenolysis of Hindered C–O Bonds.
**Conor Waldt**[1], Hansel Montalvo-Castro[1], Abdulrahman Almithn[1,2], Alvaro Loaiza[3], Craig Plaisance[3] and David Hibbitts[1], *(1)University of Florida, USA, (2)King Faisal University, Saudi Arabia, (3)Louisiana State University, USA*.

**Short Summary:**
The incorporation of P into Ni catalysts causes shifts in selectivity toward cleavage of sterically hindered C–O bonds in 2-methyltetrahydrofuran (MTHF). We explore structure-function relationships on materials isostructural to Ni2P to decouple electronic and geometric effects to provide rationale for the role of P in transition metal phosphide catalysts.

## Direct Conversion of Whole Biomass, Polysaccharides, and Carbohydrates

Session Chairs: Ana Morais, *National Renewable Energy Laboratory, USA* and Bert M. Weckhuysen, *Utrecht University, Netherlands*.

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3:45 PM **Thu-552AB-1545** Continuous Flow Valorization of Aqueous Cellulosic Biomass Feeds to Isosorbide with Sustainable Heterogeneous Catalyst.
**Majd Al-Naji**[1,2], Francesco Brandi[2,3,] Ibrahim Khalil[3] and Markus Antonietti[2], *(1)Technische Universität Berlin, Germany, (2)Max Planck Institue of Colloids and Interfaces, Germany, (3)KU Leuven, Belgium*.

**Short Summary:**
Synopsis – Sustainable and selective synthesis of isosorbide from an aqueous solution of sorbitol in a continuous-flow system using β zeolite.

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4:05 PM **Thu-552AB-1605** Selective Synthesis of Chitin-Oligosaccharides By Mechanochemical Hydrolysis over a Carbon-Based Catalyst.
**Atsushi Fukuoka**[1] and Hirokazu Kobayashi[2], *(1)Hokkaido University, Japan, (2)The University of Tokyo, Japan*.

**Short Summary:**
An activated carbon catalyst having weak acid sites hydrolyzes chitin to chitin-oligosaccharides selectively in the presence of mechanical milling. This catalyst preferentially cleaves large molecules over small oligomers, thus maximizing the selectivity and yield of chitin-oligosaccharides. Carbons easily adsorb large polysaccharides, and AC-Air can hydrolyze large polymers to small oligomers.

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4:25 PM **Thu-552AB-1625** One-Pot Synthesis of Liquid Fuel By Conversion of Lignocellulosic Biomass over Ni/H-β Zeolite.
**Odiri Siakpebru**[1], Lakshmiprasad Gurrala[1], Anoop Uchagawkar[2], Prashant Niphardkar[3], Piersen Adamson[1], Nicholas Gorschak[1], Adam Hassiba[1], Jared Bartlett[1], Vijay Bokade[3], Bala Subramaniam[2] and Ana Morais[1], *(1)University of Kansas, USA, (2)The University of Kansas, USA, (3)CSIR - National Chemical Laboratory, India*.

**Short Summary:**
The carbohydrate fraction in lignocellulosic biomass was selectively converted to liquid hydrocarbons with the retention of lignin.
The catalytic HDO of poplar using 10%Ni/H-w resulted in high selectivity to cycloalkanes.
The Lewis to Brønsted acid ratio plays a key role in the hydrogenolysis of C-O bonds present in sugars.

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4:45 PM **Thu-552AB-1645** In-Situ Catalytic Hydrotreating and Hydrocracking of Hydrothermal Liquefaction Biocrude for the Production of Liquid Transportation Fuels.
**Venu Babu Borugadda**, Thomas Conway and Ajay K Dalai, *University of Saskatchewan, Canada*.

**Short Summary:**
This study focused on the production of renewable fuels from agricultural residues via hydrothermal liquefaction followed by upgrading into transportation fuels. Biocrude is posing challenges such as high acid number, carbon chain length and viscosity. To overcome these challenges, in-situ hydrotreating, cracking was carriedout for biocrude blends with refinery distillates.

5:05 PM **Thu-552AB-1705** Maximizing Sustainable Aviation Fuel Production through Optimized Hydroprocessing of Bio-Oils.
**Jostein Gabrielsen**, Kasper Hartvig Lyng Lejre and Magnus Stummann, *Topsoe A/S, Denmark*.

**Short Summary:**
In this study, the target was to produce maximum sustainable aviation fuel yield while minimizing the loss of overall liquid fuels consisting of both sustainable aviation fuel and renewable diesel. This is best done in hydroprocessing using a bi-functional catalyst or catalyst system tailor-made to minimize yield loss.

5:25 PM **Thu-552AB-1725** Intermediate-Inspired Selectivity Control Strategies for the Catalytic Reductive Amination of Carbohydrate Toward Ethylene Polyamines.
**Benjamin Vermeeren** and Bert F. Sels, *KU Leuven, Belgium*.

**Short Summary:**
Recently, the synthesis of bio-based amines via catalytic reductive amination of carbohydrates has gained increasing interest, however, predominantly focusing on ethanolamine formation. Here, we report the selective formation of ethylene polyamines by three bottom-up strategies, each targeting a selectivity-controlling step in the reaction pathway via in-depth mechanistic insights.

## 555 AB

### THURSDAY MORNING

### Selective Oxidation Catalysis

Session Chairs: Stephanie Kwon, *Colorado School of Mines, USA* and Brent Handy, *Universidad Autónoma de San Luis Potosí, Mexico*.

9:30 AM **Thu-555AB-0930** Elucidating Facet-Dependent Redox Properties of Anatase $TiO_2$.
**Anthony Savoy**[1], Wenda Hu[2], Junrui Li[1], Libor Kovarik[2], Chaochao Dun[3], Jeffery Urban[3], Jian Zhi Hu[1], Junming Sun[1] and Yong Wang[2], *(1)Washington State University, USA, (2)Pacific Northwest National Laboratory, USA, (3)Lawrence Berkeley National Laboratory, USA*.

**Short Summary:**
To eliminate the impacts of surface heterogeneity on model catalytic surfaces, $SiO_2$ was grafted onto faceted anatase $TiO_2$ nanoparticles by selectively consuming step-edge bound hydroxyls. By passivating the contributions of step-edge sites during methanol oxidation, a more representative assessment of (101) vs (001) redox properties was obtained.

9:50 AM **Thu-555AB-0950** Implications of Pore Structure and Coordination Environment for Green Alkene Oxidation over Iron-Based Metal-Organic Frameworks.
**Rachel Yang** and Michele Sarazen, *Princeton University, USA*.

**Short Summary:**
Isometallic iron-based, carboxylate metal-organic frameworks $NH_2$-MIL-101, MIL-101, and MIL-100 are investigated for probe liquid-phase styrene oxidation by hydrogen peroxide at mild reaction conditions and differences in reactivity and selectivity are elucidated as a function of coordination environment and framework pore sizes.

10:10 AM **Thu-555AB-1010** Surface Coverage Effects for Selectivity in Vinyl Acetate Synthesis.
**Gregory Novotny**, Zhaoru Zha and Prashant Deshlahra, *Tufts University, USA*.

**Short Summary:**
Experiment and theory are used to develop a mechanistic framework that describes the effects of surface coverage on rates and selectivity for vinyl acetate synthesis on Pd(111), which can be used to identify new catalysts by incorporating relevant complexities of both coverage and composition in highly crowded surfaces.

10:30 AM ***KEYNOTE*** **Thu-555AB-1030 Selective Oxidations over Nanostructured and Well-Defined Oxide Catalysts.**
**Justin Notestein**, *Northwestern University, USA*.

**Short Summary:**
This Keynote will discuss approaches to the synthesis, characterization, and catalytic testing of well-defined and nanostructured oxide catalysts for the improved production of feedstock and intermediate chemicals via selective oxidation.

11:10 AM **Thu-555AB-1110** Poisoning Effect in the Oxidation of Higher Chain Alcohols over Dilute PdAu Alloy Catalysts.
**Jennifer Lee**[1], Amanda Filie[1], Karin Nguyen[1,2], Leigh Wilson[1], Tanya Shirman[1], Joanna Aizenberg[1], Cynthia Friend[1] and Robert Madix[1], *(1)Harvard University, USA, (2)University of Freiburg, Germany*.

**Short Summary:**
This work provides molecular-level evidence for the presence of surface-bound carboxylate species on Pd active sites during higher chain alcohol oxidation reactions over $Pd_3Au_{97}$ dilute alloy catalysts prepared using the raspberry colloid templated method and demonstrates the sensitivity of dilute alloy catalyst reactivity to molecular structure.

11:30 AM **Thu-555AB-1130** Niobium-Insertion into $\alpha_{II}$-$VOPO_4$: Tuning Catalytic Properties for Selective Oxidation.
**Frederik Rüther**[1], Rhea Machado[1], Esteban Gioria[1], Sylvia Lorraine Kunz[2], Knut Wittich[3], Patricia Löser[3], Raoul Naumann d'Alnoncourt[1], Michael Geske[1], Stephan Andreas Schunk[3,4], Robert Glaum[2] and Frank Rosowski[1,5], *(1)BasCat - UniCat BASF JointLab, Technische Universität Berlin, Germany, (2)Rheinische Friedrich-Wilhelms-Universität Bonn, Germany, (3)hte GmbH, Germany, (4)Universität Leipzig, Germany, (5)BASF SE, Catalysis Research, Germany*.

**Short Summary:**
In this work, catalyst design rules for more selective oxidations are derived from the study of $(V_{1-x}Nb_x)OPO_4$, a bulk material with tunable catalytic properties in *n*-butane oxidation. Clear property-performance correlations confirm site isolation and the electronic environment of the near-surface V as key catalytic properties for maleic anhydride formation.

## THURSDAY AFTERNOON

### Electrochemical $CO_2$ Conversion I

Session Chairs: Nirala Singh, *University of Michigan-Ann Arbor, USA* and Shu Hu, *Yale University, USA*.

1:20 PM **Thu-555AB-1320** Interfacial Engineering of Metal/Mxene Heterostructures for Electrochemical $CO_2$ Reduction to $C_1$ Products and Beyond.
**Lavie Rekhi**[1], Luan Q. Le[1] and Tej Choksi[1,2], *(1)Nanyang Technological University, Singapore, (2)Cambridge Centre for Advanced Research and Education, Singapore*.

**Short Summary:**
Tuning the electronic interactions at metal/MXene heterostructures alters their selectivity for the electrochemical reduction of $CO_2$ to syn-gas, CO, or $C_{1+}$ products. Trends in selectivity are systematized using linear scaling relations within a descriptor-based approach. A simple model to estimate the stability of metal/MXene heterostructures is also introduced.

1:40 PM **Thu-555AB-1340** Transient Kinetic Isotope Measurements Reveal Interfacial pH Swings during Electrocatalysis.
**Max Hulsey** and Yogesh Surendranath, *Massachusetts Institute of Technology, USA*.

**Short Summary:**
Interfacial pH swings determine the energy efficiency and reaction kinetics of essentially all electrocatalytic reactions. Few approaches have been reported to directly measure pH changes under electrolysis conditions. We here determine pH swings by the uptake of an acidic gas such as $CO_2$ under hydrogen evolution conditions by mass spectrometry.

2:00 PM ***KEYNOTE*** **Thu-555AB-1400 Electrochemical Systems for Carbon Dioxide Utilization. Feng Jiao**, *University of Delaware, USA*.

**Short Summary:**
We will present our recent work on a two-step tandem $CO_2$ electrolysis system, which allows us to achieve an acetate selectivity as high as 55% at high purities and concentrations. The $CO_2$-derived acetate made it possible to create an electrochemical-biological hybrid approach to produce foods from $CO_2$.

2:40 PM **Thu-555AB-1440** In-Situ Mass Transfer Characteristics in a $CO_2$RR MEA Gas Diffusion Electrode.
**Yi Xu**[1], Daniel Lee[1] and Thomas F. Jaramillo[2], *(1)Stanford University, USA, (2)SLAC National Accelerator Laboratory, USA*.

**Short Summary:**
This work demonstrates a novel platform that allows in-situ characteristics of the $CO_2$RR mass transfer mechanism in the gas diffusion electrode microporous confinements. The observation result and mechanism model are critical for $CO_2$RR catalyst and electrolyzer designs.

3:00 PM **Thu-555AB-1500** Insights into the Electrified Interface in $CO_2$ Reduction Catalysis Using Operando ATR-SEIRAS.
**Thomas F. Jaramillo**[1], Jaime Avilés-Acosta[1], Jesse Matthews[1], John Lin[1], Daniel Lee[1], Christopher Hahn[2] and Adam Nielander[3], *(1)Stanford University, USA, (2)Lawrence Livermore National Laboratory, USA, (3)SLAC National Accelerator Laboratory, USA*.

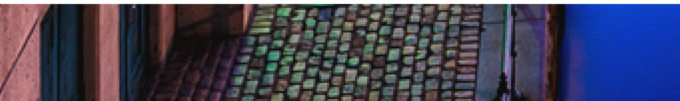
**Short Summary:**
Electrochemical carbon dioxide reduction ($CO_2$R) enables the sustainable production of chemicals and fuels from $CO_2$. Understanding the reaction microenvironment is key to enabling improved catalysis. Attenuated total reflectance – surface enhanced infrared absorption spectroscopy (ATR-SEIRAS) is developed and employed to elucidate relationships between activity, selectivity, and the microenvironment.

### Electrochemical $CO_2$ Conversion II

Session Chairs: Hongliang Xin, *Virginia Polytechnic Institute and State University, USA* and Charles T. Campbell, *University of Washington, USA*.

3:45 PM **Thu-555AB-1545** The Enhanced Performance and Stability of Metal-Free Ordered Mesoporous Nitrogenous Carbons for Oxygen Reduction Reaction.
Talla Mohan[1] and **Parasuraman Selvam**[2], *(1)Indian Institute of Technology Madras, India, (2)Kumamoto University, Japan*.

**Short Summary:**
Metal-free carbon-based electrocatalysts exhibit remarkable performance and activity retention for ORR, which may be useful in developing commercially viable alkaline fuel cells.



4:05 PM **Thu-555AB-1605** Understanding and Controlling Chemical Transformations and Fuel Synthesis at Electrocatalytic Interfaces.
**Marcel Schreier**, *University of Wisconsin-Madison, USA; University of Wisconsin-Madison, USA*.

**Short Summary:**
Producing fuels and chemicals using renewable electricity holds the promise to enable a sustainable economy. I will show how fundamental understanding of the interfacial processes occurring in electrocatalytic reactions, such as $CO_2$ reduction, can be exploited to expand the reaction scope of electrocatalysis to the transformation of complex substrates.

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4:25 PM **Thu-555AB-1625** Enhanced $CO_2$ Capture and Conversion at Organic Ligands - Inorganic Surface Interfaces.
Mingyu Wan, Zhiyong Gu and **Fanglin Che**, *University of Massachusetts Lowell, USA*.

**Short Summary:**
This theoretical work presents a future ligand-modulated electrocatalyst design, which could promoted $CO_2$ capture, first-proton transfer activation, and its selectivity to $C_2$ via providing dual organic-inorganic active sites at the aminothiolate/Cu interface.

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4:45 PM **Thu-555AB-1645** DFT Study of Electro-Organocatalysts for Reduction of $CO_2$ to Multicarbon Products.
**Craig Plaisance** and Foroogh Khezeli, *Louisiana State University, USA*.

**Short Summary:**
In this study, we designed a hybrid system by using organocatalyst which was able to reduce $CO_2$ to C-H bond products at reasonable pH and potential and it also showed the potential to form multicarbon products via reductive aldol condensation.

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5:05 PM **Thu-555AB-1705** Halogen-Incorporated Sn Catalysts for Selective Electrochemical $CO_2$ reduction to Formate.
**Tian Wang**[1], Hongbin Yang[2], Bin Liu[3] and Sibudjing Kawi[1], *(1)National University of Singapore, Singapore, (2)Suzhou University of Science and Technology, China, (3)Nanyang Technological University, Singapore*.

**Short Summary:**
In this work, the introduction of halogen into Sn effectively tuned the electronic structure, greatly promoted the adsorption of *OCHO while suppressed the *CO adsorption, which significantly boosted the production of formate. The dynamic evolution of catalyst under cathodic potential is also monitored.

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5:25 PM **Thu-555AB-1725** Heterostructured Bi-$Cu_2s$ Nanocrystals for Efficient $CO_2$ Electroreduction to Formate.
**Xue Han**[1] and Huiyuan Zhu[2], *(1)Virginia Polytechnic Institute and State University, USA, (2)University of Virginia, USA*.

**Short Summary:**
We have reported a one-pot synthesis of heterostructured Bi-$Cu_2S$ nanocrystals for the $ECO_2RR$ toward formate production. This work highlights a unique design strategy of *p*-block metal and TMC heterostructures to fine tailor active sites for advanced electrocatalysis.

## 556 AB

### THURSDAY MORNING

### Design and Synthesis of Single-Atom & Cluster Catalysts

Session Chairs: Casey O'Brien, *University of Notre Dame, USA* and Chae Jeong-Potter, *National Renewable Energy Laboratory, USA*.

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9:30 AM **Thu-556AB-0930** Strikingly Distinct Behaviors of Pt Single Atoms with Fine-Tuned Coordination Environments in Different Catalytic Oxidation Reactions.
Wei Tan[1,2], Shaohua Xie[1], Duy Le[1], Dave Austin[1], Sampyo Hong[3], Fei Gao[2], Lin Dong[2], Talat Rahman[1] and **Fudong Liu**[1], *(1)University of Central Florida, USA, (2)Nanjing University, China, (3)Brewton-Parker College, USA*.

**Short Summary:**
$CeO_2$ supported Pt single atom ($Pt_1$) catalysts with precisely tuned coordination environments were successfully constructed by a simple calcination temperature-control strategy, which exhibited strikingly distinct behaviors for CO oxidation and $NH_3$ oxidation due to the different $Pt_1$ local coordination structures and their different privileges in reactants activation and $H_2O$ desorption.

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9:50 AM **Thu-556AB-0950** The Encapsulation of Metal Nanoclusters into Zeolites to Fabricate Tailor-Made Catalysts and Adsorbents.
**Zhendong Liu**, *Tsinghua University, China*.

**Short Summary:**
Encapsulating of metal nanoclusters into zeolites combines the merits of both parts and greatly enriches their functionalities. New synthesis methods are significant to fabricating such bifunctional materials, tailoring their properties and opening up new applications. This talk focuses on how to create this class of materials for catalysis and adsorption.

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10:10 AM **Thu-556AB-1010** Role of Ceria-Supported Single Atoms in Hydrogenation Reactions.
**Honghong Shi**, Linxiao Chen, Janos Szanyi, Libor Kovarik, Johannes A. Lercher and Oliver Y. Gutierrez, *Pacific Northwest National Laboratory, USA*.

**Short Summary:**
We use the hydrogenation of crotonaldehyde as a probe reaction to interrogate the nature of activated hydrogen and its transfer mechanisms to adsorbed organic molecules. Our work correlates the structural features of single atom catalysts with reaction kinetics to identify requirements at molecules and active sites for hydrogen transfer.

10:30 AM **Thu-556AB-1030** Reversible Transformation of Pt Single Atoms and Subnanometer Clusters Supported on CeOx Nanoglues: Contrasting Catalytic Properties for Ethylene Hydrogenation.
Yizhen Chen[1], Jiankang Zhao[2], Xiao Zhao[3], Xu Li[2], Nan Zhang[2], Jie Zeng[4], Miquel Salmeron[3], Jingyue Liu[5] and **Bruce Gates**[6], *(1)University of California - Davis, USA, (2)National Research Center for Physical Sciences at the Microscale, University of Science and Technology of China, Hefei, China, (3)Lawrence Berkeley National Laboratory, USA, (4)University of Science and Technology of China, China, (5)Arizona State University, USA, (6)University of California, Davis, USA*.

**Short Summary:**
The data provide a rigorous, fundamental comparison of the catalytic properties of isolated Pt cations and subnanometer Pt clusters isolated and stabilized on $CeO_x$ islands stably dispersed on $SiO_2$—the catalysts were stable in (low-temperature) operation but were reversibly and repeatedly interconverted by high-temperature reduction/oxidation treatments.

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10:50 AM **Thu-556AB-1050** Defective Ceria Created by Oxy-Hydrogen Flame and Its Influences on Pt Dispersion, Pt-Ceria Interaction and Catalytic Hydrogenation.
**Ali Kamali**[1] and Dongxia Liu[2], *(1)University of Maryland, College Park, USA, (2)University of Maryland, USA*.

**Short Summary:**
The simple oxy-hydrogen flame treatment used to create defects (i.e., oxygen vacancies and $Ce^{3+}$ state) in ceria under vacuum condition. These defects are stable and enabled the reduced ceria substrate with a high redox capability. Consequently, defective Pt/ceria enabled strong metal-support interaction and higher 3-VA selectivity in 3-NS hydrogenation.

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11:10 AM **Thu-556AB-1110** Successive Strong Electrostatic Adsorptions of $[RhCl_6]^{3-}$) on $WO_x$-$CeO_2$ to Preserve Rh Clusters from Sintering Under $H_2$ at 600°C.
Jeffrey T. Miller[1], Neil Schweitzer[2], Mimoun Aouine[3], Philippe Vernoux[3], Abdelmalik Boufar[4], Juliette Blanchard[4], Jean-Marc Krafft[4], Christophe Méthivier[4], Céline Sayag[4], Mickaël Sicard[5], Frédéric Ser[5] and **Cyril Thomas**[4], *(1)Davidson School of Chemical Engineering, Purdue University, USA, (2)Northwestern University, USA, (3)Université de Lyon, CNRS, France, (4)Sorbonne Université, France, (5)ONERA, France*.

**Short Summary:**
The present study demonstrates that the presence of oxotungstates (1.3 W/nm2) coupled with the selective deposition of Rh on the $CeO_2$ surface (via successive strong electrostatic adsorptions of $[RhCl_6]^{3-}$) prevents Rh sintering after reduction at 600°C under $H_2$ compared to a W-free $CeO_2$ support.

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11:30 AM **Thu-556AB-1130** Highly Active and Stable Catalysts for Automobile Exhaust Treatment.
**Hao Xu**[1], Weixin Huang[1], Dong Jiang[1] and Yong Wang[1,2], *(1)Washington State University, USA, (2)Pacific Northwest National Laboratory, USA*.

**Short Summary:**
Well-controlled structural configuration of metal atoms is crucial for promoting catalytic activity and thermal stability for automobile exhaust aftertreatment. The developed methods including thermal-shock synthesis and support modification with a transition metal could lead to the formation of stabilized active sites, which can also be applied to other catalytic systems.

## THURSDAY AFTERNOON

## Design and Synthesis of Supported Catalysts

Session Chairs: Biswanath Dutta, *National Energy Technology Laboratories, USA* and Kostas Goulas, *Oregon State University, USA*.

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1:20 PM ***KEYNOTE*** **Thu-556AB-1320 Designing Multifunctional Catalysts for Cascade Reactions and Biorefining. Karen Wilson** and Adam Lee, *Griffith University, Australia*.

**Short Summary:**
Biomass is a sustainable carbon source and low cost solution to transportation fuels and organic chemicals. Transformation of functional bioderived molecules may involve cascade processes, with multicomponent catalysts acting in concert to promote sequential reactions. This presenation will discuss innovations in catalyst/process design for cascade reactions of relevance to biorefineries.

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2:00 PM **Thu-556AB-1400** Synthesis Strategies for the Preparation of Supported Transition Metal Catalysts.
**Alyssa Love**, Stuart Soled, Vera Grankina and Chris Kliewer, *ExxonMobil Technology and Engineering Center, USA*.

**Short Summary:**
This work extends previously discovered use of bifunctional organics to the improved dispersion of noble metals on silica to the preparation of well-dispersed silica-supported transition metals (Co, Ni, Cu). The development of a gravimetric $N_2O$ chemisorption technique to quantitatively assess metal dispersion is also highlighted.

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2:20 PM **Thu-556AB-1420** Synthesis and Characterization of Zeolite-Supported Platinum Catalysts with Controlled Platinum Nanoparticle Locations.
Kaan Yalcin[1], Noah Felvey[1], Ram Kumar[2], **Alexander Katz**[2], Bruce Gates[3], Ambarish Kulkarni[3], Ron Runnebaum[1] and Coleman Kronawitter[3], *(1)University of California, Davis, USA, (2)University of California, Berkeley, USA, (3)University of California - Davis, USA*.

**Short Summary:**
Noble-metal-containing zeolites are widely used hydrocarbon-conversion catalysts, having activities and stabilities during reduction/oxidation (reaction/regeneration) cycles that depend on the metal particle size and location (inside or outside the zeolite)—and we show how to control these by choice of synthesis conditions for Pt/HZSM-5.

2:40 PM **Thu-556AB-1440** Hydrogenation of Dimethyl Oxalate to Ethylene Glycol over $SiO_2$-Supported Cu- and Ag-Based Catalysts: Insights and Prospects.
Nicolas Gleason-Boure, Xinbin Yu and **Christopher Williams**, *University of South Carolina, USA*.

**Short Summary:**
Hydrogenation of dimethyl oxalate (DMO) to ethylene glycol (EG)nis successfully used in industry and its performance has been significantly improved via modification of preparation methods, promoters, and support. Through synthesis, characterization, and evaluation of Cu- and Ag-based catalysts, the interplay of oxidation state, hydrogen activation, and support structure is elucidated.

3:00 PM **Thu-556AB-1500** Effects of Titania Structure on Rh and Ir Catalysts – Strategies for Tuning the Selectivity Toward Hyperpolarized Hydrogenation Products for Parahydrogen-Enhanced Nuclear Magnetic Resonance.
**Helena Hagelin-Weaver**, Hanqin Zhao, Michelle Lapak, Bochuan Song, Diana Choi and Clifford R. Bowers, *University of Florida, USA*.

**Short Summary:**
Rhodium and iridium catalysts supported on anatase and rutile titania nanoparticles were synthesized and tested for activity and pairwise selectivity (addition of one parahydrogen molecule) in the hydrogenation of propene to hyperpolarized propane after reductive treatments at different temperatures. Both the titania structure and the reduction temperature influence the selectivity.

## Design and Synthesis of Bulk Materials

Session Chairs: Al Maglio, *BASF, USA* and Dmitry Murzin, *Åbo Akademi University, Finland*.

3:45 PM **Thu-556AB-1545** Probing the Intrinsic Activity of Nanofacets on Anatase $TiO_2$ Nanocrystals Synthesized Using Strongly Bonded F–.
**Junrui Li**[1], Anthony Savoy[1], Wenda Hu[2], Chaochao Dun[3] and Yong Wang[1], *(1)Washington State University, USA, (2)Pacific Northwest National Laboratory, USA, (3)Lawrence Berkeley National Laboratory, USA*.

**Short Summary:**
We report a facile method to remove the F– that is commonly used in the synthesis of $TiO_2$ nanofacets without damaging well-defined morphologies. F– has been found to significantly enhance the dehydration rate for methanol and isopropanol reactions, while clean $TiO_2$ nanofacet has intrinsically higher oxidative dehydrogenation rate.

4:25 PM **Thu-556AB-1625** Transforming $CeO_2$ Nanoparticles into Atomically Dispersed Ce+3 Ions on Alumina Significantly Enhances Catalytic Activity.
**Konstantin Khivantsev**[1], Hien Pham2, Mark Engelhard[1], Hristiyan Aleksandrov[3], Georgi Vayssilov[3], Shari Li[1], Jeffrey T. Miller[4], Yipeng Sun[5], Pascaline Tran[5], Janos Szanyi[1], Abhaya Datye2 and Yong Wang[1], *(1)Pacific Northwest National Laboratory, USA, (2)University of New Mexico, USA, (3)University of Sofia, Bulgaria, (4)Davidson School of Chemical Engineering, Purdue University, USA, (5)BASF Corporation, USA*.

**Short Summary:**
Our findings highlight previously unknown phenomena that explain how ceria/alumina (TWC and CO oxidation) catalysts respond dynamically to varying atmospheres and maintain high activity even after exposure to extreme aging conditions.

4:45 PM **Thu-556AB-1645** Synthesis of Hierarchical Siliceous Zeolites By Post-Synthetic Surfactant Templating.
**Kaivalya Gawande**, Wei Fan and William Curtis Conner, *University of Massachusetts Amherst, USA*.

**Short Summary:**
Surfactant-templating is a promising method to synthesize hierarchy in microporous zeolites but the lack of fundamental understanding of the mechanism limits its application to an array of industrially relevant aluminosilicates. And hence we reported a meticulous study of the effect of various parameters involved to understand the phenomenon in detail.

5:05 PM **Thu-556AB-1705** Comparison of Sn Electrocatalyst Thin Films for ATR-FTIR Applications in $CO_2$ Reduction.
**Yuval Fishler**[1,2,3], Adam Holewinski[1] and Wilson Smith[1], *(1)University of Colorado Boulder, USA, (2)Renewable and Sustainable Energy Insitute, USA, (3)National Renewable Energy Laboratory, USA*.

**Short Summary:**
In this work we established a synthesis route for electrocatalysts for ATR-FTIR and ATR-SEIRAS methods. Specifically for $CO_2$ conversion mechanistic insights purposes.

5:25 PM **Thu-556AB-1725** Self-Assembled $SiO_2$ Nanoparticles as Ordered Mesoporous Support Material for Ni/$SiO_2$ Heterogeneous Catalysts.
**Kelly J.H. Brouwer**, Kristiaan H. Helfferich, Petra E. de Jongh and Alfons van Blaaderen, *Utrecht University, Netherlands*.

**Short Summary:**
Self-assembly of nanoparticles is a powerful technique to build ordered mesoporous support materials. By combing monodisperse $SiO_2$ nanoparticles, support materials can be formed with 3D ordered pores, great synthetic control and tunable (meso)pore size. In this work we focus on Ni/$SiO_2$ catalysts made by self-assembly of monodisperse $SiO_2$ nanoparticles.

4:05 PM **556-AB-1605** Catalytic Sites Contiguity Study of the Ni/MgO-$Al_2O_3$ Catalyst for $CO_2$ Reforming of $CH_4$ Using STEM-EDX.
**Hui Wang**[1], Christian Patzig[2] and Yongfeng Hu[1], *(1)University of Saskatchewan, Canada, (2)Fraunhofer Institute for Mechanics of Materials, Germany*.

**Short Summary:**
*Catalytic Sites Contiguity* was created to describe the geographical orientation of the catalytic sites on the catalyst surface and the mutual accessibility of the adsorbed species. This presentation reports the visual study of the catalytic sites contiguity of Ni/MgO-$Al_2O_3$ catalyst that we developed for $CO_2$ reforming of methane using STEM-EDX.

# Ballroom A

## THURSDAY MORNING

### Alkane Dehydrogenation III

Session Chairs: Viktor Cybulskis, *Syracuse University, USA* and Daniel Curulla-Ferre, *TotalEnergies, Belgium*.

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9:30 AM **Thu-BLRMA-0930** Synthesis of SBA-15 Supported Metals and Metal Oxides by Atomic Layer Deposition for High Pressure Reactions.
**Ching-Yu Wang**, Raymond J. Gorte and John M. Vohs, *University of Pennsylvania, USA*.

**Short Summary:**
In this work, we have modified the surface of SBA-15 with metal oxides by ALD and incorporated catalytic metals into SBA-15 by vapor phase infiltration. Pt/SBA-15 deactivated rapidly at lower pressures but was stable at higher pressures. Such behavior can be attributed to uniform mesopore structure of SBA-15.

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9:50 AM **Thu-BLRMA-0950** From Pulses to Pellets to Packed Beds: Understanding $CrO_x/Al_2O_3$ Catalyst Deactivation during Propane Dehydrogenation through Transient Kinetic Analysis and Multiscale Modeling.
**Nicholas Thornburg**[1], Meagan F. Crowley[1], Adam C. Yonge[2], Hariswaran Sitaraman[1], Dingqi Nai[2], M. Ross Kunz[3], Yu-Yen Chen[3], Rong Xing[4], Mingyong Sun[4], Lars Grabow[5], Rebecca Fushimi[3], Andrew Medford[2] and Peter N. Ciesielski[1], *(1)National Renewable Energy Laboratory, USA, (2)Georgia Institute of Technology, USA, (3)Idaho National Laboratory, USA, (4)Clariant Corporation, USA, (5)University of Houston, USA*.

**Short Summary:**
This presentation leverages dynamic catalyst science experiments and informatics-based mechanism determination to develop transient multiscale models that predict supported $CrO_x/Al_2O_3$ catalyst deactivation phenomena for industrial propane dehydrogenation. These findings provide actionable physicochemical insights into catalyst evolution to guide practical improvements for advantaged catalyst formulation and commercial reactor operation.

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10:10 AM **Thu-BLRMA-1010** PtSn/DeAlBEA Catalysts for Propane Dehydrogenation.
**Natalie Lefton** and Alexis Bell, *University of California, Berkeley, USA*.

**Short Summary:**
PtSn/DeAlBEA catalysts show evidence for highly dispersed platinum species at low loadings (CO-FTIR). The TOF for propane dehydrogenation is highest for the lowest Pt/Al ratio. Kinetic studies suggest that the reaction occurs over a single Pt site, independent of Pt/Al and consistent with small nanocluster formation at higher Pt/Al ratios.

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10:30 AM **Thu-BLRMA-1030** Microwave-Assisted Direct Propane Dehydrogenation over $PtSn/SiO_2$ Catalysts.
**Yeonsu Kwak**[1], Cong Wang[1], Kewei Yu[1], Weiqing Zheng[1], Himanshu Goyal[2] and Dionysios Vlachos[1], *(1)University of Delaware, USA, (2)Indian Institute of Technology Madras, India*.

**Short Summary:**
This work features microwave irradiation (MW) for nonoxidative propane dehydrogenation (PDH). To exclude localized thermal effects, MW is investigated at a representative temperature setup and compared with conventional heating. The intact active site density of PtSn nanoparticles originates the remarkable durability of MW PDH at low temperatures without $H_2$ addition.

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10:50 AM **Thu-BLRMA-1050** Highly Selective Propane Dehydrogenation with Dilute Pt-Cu Alloy Catalysts.
**Baraa Werghi**[1], Shikha Saini[2], Pin-Hung Chung[1], Frank Abild-Pedersen[2], Simon Bare[2] and Matteo Cargnello[1], *(1)Stanford University, USA, (2)SLAC National Accelerator Laboratory, USA*.

**Short Summary:**
We present the catalytic behavior of novel γ-alumina-supported platinum/copper nanocrystals (NC) prepared by a colloidal approach affording particles with controlled size and composition. We tailored the design of our bimetallic catalyst to generate Cu rich structures that showed remarkable enhancement in the reaction activity and selectivity

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11:10 AM **Thu-BLRMA-1110** Co(II) Monomers Dispersed on $SiO_2$ and $Al_2O_3$ as Stable and Active Lewis Acid-Base Pairs for Alkane Dehydrogenation.
Nicholas Jaegers[1], Biswanath Dutta[1], Vardan Danghyan[1], Junnan Shangguan[1], **Carlos Lizandara**[2], Guang Miao[1], Joseph Dellamorte[2] and Enrique Iglesia[1], *(1)University of California, Berkeley, USA, (2)BASF Corporation, USA*.

**Short Summary:**
Co-catalyzed alkane dehydrogenation arises from the presence of dispersed Co(II) monomers which exhibit rates that exceed those of industrial catalysts. The developed synthetic protocol enables the control of the CoO domain distribution on the support surface to improve the utilization of a low-cost, stable catalyst for the alkane dehydrogenation reactions.

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11:30 AM **Thu-BLRMA-1130** Highly Dispersed $CO_2$+ Clusters As Coke-Resistant Catalyst for Selective Propane Dehydrogenation.
**Fabian Ebert**[1], Piyush Ingale[1], Geumah Lee[1], Sarah Vogl[2], Christopher Schlesiger[2], Sebastian Praetz[2], Michael Geske[1], Raoul Naumann d'Alnoncourt[1], Esteban Gioria[1], Arne Thomas[2] and Frank Rosowski[1,3], *(1)BasCat - UniCat BASF JointLab, Technische Universität Berlin, Germany, (2)Technische Universität Berlin, Germany, (3)BASF SE, Catalysis Research, Germany*.

**Short Summary:**
A catalyst with highly dispersed cobalt sites, incorporated into a mesoporous alumina structure was synthesized via a sol-gel route. The catalyst shows outstanding performance for propane dehydrogenation in terms of deactivation and coke formation. Characterizations evidence that the stabilized $CO_2$+ sites are responsible for the excellent performance.

# THURSDAY AFTERNOON

## Alkane Dehydrogenation IV

Session Chairs: Elaine Gomez, *ExxonMobil,* and John Barton, *The Dow Chemical Company, USA*.

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1:20 PM **Thu-BLRMA-1320** Effect of Dealumination on Acid-Base Characteristics of Zn-BEA Zeolites and Their Catalytic Performance in $CO_2$-Mediated Propane Dehydrogenation to Propylene.
**Stanislaw Dzwigaj**, *Sorbonne-Universite, France*.

**Short Summary:**
The results of this work indicate that regulation of acid-base characteristics of BEA zeolites by full dealumination provides an improved catalytic performance of ZnSiBEA in $CO_2$-PDH. The advantages of propylene production using Zn-BEA catalysts with the involvement of $CO_2$ are demonstrated.

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1:40 PM **Thu-BLRMA-1340** Non-Oxidative Propane Dehydrogenation to Propene over Anatase $TiO_2$-X.
Iqtidar Ali Khan, Asmae Bouziani and **Gokhan Celik**, *Middle East Technical University, Turkey*.

**Short Summary:**
We demonstrate the use of bulk titania as an active material for propane dehydrogenation. Titania samples were synthesized using sol-gel technique at different pH. The dehydrogenation activity tests over titania samples revealed a volcano-shaped curve of propene yield vs volume 1M HCl added during the sol-gel synthesis.

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2:00 PM **Thu-BLRMA-1400** Heterolytic C-H Activation Routes in Catalytic Dehydrogenation of C2–C7 Alkanes on Lewis Acid-Base Pairs at Chemically-Treated $ZrO_2$ Surfaces.
**Nicholas Jaegers**[1], Vardan Danghyan[1], Junnan Shangguan[1], Janik Hense[1], Prashant Deshlahra[2], Carlos Lizandara[3] and Enrique Iglesia[1], *(1)University of California, Berkeley, USA, (2)Tufts University, USA, (3)BASF Corporation, USA*.

**Short Summary:**
Kinetic assessments of alkane dehydrogenation rates on earth-abundant $ZrO_2$, possible only by exposing the active Lewis acid-base pairs, implicate C–H abstraction from the terminal methyl group to form a surface-stabilized carbanion as the rate determining step. The microscopic reversibility of the reaction enables the accurate prediction of alkene hydrogenation rates.

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2:20 PM **Thu-BLRMA-1420** Removal of Surface Titrants from Lewis Acid-Base Pairs By Thermal and Chemical Treatments: Catalytic Consequences for Propane Dehydrogenation Rates on $ZrO_2$.
**Vardan Danghyan**[1], Junnan Shangguan[1], Nicholas Jaegers[2], Joseph Dellamorte[3], Carlos Lizandara[3], Craig Cain-Borgman[3] and Enrique Iglesia[1], *(1)University of California, Berkeley, USA, (2)Pacific Northwest National Laboratory, USA, (3)BASF Corporation, USA*.

**Short Summary:**
Lewis acid-base pairs on $ZrO_2$ catalyze heterolytic cleavage of C–H bonds, but are titrated by $H_2O$ and $CO_2$. This study demonstrates that such titrants can be removed by chemical reactions. Exposure to dimethyl ether leads to >100-fold increase in propane dehydrogenation rates and to >99.7% propene selectivity at 723 K.

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2:40 PM **Thu-BLRMA-1440** Designing Highly Stable Catalysts for the Oxidative Dehydrogenation of Propane with Carbon Dioxide: Vanadium Supported in Microporous Materials..
Michiel Dusselier, Marco Rigamonti, Meera Shah and **Jose Mendoza Mesa**, *KU Leuven, Belgium*.

**Short Summary:**
A clear look into the desirable characteristics that an industrially viable ODPH catalyst should have. Vanadium supported in zeolites have superior stability owing to the high mitigation of coke formation, with high activity/selectivity in the direction of the defined milestones. These materials are on their way to industrial application.

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3:00 PM **Thu-BLRMA-1500** Hydroxylation-Dehydration Bifunctional Cascades for Catalytic Ethane Dehydrogenation on Cu-Redox and Brønsted-Acid Sites.
**Andrew Hwang**, Ihab Elmasri and Enrique Iglesia, *University of California, Berkeley, USA*.

**Short Summary:**
Reactions of ethane with dioxygen on Cu(II)-exchanged zeolites form ethene and $CO_2$ via bifunctional cascades involving Cu-mediated alkane hydroxylation and acid-mediated alkanol dehydration.

## Alkane Dehydrogenation (V), Catalytic Cracking and Isomerization

Session Chairs: Clark Miller, *Phillips 66, USA* and Siris Laursen, *University of Tennessee, USA*.

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3:45 PM **Thu-BLRMA-1545** Ga+-Exchanged Fe-Substituted Zeolites Are Highly Stable and Selective Catalyst for Propane Dehydrogenation.
**Yong Yuan** and Raul Lobo, *University of Delaware, USA*.

**Short Summary:**
Ga/[Fe]zeolites catalysts, inlcuding Ga/[Fe]Beta, Ga/[Fe]ZSM-5 and Ga/[Fe]-CHA, have been first discovered as an effective catalyst for propane dehydrogenation with high propylene selectivity (96%). It provides guidance for developing Ga-zeolites towards propane dehydrogenation via synthesizing heteroatom-containing zeolites instead of traditional Al-containing zeolites.

4:05 PM **Thu-BLRMA-1605** Metal-Doped AlN Catalysts for Propane Dehydrogenation.
**Mona Abdelgaid** and Giannis Mpourmpakis, *University of Pittsburgh, USA*.

**Short Summary:**
Catalytic propane dehydrogenation (PDH) holds great promise for filling the propylene supply-demand gap. We applied first-principles-based multiscale simulations and discovered novel metal-doped AlN PDH catalysts exhibiting high activity due to their ability to activate C-H bonds. The introduced AlN-based catalysts outperform in activity many other catalysts previously suggested in literature.

4:25 PM **Thu-BLRMA-1625** Ceramic Membrane Reactor for *in Situ* High-Temperature $H_2$ Separation during Propane Dehydrogenation.
Isabel Ibarra[1], **Ryan Alcala**[1], Leonard Ruggiero[1], Ian Alsobrook[1], Abhaya Datye[1], Hiroki Nagasawa[2] and Jeffrey Brinker[1], *(1)University of New Mexico, USA, (2)Hiroshima University, Japan*.

**Short Summary:**
The use of hydrogen-selective molecular sieve type inert membranes under reaction conditions at high temperature (~500°C) will allow significantly higher yields at lower operating temperatures for endothermic dehydrogenation reactions. The portion of catalyst in contact with the membrane then promotes the forward reaction further upon the selective removal of $H_2$.

4:45 PM **Thu-BLRMA-1645** Performance Prediction of FCC SOx Reduction Additives: From Lab Bench Scale Microreactors to Commercial Units.
**Xunhua Mo**, Hongbo Ma, Charles Kanyi, Mehdi Allahverdi and Paul Diddams, *Johnson Matthey, USA*.

**Short Summary:**
This paper reports the development of performance evaluation protocols of Fluid Catalytic Cracking (FCC) SOx reduction additives using bench scale microreactors. Commercial trial data were used to validate the lab testing methodologies, and insights on the root causes leading to different performances under different conditions will also be addressed.

5:05 PM **Thu-BLRMA-1705** Role of Silica/Alumina Ratio (SAR) in ZSM-5 Frameworks in Catalyzing Isomerization vs. Cracking Reactions.
CP Kelkar and **James Fu**, *BASF Corporation, USA*.

**Short Summary:**
Although ZSM-5 has been extensively used in catalytic cracking, the role of acid site density (SAR) of ZSM-5 in catalyzing isomerization vs. cracking reaction is still unclear. This work will systematically compare performance of ZSM-5's with widely differing SAR's.

5:25 PM **Thu-BLRMA-1725** Cracking of Light Cycle Oil in Presence of Hydrogen Donor into BTX Fraction over Bifunctional Monometallic and Bimetallic Catalysts.
**Akshata Ramteke**, Divesh Bhatia and Kamal Pant, *Indian Institute of Technology Delhi, India*.

**Short Summary:**
Novel bifunctional catalysts are prepared for the selective hydrocracking of light cycle oil into monoaromatics such as benzene, toluene, and xylene. Instead of hydrogen at high pressure, a hydrogen donor is used to achieve a high BTX yield, which has a potential to reduce the costs of the overall process.

## Ballroom BC

### THURSDAY MORNING

### Advances in Operando X-Ray Absorption Spectroscopy

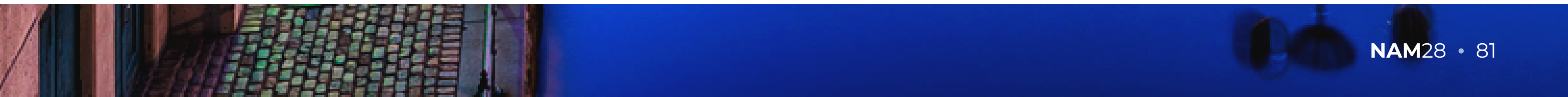
Session Chairs: David Yancey, *Dow, USA* and Jose Rodriguez, *Brookhaven National Laboratory, USA*.

9:30 AM **Thu-BLRMBC-0930** Limits of Detection for EXAFS Characterization of Single Atom Catalysts.
**Jordan Finzel**[1], Phil Christopher[2] and Simon Bare[3], *(1)University of California Santa Barbara, USA, (2)University of California, Santa Barbara, USA, (3)SLAC National Accelerator Laboratory, USA*.

**Short Summary:**
We determine limits of detection for clustered species when characterizing single atom catalysts using EXAFS. Metallic clusters can be identified as a subpopulation at ~10 at%, but oxidized clusters may elude detection even at 40%. Inherent properties of oxide structures can completely inhibit differentiation of small clusters and isolated species.

9:50 AM **Thu-BLRMBC-0950** Revealing Structural Complexity in Catalyst via Advanced X-Ray Absorption Spectroscopy Data Analysis.
**Jiyun Hong**, Adam Hoffman and Simon Bare, *SLAC National Accelerator Laboratory, USA*.

**Short Summary:**
X-ray absorption spectroscopy (XAS) is a valuable technique that can probe the catalyst structures. By applying advanced XAS data analysis methods, we should strive to fully interpret all the information that the XAS data entails and reveal structural complexity of catalyst in concrete detail.



10:10 AM **Thu-BLRMBC-1010** Quantifying the Site Heterogeneity in Atomically Dispersed Catalyst Using Automated Workflow for XAS Analysis.
**Rachita Rana**[1], Ambarish Kulkarni[2], Simon Bare[3] and Adam Hoffman[3], *(1)University of California, USA, (2)University of California - Davis, USA, (3)SLAC National Accelerator Laboratory, USA*.

**Short Summary:**
The goal of this talk is to demonstrate the ability of QuantEXAFS to measure the site heterogeneities using EXAFS and DFT. An automated workflow of combined experimental and computational methods to quantify sites in atomically dispersed catalysts, this leads to a better understanding of targeted site-controlled synthesis, activity, and stability.

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10:30 AM **Thu-BLRMBC-1030** Bridging the Gap between the X-Ray Absorption Spectroscopy and the Computational Catalysis Communities in Heterogeneous Catalysis: A Perspective on the Current and Future Research Directions.
**Ambarish Kulkarni**[1], Rachita Rana[1], Fernando Vila[2] and Simon Bare[3], *(1)University of California, Davis, USA, (2)University of Washington, USA, (3)SLAC National Accelerator Laboratory, USA*.

**Short Summary:**
Recognizing the tremendous impact of XAS and data-centric tools on catalysis science, it is now timely to examine the opportunities and challenges associated with using XAS to probe the structure and properties of the active site(s). This talk aims to bridge the gap between the theory and experimental researchers.

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10:50 AM **Thu-BLRMBC-1050** $CO_2$ Hydrogenation to Methanol over Silica Supported Ni-Ga Alloy Nanoparticles: On the Structural Factors Driving Catalyst Activity and Selectivity.
**Nora Zimmerli**, Lukas Rochlitz, Paula Macarena Abdala, Christoph Müller and Christophe Copéret, *ETH Zürich, Switzerland*.

**Short Summary:**
Here, we present a structure-performance analysis of Ni-Ga alloy nanoparticles (ca. 2 nm) supported on silica for the hydrogenation of $CO_2$ to methanol. We combine in-situ/operando X-ray total scattering with X-ray absorption and IR spectroscopies to resolve the structures of the catalysts at the nm and sub-nm scales.

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11:10 AM **Thu-BLRMBC-1110** Recent Developments of High-Resolution X-Ray Spectroscopic Methods for Catalysis at NSLS-II..
**Eli Stavitski**[1], David Dean[2], Denis Leshchev[1] and Jeffrey T. Miller[3], *(1)Brookhaven National Laboratory, USA, (2)Purdue University, USA, (3)Davidson School of Chemical Engineering, Purdue University, USA*.

**Short Summary:**
In this contribution we review recent innovations at the National Synchrotron Light Source II (NSLS-II) which enable applications of High Resolution X-ray spectroscopy to catalytic systems as well as several examples to demonstrate the advantages of these techniques.

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11:30 AM **Thu-BLRMBC-1130** Modulation Excitation XAFS Zooms in on Reaction-Induced Restructuring in Pd-Au Bimetallic Catalyst.
**Prahlad Kumar Routh**[1], Evgeniy Redekop[2], Maarten Nachtegaal[3], Adam Clark[4] and Anatoly Frenkel[1,5], *(1)Stony Brook University, USA, (2)University of Oslo, Norway, (3)Paul Scherrer Institute, Switzerland, (4)Paul Scherrer Institut, Switzerland, (5)Brookhaven National Laboratory, USA*.

**Short Summary:**
Direct measurement of the active species is a challenge, given the heterogeneity associated with active sites and the absence of a technique which can selectively measure the active species and its dynamic evolution as the reaction conditions progress. ME-XAFS shows such atmosphere-dependent dynamic characterization of active species in Pd-Au nanocatalysts.

## THURSDAY AFTERNOON

## Time-Resolved X-Ray Absorption Spectroscopy

Session Chairs: Melissa Cendejas, *SLAC National Accelerator Laboratory, USA* and Timothy Carroll, *Clariant, USA*.

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1:20 PM **Thu-BLRMBC-1320** Shedding Light on the Interplay of Synergistic Effects and Dynamic Behavior of Multi-Metal Catalysts By Operando X-Ray Spectroscopy.
**Nina S. Genz**[1], Adam Hoffman[2], Christopher Goodwin[3], Patrick Lömker[3], Anders Nilsson[3], Florian Meirer[1], Simon Bare[2] and Bert M. Weckhuysen[1], *(1)Utrecht University, Netherlands, (2)SLAC National Accelerator Laboratory, USA, (3)Stockholm University, Sweden*.

**Short Summary:**
We used a multimodal operando X-ray spectroscopy approach, i.e., operando quick-X-ray absorption spectroscopy with modulation excitation experimentation and high-pressure X-ray photoelectron spectroscopy, to unravel key information on synergistic effects and dynamic behavior of multi-metal $CO_2$ hydrogenation catalysts, being particularly important for the rational design of next generation $CO_2$ valorization catalysts.

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1:40 PM **Thu-BLRMBC-1340** Tuning Catalyst Activity, Stability, and Selectivity through Fundamental Understanding.
**Charlotte Vogt**, *Technion - Israel Institute of Technology, Israel*.

**Short Summary:**
Bottom-up catalyst design for improved activity has been a desire driving catalysis research for over a century. I will discuss some of the limitations in our current understanding and prediction of catalyst activity and design through fundamental understanding from theory and operando spectroscopy in heterogeneous thermocatalysis, and electrocatalysis.

2:00 PM **Thu-BLRMBC-1400** Unravelling the Reactivity of Different Pd Species over $Al_2O_3$ in Methane Combustion.
**Xiang Yu**, Xinwei Ye, Nina S. Genz, Florian Meirer, Matteo Monai and Bert M. Weckhuysen, *Utrecht University, Netherlands*.

**Short Summary:**
Combining HAADF-STEM, operando quick-EXAFS, operando FT-IR and DFT calculations, we revealed the evolution of Pd on gamma alumina and defective alumina under catalytic reaction conditions, as well as the mechanism of methane oxidation catalyzed by Pd particles, clusters and single atoms.

2:20 PM **Thu-BLRMBC-1420** Identifying Active Sites in Ga-Based Propane Dehydrogenation Catalysts Using Operando X-Ray Absorption Spectroscopy.
**Jason A. Chalmers**[1], Fernando Vila[2], Simon Bare[3] and Susannah Scott[1], *(1)University of California, Santa Barbara, USA, (2)University of Washington, USA, (3)SLAC National Accelerator Laboratory, USA*.

**Short Summary:**
We characterized the structure of Ga on several propane dehydrogenation catalysts using *operando* XAS. The superior stability and activity of Ga/HZSM-5 is consistent with more Ga(I) active sites which are stabilized by the support. In contrast, Ga/$\gamma$-$Al_2O_3$ does not stabilize Ga(I) sites under the reaction conditions, resulting in significant deactivation.

2:40 PM ***KEYNOTE*** **Thu-BLRMBC-1440 Operando Transient X-Ray Spectroscopy Provides Insight in the Catalytic Active Site.**
**Maarten Nachtegaal**, *Paul Scherrer Institute, Switzerland*.

**Short Summary:**
Operando quick scanning X-ray absorption spectroscopy (XAS) combined with transient experimentation provides new insights into relevant catalytic processes: heterogeneous Wacker oxidation of ethylene, the oxygen evolution reaction and NOx reduction in automotive gas after treatment systems.

## Design and Synthesis of Carbon-Based Materials

Session Chairs: Kara Stowers, *Brigham Young University, USA* and Levi Thompson, *University of Delaware, USA*.

3:45 PM **Thu-BLRMBC-1545** Tuning the Work Function of Carbon Supports to Enhance the Selectivity of Supported Metal Nanoparticles.
Hamed Bateni[1,2], **Deep M. Patel**[1,2], Laura M. Snyder[1,2], Prathamesh T. Prabhu[1,2], Prerana Carter[1,2], Luke Roling[1,2] and Jean-Phillippe Tessonnier[1,2], *(1)Iowa State University, USA, (2)Center for Biorenewable Chemicals (CBiRC), USA*.

**Short Summary:**
The work function of carbon supports was engineered via oxygen functionalization to induce a charge transfer at the interface with the metal active phase. In the case of Pd/C, a 1.0 eV change in support WF induced a 25-point enhancement in selectivity for the hydrogenation of cinnamaldehyde.

4:05 PM **Thu-BLRMBC-1605** Engineering Mesoporous Carbon Pellets As Catalyst Support for Catalytic Conversion of Biomass.
**Lianjun Liu**, *ADM Company, USA*.

**Short Summary:**
We have successfully engineered mesoporous carbon pellets by controlling the binder system and pyrolysis process. Although the carbon – supported bimetallic catalyst had slightly lower metal dispersion and bigger particle size compared with commercial AC, it demonstrated higher selectivity for glycerol hydrogenolysis.

4:25 PM **Thu-BLRMBC-1625** In-Situ Synthesis of Carbon Nanotubes-Conductive Carbon Hybrids Materials for Energy Storage.
**Ricardo Prada Silvy**, *Chasm Advanced Materials, USA*.

**Short Summary:**
In-situ growth of carbon nanotubes (CNTs) was carried out to create a new category of carbon nanotubes-graphite hybrid materials to be use in the manufacturing of advanced Li-ion battery electrodes. A novel catalyst preparation method using surfactant solutions is described.

4:45 PM **Thu-BLRMBC-1645** Renewable Activated Carbon Sorbents from Food Waste for Adsorptive Desulfurization of Liquid Hydrocarbon Fuels.
**Henry Sokol** and Julia Valla, *University of Connecticut, USA*.

**Short Summary:**
Renewable activated carbon sorbents prepared from food waste have shown remarkable adsorption capacity for sulfur compounds in hydrocarbon fuels. The steam activation process allows for tuning of the morphology and pore structure of the materials, enabling the synthesis of optimal sorbents for adsorptive desulfurization and other applications.

5:05 PM **Thu-BLRMBC-1705** Polymeric Microphotoreactor Functionalized with Carbon Nitride for Continuous-Flow Organic Synthesis.
**Alessandra Sivo**, Vincenzo Ruta, Mark Bajada and Gianvito Vile, *Politecnico di Milano, Italy*.

**Short Summary:**
Herein, we present polymeric microphotoreactor functionalized with carbon nitride as a new class of structured reactors merging the features of polymer science with heterogeneous catalysis. The optimal performance of the microreactor towards methylene blue degradation demonstrates that the system can find applications in other light-driven chemical processes.

5:25 PM **Thu-BLRMBC-1725** Suppressing Undesired Formation of $H_2O_2$ on Fe-N-C Electrocatalysts By Microwave-Assisted Treatments.
Yusaku Yamazaki, Shin Mukai and **Isao Ogino**, *Hokkaido University, Japan*.

**Short Summary:**
The durability of iron- and nitrogen-doped carbon (Fe-N-C) electrocatalysts is a significant challenge for their applications to polymer electrolyte fuel cells. We report that post-synthetic treatments of Fe-N-C catalysts, derived from ZIF-8-based materials, suppress the formation of undesired peroxide by-products during ORR while retaining the ORR activity.

## Ballroom DE

### THURSDAY MORNING

### Exploring the Reaction Energy Landscape

Session Chairs: Neeraj Rai, *Mississippi State University, USA* and Guoxiang Hu, *Queens College, USA*.

9:30 AM **Thu-BLRMDE-0930** Intermetallic Rh-Zn Heterogeneous Catalyst for Highly Active Hydroformylation.
Geet Gupta, Minda Chen, Wenyu Huang and **Luke Roling**, *Iowa State University, USA*.

**Short Summary:**
A RhZn intermetallic nanoparticle catalyst is shown to demonstrate heterogeneous hydroformylation performance exceeding homogeneous benchmarks. Density functional theory calculations identify active facets based on surface energy calculations under reaction conditions and show the crucial role of mixed Rh and Zn surface atoms in determining hydroformylation activity.

9:50 AM **Thu-BLRMDE-0950** Machine Learning Based Prediction of Activation Energies for Chemical Reactions on Metal Surfaces.
Daniel J. Hutton[1], Kari E. Cordes[1], Carine Michel[2] and **Florian Goeltl**[1], *(1)The University of Arizona, USA, (2)CNRS - ENS de Lyon, France*.

**Short Summary:**
We use generalized BEP relationships to predict activation energies for chemical reactions on metal surfaces. In combination with machine learning, our method significantly outperforms state of the art methods for activation energy predictions and might play a critical role for catalyst design in the future.

10:10 AM **Thu-BLRMDE-1010** Beyond Conventional Transition State Theory in Catalysis: Applications of Matrix Completion Methods.
**Selin Bac**, Stephen Jon Quiton, Kareesa Kron, Jeongmin Chae, Urbashi Mitra and Shaama Mallikarjun Sharada, *University of Southern California, USA*.

**Short Summary:**
This work aims to use matrix completion methods to predict eigenvalues of otherwise computationally expensive Hessians. These eigenvalues along the minimum energy path are necessary for variational transition state theory rate calculations. Our HVMC and PVMC methods will, therefore, allow the use of such sophisticated theories at lower costs.

10:30 AM **Thu-BLRMDE-1030** Adsorb-ML: Accelerating Adsorption Energy Calculations with Machine Learning.
**Muhammed Shuaibi**[1], Janice Lan[1], Aini Palizhati[2], Brandon Wood[1], Brook Wander[2], Abhishek Das[1], Matt Uyttendaele[1], C. Lawrence Zitnick[1] and Zachary Ulissi[2], *(1)Meta AI, USA, (2)Carnegie Mellon University, USA*.

**Short Summary:**
We introduce AdsorbML, a hybrid ML+DFT algorithm to find the minimum binding energy - the adsorption energy. We show that state of the art graph neural networks (SCN, GemNet-OC) are accurate enough to find comparable low-energy binding sites ~86% of times at ~1400x speedup over DFT alone.

10:50 AM **Thu-BLRMDE-1050** Efficient Prediction of Enthalpy of Linear Hydrocarbon Adsorbates on Pt(111) Using Unsupervised and Supervised Machine Learning.
**Jinwoong Nam**[1], Charanyadevi Ramasamy[1], Daniel E. Raser[1], Gustavo L. Barbosa Couto[1], Lydia Thies[2], David Hibbitts[2] and Fuat Celik[1], *(1)Rutgers, The State University of New Jersey, USA, (2)University of Florida, USA*.

**Short Summary:**
A new framework of machine learning application for predicting enthalpies of the adsorbates is developed. The adsorbates are clustered first based on the chemical insights into potential interactions between adsorbates and the surface, followed by the proper application of machine learning regression models.

11:10 AM **Thu-BLRMDE-1110** Generalized Prediction of O and OH Surface Adsorption on Transition Metal Oxides from Bulk Descriptors.
Benjamin Comer[1,2], Neha Bothra[1,2], Frank Abild-Pedersen[1], Michal Bajdich[1] and **Kirsten T. Winther**[1], *(1)SLAC National Accelerator Laboratory, USA, (2)Stanford University, USA*.

**Short Summary:**
I will discuss our recent work on developing accurate and generalizable ML models for O and OH adsorption energies on ($A_xO_y$) transition metal oxide surfaces. We utilize the integrated COHP of the bulk metal-oxygen bond to improve the adsorption energy prediction across crystal structures and oxidation states.

11:30 AM **Thu-BLRMDE-1130** Dechlorination Decomposition of Mustard Gas: A Thermodynamic Analysis on Pt and Cu Catalysts Supported on Rutile-$TiO_2$(110).
**David Jiang**[1] and Philippe Sautet[2], *(1)University of California, USA, (2)University of California, Los Angeles, USA*.

**Short Summary:**
Neutralization of the blistering and carcinogenic chemical warfare agent known as mustard gas under ambient temperature conditions has been explored via computational modelling of its decomposition pathway on Pt single atom catalysts and highly dispersed Cu clusters.

## THURSDAY AFTERNOON

## Heteroatom Chemistry and Oxidation

Session Chairs: Edwin Yik, *M2X Energy Inc., USA* and Jiahan Xie, *Braskem America, USA*.

1:20 PM **Thu-BLRMDE-1320** Trends in C–X Hydrogenolysis: Effects of Metal Type and Electronic Environment.
**Nikki Kragt**[1], Abdulrahman Almithn[1], Jalal Tavana[2], Mohammed Al-Gharrawi[2], Thomas J. Schwartz[2] and David Hibbitts[1], *(1)University of Florida, USA, (2)University of Maine, USA*.

**Short Summary:**
Hydrogenolysis reactions are ubiquitous in many industrial processes, including biomass conversion, chemical recycling of plastics, and pharmaceutical syntheses. We explore hydrogenolysis trends on Pt-group metals with the goal of understanding mechanisms of heteroatom removal, and, through this understanding, inform catalyst design and chemical process development.

1:40 PM **Thu-BLRMDE-1340** Propene Ammoxidation By Forced Dynamic Operation over Bismuth Molybdate Based Catalysts.
**Zhuoran Gan**[1], Lars Grabow[2] and William Epling[1], *(1)University of Virginia, USA, (2)University of Houston, USA*.

**Short Summary:**
Forced dynamic operation (FDO) was employed in the ammoxidation of propene to acrylonitrile (ACN) over Bismuth Molybdate (BMO) based catalysts. FDO shown promising ACN yield compared to steady-state operations (SSO). ACN production during FDO is correlated with lattice O of BMO based catalysts.

2:00 PM **Thu-BLRMDE-1400** Lowering the Operating Temperature of Au Acetylene Hydrochlorination Catalysts Using Oxidized Carbon Supports.
**Samuel Pattisson**[1], Simon Dawson[1], Grazia Malta[1], Nicholas Dummer[1], Louise Smith[1], Anna Lazaridou[1], David Morgan[1], Simon Freakley[2], Simon A. Kondrat[3], Joost Smit[4], Peter Johnston[4] and Graham Hutchings[1], *(1)Cardiff Catalysis Institute, Cardiff University, United Kingdom, (2)University of Bath, United Kingdom, (3)Loughborough University, United Kingdom, (4)Johnson Matthey, United Kingdom*.

**Short Summary:**
The functionalization of carbon supports for gold acetylene hydrochlorination catalysts was found to dramatically increase overall activity and enable operation at lower temperatures. This is a key finding that could enable the production of lower light-off catalysts and provide a drop-in replacement for toxic mercuric chloride catalysts in existing reactors.

2:20 PM **Thu-BLRMDE-1420** Promotional Effect of Co Cations on the Catalytic Activity of Co/ZSM-5 in 1,2-Dichloroethane Dehydrochlorination for the Production of Vinyl Chloride Monomer.
**HyeongDong Jung**[1], Yong Hyun Lim[1], Kihun Nam[1], Jae-Soon Choi[2], Jungup Bang[2], Sangjin Kim[2] and Do Heui Kim[1], *(1)Seoul National University, Korea, Republic of (South), (2)LG Chem Ltd, Korea, Republic of (South)*.

**Short Summary:**
The introduced Co cations changed the acid site distribution, turning Brønsted acid sites into more active Lewis acid sites which were active site for the DCE dehydrochlorination, enhancing catalytic activity, VCM selectivity and reusability of the catalyst.

2:40 PM **Thu-BLRMDE-1440** Investigation of Dynamic VPO Catalyst Behaviour through Phosphorous Dosing Under Transport Limitation Free Conditions.
**Scott D. Anderson**[1], Martin Kutscherauer[1,2], Sebastian Boecklein[2], Gerhard Mestl[2], Gregor D. Wehinger[1] and Thomas Turek[1], *(1)Clausthal University of Technology, Germany, (2)Clariant AG, Germany*.

**Short Summary:**
Dynamic behaviour of vanadium phosphorous oxide catalysts is investigated via dosing of trimethyl phosphate on the nanolitre scale. Partial oxidation of *n*-butane is conducted in a transport limitation free μ-reactor. Results demonstrate how we can vary the catalyst activity via different reactor temperatures and TMP dosing.

3:00 PM **Thu-BLRMDE-1500** Optimization of Reduction Process to Maximumly Activate Supported Metal Oxide Catalysts.
**Justin X. Wang**, Prasomsri Prasomsri, Samantha Sargent and Yeping Cai, *Clariant Corporation, BU Catalysts, USA*.

**Short Summary:**
With DoE program, effect of moisture content, impurities, gas space velocities, $H_2$ concentration, temperature and pressure on industrial activation processes was investigated. Optimized reduction and stabilization processes were identified to maximize the activation of the metal oxide catalysts. The development was confirmed at a commercial process.

## Selective Catalytic Reduction of NOx I

Session Chairs: Chip Roberts, *Toyota Research Institute - North America, USA* and Enrico Tronconi, *Politecnico di Milano, Italy*.

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3:45 PM **Thu-BLRMDE-1545** Dual-Site RHC and OHC Transient Kinetic Analysis Enables Prediction of the Low-T Steady-State Standard SCR Rates on a Cu-CHA Catalyst.
Nicole Daniela Nasello[1], Nicola Usberti[1], Umberto Iacobone[1], Federica Gramigni[1], Wenshuo Hu[2], Shaojun Liu[2], Isabella Nova[1], Xiang Gao[2] and **Enrico Tronconi**[1], *(1)Politecnico di Milano, Italy, (2)Zhejiang University, China*.

**Short Summary:**
Mechanistic aspects of the *reduction* and *oxidation half cycles* of the Standard SCR reaction over a Cu-CHA catalyst are addressed by transient redox experiments and kinetic modelling analysis. The present results provide a stoichiometrically and kinetically consistent closure of the Cu redox mechanism in the low temperature Standard $NH_3$-SCR chemistry.

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4:05 PM **Thu-BLRMDE-1605** First-Principles Insights into the Reduction Half Cycle of the LT $NH_3$-SCR over Cu-CHA Under Wet Conditions.
**Gabriele Contaldo**, Matteo Ferri, Chiara Negri, Isabella Nova, Matteo Maestri and Enrico Tronconi, *Politecnico di Milano, Italy*.

**Short Summary:**
The study focuses on the so far neglected role of $H_2O$ on the reduction half step of $NH_3$-SCR over Cu-CHA. The results reveal the relevant contribution of entropic losses in inhibiting the RHC rate, while strong enthalpic stabilization effects decrease the apparent activation enthalpy due to disperive forces.

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4:25 PM **Thu-BLRMDE-1625** Reaction Kinetics of $NH_3$-SCR over Cu-CHA from First Principles.
**Yingxin Feng**[1], Henrik Grönbeck[1], Ton V.W. Janssens[2], Peter N.R. Vennestrøm[2], Jonas Jansson[3], Magnus Skoglundh[1] and Derek Creaser[1], *(1)Chalmers University of Technology, Sweden, (2)Umicore Denmark ApS, Denmark, (3)Volvo Group Trucks Technology, Sweden*.

**Short Summary:**
In this work, we access to first principles microkinetic models for $NH_3$-SCR over Cu-CHA, which rationalizes previous phenomenological models and links the kinetic behavior with fundamental materials properties. Moreover, the new insights form a basis for further improvements of the catalyst.

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4:45 PM **Thu-BLRMDE-1645** Effects of Hydrothermal Ageing on the Nature of Active Sites in Cu-Exchanged Small Pore Zeolites.
**Andreas Jentys**[1], Rachit Khare[1], Mirjam Wenig[1] and Johannes A. Lercher[1,2], *(1)Technical University of Munich, Germany, (2)Pacific Northwest National Laboratory, USA*.

**Short Summary:**
Selective catalytic reduction of $NO_x$ with $NH_3$ using Cu-exchanged small-pore zeolites is currently the leading technology to mitigate $NO_x$ emissions from engine exhaust. Using operando X-ray absorption spetroscopy we elucidate the effects of hydrothermal ageing on the dynamic nature of active sites in Cu-SSZ-13 and Cu-SSZ-39 during $NH_3$-SCR.

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5:05 PM **Thu-BLRMDE-1705** Correlating Static Cu Dimer Changes to SCR Rate Changes after Sulfur Poisoning on Cu-SSZ-13 Catalysts.
Yu-Ren Chen[1], **Poonam Rani**[1], Keka Mandal[1], Rohil Daya[2], Chris Paolucci[1] and William Epling[1], *(1)University of Virginia, USA, (2)Cummins Inc., USA*.

**Short Summary:**
To understand SCR rate changes after sulfur poisoning, this study explored the changes in the amounts of static Cu dimers by using CO titration before and after sulfur exposure. The reduction in $CO_2$ formation after sulfur exposure can be correlates with the interaction of sulfur with Cu dimers in catalyst.

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5:25 PM **Thu-BLRMDE-1725** Mechanistic Insights on the Deactivation during Temperature-Cycled Sulfur Exposure over Cu-SSZ-13.
**Rohil Daya**, Yuhui Zha, Hongmei An, Lai Wei, Unmesh Menon, Dylan Trandal and Ashok Kumar, *Cummins Inc., USA*.

**Short Summary:**
Reactor experiments are utilized to propose a kinetic model for the sulfation of active Cu sites and loss of Brønsted acidity during temperature-cycled sulfur exposure over Cu-SSZ-13. This model considers bisulfite formation and oxidation to bisulfates over ZCuOH sites, in addition to sulfur-assisted dealumination process and formation of Al sulfates.

## Rotunda

### THURSDAY MORNING

## Carbon Dioxide Capture and Conversion

Session Chairs: Daniel Haynes, *National Energy Technology Laboratory, USA* and Gabriella Garbarino, *University of Genova, Italy*.

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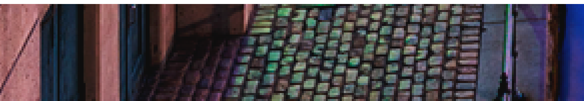
9:30 AM **Thu-RTND-0930** Novel Hierarchical Sorbent-Catalysts for Sorption-Enhanced Hydrogen Production-$CO_2$ Intensification Technologies.
**Diana Iruretagoyena Ferrer**[1,2], Paul Fennell[1], Ronny Pini[1], Nilay Shah[1], David Chadwick[1] and Aida Gutiérrez-Alejandre[2], *(1)Imperial College London, United Kingdom, (2)National Autonomous University of Mexico, Mexico*.

**Short Summary:**
Hydrogen is a key clean fuel. The sorption-enhanced $H_2$ process is a promising intensification strategy to boost the amount of $H_2$ produced with efficient $CO_2$ capture and storage. We have developed novel hierarchical sorbent-catalysts for this technology with remarkable performance in terms of activity, kinetics and stability.



9:50 AM **Thu-RTND-0950** Could a Switchable Catalyst Become an Efficient Dual Functional Material for $CO_2$ Capture and Utilization? An Operando DRIFT Study to Elucidate the Underlying Mechanism.
**Loukia-Pantzechroula Merkouri**[1], Luis F. Bobadilla[2], Juan Luis Martín-Espejo[2], Melis Duyar[1] and Tomas Ramirez Reina[1,2], *(1)University of Surrey, United Kingdom, (2)University of Seville-CSIC, Spain*.

**Short Summary:**
Operando DRIFTS was performed to investigate the mechanism of $CO_2$ capture and conversion of switchable Dual Function Materials (DFMs). These materials open up possibilities in flexible chemical production from $CO_2$, through a combination of $CO_2$ adsorption and subsequent chemical transformation (methanation, reverse water gas shift or dry reforming of methane).

10:10 AM **Thu-RTND-1010** In-Situ $CO_2$ Capture and Catalytic Methanation Using Ni/Alkaline Earth Carbonate Dual Function Materials.
**Xianyue WU**[1], Wen Liu[1], Ocean Cheung[2] and Ribooga Chang[2], *(1)Nanyang Technological University, Singapore, (2)Uppsala University, Sweden*.

**Short Summary:**
The idea of this work is to directly load Ni onto alkaline carbonates to simulate $CO_2$ DFMs. Both two-step carbonation and conventional one-step $CO_2$ hydrogenation schemes are studied to evaluate these DFMs' performance and investigate the hydrogenation mechanism. A correlation between the two schemes is proposed.

10:30 AM **Thu-RTND-1030** Understanding Catalyst-Sorbent Interactions in a Dual-Function Material for $CO_2$ Capture and Methanation.
**Shradha Sapru**, Arun Majumdar and Matteo Cargnello, *Stanford University, USA*.

**Short Summary:**
This work highlights the crucial role Ru plays in activating the sorbent for $CO_2$ capture, in addition to its role as a catalyst. It also demonstrates the dependence of $CO_2$ capture and conversion on the proximity between the sorbent and catalyst, paving the way to design more efficient dual-function materials.

10:50 AM **Thu-RTND-1050** Insights on Dual Function Materials (DFM) for $CO_2$ Capture and Hydrogenation from Flue Gases By Spatially Resolved Operando FT-IR.
**Alessandro Porta**, Roberto Matarrese, Carlo Giorgio Visconti and Luca Lietti, *Politecnico di Milano, Italy*.

**Short Summary:**
Dual Function Materials (DFM) are promising materials for direct $CO_2$ capture and methanation. DFM materials have been tested with operando FTIR spectroscopy and microreactor experiments and new insights on DFMs performances and reaction mechanism have been obtained, allowing for the rational design of new formulations.

11:10 AM ***KEYNOTE*** **Thu-RTND-1110** $CO_2$ **Capture, Concentration, and Conversion.** Bianca Ceballos, Jeff Barlow and **Jenny Yang**, *University of California, Irvine, USA*.

**Short Summary:**
Closing the anthropogenic carbon cycle requires selective valorization of $CO_2$ and efficient methods for capture and concentration from dilute streams. Strategies for addressing the challenge of product selectivity in electrocatalytic $CO_2$ reduction, as well as combined $CO_2$ capture and conversion will be discussed.

## THURSDAY AFTERNOON

## Methane Oxidation to Methanol

Session Chairs: Robert Davis, *University of Virginia, USA* and James Harris, *The University of Alabama, USA*.

1:20 PM **Thu-RTND-1320** Computationally Guided Discovery of Stable Metal-Organic Frameworks That Are Promising Methane-to-Methanol Catalysts.
**Husain Adamji**[1], Aditya Nandy[1,2], Ilia Kevlishvili[1], Yuriy Roman[1] and Heather Kulik[1,2], *(1)Massachusetts Institute of Technology, USA, (2)MIT, USA*.

**Short Summary:**
Combining machine-learning and density-functional-theory to repurpose experimentally synthesized MOFs for methane-to-methanol, we find several stable Mn MOFs with methane-to-methanol potential that exhibit great metal-local structural diversity. Our computational workflow can guide experimentation to discover new MOFs for methane-to-methanol ultimately mitigating global warming driven by waste methane emissions.

1:40 PM **Thu-RTND-1340** Quantifying the Upper Limit of Methane Activation Rates in Cu-Exchanged Zeolites Using Exhaustive DFT Calculations and Machine Learning Based Force Fields.
**Jiawei Guo**, Ty Sours, Sam Holton, Chenghan Sun and Ambarish Kulkarni, *University of California - Davis, USA*.

**Short Summary:**
The overarching goal is to leverage DFT calculations and ML-FF to exhaustively sample all relevant Cu species (>16,000) within 52 distinct zeolite topologies. This enables evaluating the catalytic performance of every single unique CuOCu site (>5,000) and predicting the ensemble average and maximum possible performance of a given topology.

2:00 PM **Thu-RTND-1400** Effects of Cu-CHA Composition, Structure, and Pretreatment on Catalytic Partial Methane Oxidation to Methanol.
**Andrew Mikes** and Raj Gounder, *Purdue University, USA*.

**Short Summary:**
Cu-CHA zeolites of varying Cu densities and Al arrangements exhibit different selectivities and apparent reaction orders during catalytic partial methane oxidation, implying differences in the nature of Cu active sites, whose structures were identified and quantified using XANES and UV-Vis spectroscopy.

2:20 PM **Thu-RTND-1420** Control of Distribution of Framework Al Atoms in 8-Ring Zeolites and Its Impact on Catalysis for Activation of $N_2O$ with $CH_4$.
Peipei Xiao[1], Kengo Nakamura[1], Yao Lu[1], Yong Wang[1], Hermann Gies[2] and **Toshiyuki Yokoi**[1], *(1)Tokyo Institute of Technology, Japan, (2)Ruhr University Bochum, Germany*.

**Short Summary:**
AEI-type aluminosilicate zeolites with different Al distributions were prepared. Metal species, Cu and Fe, were introduced onto the zeolites *via* the ion-exchanged method. Thus prepared AEI-type zeolites were applied as catalyst for activation of $N_2O$ with $CH_4$, continuous oxidation of methane reaction was carried out by using $N_2O$ as oxidant.

2:40 PM **Thu-RTND-1440** Elucidating the Active Sites for Selective Oxidation of Methane to Methanol over Cu-SSZ-13 Zeolite.
**Jie Zhu**, Ran Zhu, Husain Adamji and Yuriy Román-Leshkov, *Massachusetts Institute of Technology, USA*.

**Short Summary:**
The catalytic activity and selectivity of Cu-SSZ-13 zeolites for continuous methane oxidation were found to vary with the preparation method. The sample showing full selectivity towards methanol and dimethyl ether under the reaction condition provides insight into the structure of the copper sites that are capable of oxidizing methane selectively.

3:00 PM WITHDRAWN: Small Pore-Zeolite Based Catalysts for Methane to Methanol.

## Insights into Catalysis I

Session Chairs: Michele Sarazen, *Princeton University, USA* and Gina Noh, *The Pennsylvania State University, USA*.

3:45 PM **Thu-RTND-1545** Coordination Sphere of Solid Acid Sites and Their Catalytic Consequences in Dehydration and C-O Scission Catalysis.
**Guangming Cai**, William Broomhead and Cathy Chin, *University of Toronto, Canada*.

**Short Summary:**
We connect the thermochemical properties of solid Brønsted and Lewis acid sites and their vicinal coordination environments to their turnovers in C-O bond scission in alkanols.

4:05 PM **Thu-RTND-1605** The Nature of Methanol Diffusion Dynamics in H-ZSM-5 As a Function of Si/Al Ratio: A Quasi-Elastic Neutron Scattering (QENS) Study.
**Santhosh Matam**[1,2], Alex O'Malley[2,3], Ian Silverwood[2,4] and C. Richard A. Catlow[1,2,5], *(1)Cardiff University, United Kingdom, (2)UK Catalysis Hub at Harwell, United Kingdom, (3)University of Bath, United Kingdom, (4)ISIS Facility, STFC Rutherford Appleton Laboratory, United Kingdom, (5)University College London, United Kingdom*.

**Short Summary:**
Zeolite ZSM-5 is the key in many commercially important processes involving methanol, such as MTH and alkylation. Here we demonstrate that the nature of methanol diffusion dynamics is dependent on the Si/Al ratio of the zeolite and measurement temperature.

4:25 PM **Thu-RTND-1625** Elucidation of the Roles of Water on the Reactivity of Surface Intermediates in Carboxylic Acid Ketonization on $TiO_2$.
Fan Lin[1], Wenda Hu[1,2], Nicholas Jaegers[1,2], Feng Gao1, Jian Zhi Hu[1,2], Huamin Wang[1] and **Yong Wang**[1,2], *(1)Pacific Northwest National Laboratory, USA, (2)Washington State University, USA*.

**Short Summary:**
The inhibition effect of $H_2O$ on the carboxylic acid ketonization over $TiO_2$ catalysts was investigated. We demonstrated that the presence of $H_2O$ increases the coverage of the less reactive bridging bidentate carboxylate associated with adsorbed $H_2O$ molecule, leading to a lower ketonization activity on hydrated $TiO_2$.

4:45 PM **Thu-RTND-1645** Can the Rate of a Catalytic Turnover be Altered by a Ligand in the Absence of Direct Binding Interactions?.
Jacklyn N. Hall and **Praveen Bollini**, *University of Houston, USA*.

**Short Summary:**
This work reports a methodology for kinetic analysis that provides unambiguous quantitative characterization of site uniformity in redox catalysis. Resulting kinetic features reveal second sphere coordination effects in which ligands alter redox parameters even in the absence of direct bonding interactions with the primary active site.

5:05 PM **Thu-RTND-1705** Revealing Molecular-Level Catalytic and Inhibitory Interactions during the Co-Pyrolysis of Cellulose and Plastics.
**Fuat Sakirler**, Mihriye Doga Tekbas and Hsi-Wu Wong, *University of Massachusetts Lowell, USA*.

**Short Summary:**
Co-pyrolysis of cellulose and plastics are studied by microreactor experiments and DFT. Levoglucosan, 5-hydroxymethylfurfural, and glycolaldehyde are selected as key cellulose-derived pyrolysis products of interest, and the catalytic and inhibitory effects of the ether and aromatic moieties in plastics on the formation kinetics of these products are elucidated.

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5:25 PM **Thu-RTND-1725** Strategies for Controlling Surface Coverage during Methane Partial Oxidation.
**Shengguang Wang**[1,2], Yu Liu[1] and Lars Grabow[1,2], *(1)University of Houston, USA, (2)Center for Programmable Energy Catalysis (CPEC), USA*.

**Short Summary:**
While methane conversion processes share underlying reaction networks, methane partial oxidation stands out as the only reaction that proceeds faster as the particle size increases. We have successfully attributed the origin of the particle size effects to the excess oxygen and evaluated the strategy of catalyst design.

# Friday, June 23, 2023

## 551 AB

### FRIDAY MORNING

### Advanced Approaches to Kinetic Modeling

Session Chairs: Srinivas Rangarajan, *Lehigh University, USA* and Thomas Senftle, *Rice University, USA*.

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8:00 AM **Fri-551AB-0800** Modeling Solvent Confinement in Zeolite Pores and Its Impact on Epoxidation Catalysis.
Vijaya Sundar Jeyaraj and **Alexander V. Mironenko**, *University of Illinois Urbana-Champaign, USA*.

**Short Summary:**
Predicting the stability of transition states in presence of external stimuli is important in modeling efficient catalytic process. Here, we develop a simulation protocol for fast and accurate estimation of the adsorption enthalpy of epoxides in transition metal substituted zeolite frameworks from dilute liquid solution.

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8:20 AM **Fri-551AB-0820** Validating Kinetic Models for Ethylene Epoxidation over Silver.
**Lilliana Brandao** and Christian Reece, *Harvard University, USA*.

**Short Summary:**
We have implemented three kinetic models for ethylene epoxidation over Ag in a home-built Temporal Analysis of Products (TAP) simulation software to numerically recreate previous TAP experiments. While no model recreated the experimental results precisely, one appears to recreate experimental trends with modification of the oxygen desorption pathway.

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8:40 AM **Fri-551AB-0840** Kinetic Monte Carlo Simulations of Surface Kinetics on Heterogeneous Computing Architectures.
**Craig Daniels**, Kyungjoo Kim, Nathan Roberts, Habib Najm and Judit Zádor, *Sandia National Laboratories, USA*.

**Short Summary:**
We present a new open-source software “KinCat” for performing KMC simulations on a 2D lattice. KinCat is compatible with a variety of computing architectures, utilize multiple KMC algorithms, and naturally manage the complexity of lateral interactions. We illustrate the accuracy of the simulator and examine its scalability and performance.

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9:00 AM **Fri-551AB-0900** Using Reaction Mechanism Generator (RMG) to Automate Kinetic Monte Carlo Simulation Setup.
**Sevy Harris** and Richard West, *Northeastern University, USA*.

**Short Summary:**
This work automates the generation of kinetic Monte Carlo (KMC) simulation input files using Reaction Mechanism Generator (RMG). This allows users to leverage existing thermodynamic and kinetic databases to populate more detailed simulations which can account for spatial inhomogeneities on the reacting surface.

### Elucidation of Active Sites

Session Chairs: Brandon Bukowski, *Northwestern University, USA* and Fuat Celik, *Rutgers, The State University of New Jersey, USA*.

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9:40 AM **Fri-551AB-0940** Modeling the Roles of Rigidity and Dopants in Single-Atom Methane-to-Methanol Catalysts.
**Haojun Jia** and Heather Kulik, *MIT, USA*.

**Short Summary:**
We develop an understanding of the relationship of SACs to these homogeneous analogues by comparing the energetics and structure of the direct metal-coordinating environment in the presence of 2p (i.e., N or O) and 3p (i.e., P or S) dopants for the methane-to-methanol catalysts.

10:00 AM **Fri-551AB-1000** Investigating the Effect of Near-Surface Structure and Composition on the Catalytic Activity of High-Entropy Alloys.
**Gaurav Deshmukh**[1], Fei Xu[2], Qingzhe Xin[2], Canhui Wang[2], Chao Wang[2] and Jeffrey Greeley[1], *(1)Purdue University, USA, (2)Johns Hopkins University, USA*.

**Short Summary:**
A workflow combining density functional theory calculations, catalysis informatics tools, and experiments is utilized to efficiently probe the influence of Pt-skin formation on the oxygen reduction activity of Pt-based high-entropy alloys with non-precious metals. Moreover, strategies are discussed to couple this workflow with an in-house graph convolutional network.

10:20 AM **Fri-551AB-1020** Design of Active Sites in Bimetallic NO Decomposition Catalysis.
**Joakim Halldin Stenlid**[1,2], Verena Streibel[1,2], Tej Choksi[3] and Frank Abild-Pedersen[2], *(1)Stanford University, USA, (2)SLAC National Accelerator Laboratory, USA, (3)Nanyang Technological University, Singapore*.

**Short Summary:**
To traverse the vast design space of bimetallic nanocatalysts, we use a physics-based approach that evaluates site-specific catalytic activities using site-stability as sole descriptor. The site-stability is sensitive to structural and compositional variations around the site and its instantaneous evaluation enables accelerated screening of bimetallic nanocatalysts in, e.g., NO decomposition.

10:40 AM **Fri-551AB-1040** Identification of Active Site for Ethane Dehydrogenation on Platinum Catalyst Using Bayesian Analysis.
**Mubarak Bello** and Andreas Heyden, *University of South Carolina, USA*.

**Short Summary:**
Using Bayesian analysis this study found evidence for both Pt(111) and Pt(211) as active sites for the ethane dehydrogenation reaction on Platinum catalysts. Thus, this study helps reconcile the apparent conflict in the literature on the computationally predicted and experimentally identified active site during catalysis at various reaction conditions.

11:00 AM **Fri-551AB-1100** TDDFT Study of the V K-Edge XANES of the Vanadium Complexes.
**Jun Yi**[1], Ying Zhu[2], Yuezhi Mao[3], John Herbert[2] and Zhou Lin[4], *(1)University of Massachusetts, USA, (2)The Ohio State University, USA, (3)San Diego State University, USA, (4)University of Massachusetts Amherst, USA*.

**Short Summary:**
We performed real-time time-dependent density functional theory (RT-TDDFT) calculations to calculate V k-edge XANES spectra for vanadium(V) complexes. Based on our calculation, we have reproduce experimental observation and interpret the spectra features.

11:20 AM **Fri-551AB-1120** Tight Binding Models for the Electronic Structure of Bimetallic Catalysts.
**Filippo Balzaretti**, *Stanford University, USA; SLAC National Accelerator Laboratory, USA*.

**Short Summary:**
Shifts of the d-band center relate to catalytic activity trends. Electronic structure calculations of complex nanoparticles, though, are demanding for DFT. Methods such as DFTB are 103 times faster and provide transferable results. With this contribution we present the effectiveness of this approach when applied to several bimetallic catalysts.

11:40 AM WITHDRAWN: Effect of Heterogeneity of Silica-Supported Co(II) Sites on Small Alkane Dehydrogenation Kinetics: A Theoretical Study.
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## 552 AB

### Conversion of Biomass-Derived Oxygenates II

Session Chairs: Lucas Ellis, *Oregon State University, USA* and Wei Fan, *University of Massachusetts Amherst, USA*.

8:00 AM **Fri-552AB-0800** Oxidative Dehydrogenation of Glycerol-Derived Secondary Alcohols on Silica-Supported Platinum Nanoparticles.
**Sydney Foster**, Shuai Qian, Jason Bara and James Harris, *The University of Alabama, USA*.

**Short Summary:**
Biodiesel waste glycerol is an underutilized source of inexpensive and valuable carbon. Successful oxidative dehydrogenation of glycerol-derived symmetric diether alcohols on platinum and platinum-bismuth bimetallic nanoparticles was studied with various silica supports. Appreciable catalytic activity was observed for these relative to other secondary aliphatic alcohols.

8:20 AM **Fri-552AB-0820** Elucidating Nanoscale Influences on the Competitive Adsorption and Aqueous Phase Reforming of Mixed Carboxylic Acid Systems.
**Alyssa Hensley**[1], Ayodeji Omoniyi[1], Giulia Zoppi[2], Samir Bensaid[2], Raffaele Pirone[2] and Giuseppe Pipitone[2], *(1)Stevens Institute of Technology, USA, (2)Polytechnic of Turin, Italy*.

**Short Summary:**
A critical challenge that continues to plague the catalytic upgrading of biomass is its chemical complexity. Typically, studies are performed on idealized systems containing a single reactant molecule type. Here, we investigate the influence of multi-component aqueous phase mixtures of biomass-derived carboxylic acids on the reactivity of solid-liquid interfaces.

8:40 AM **Fri-552AB-0840** Probing Outer-Sphere Interactions in Nanoporous Catalysts with Lactic Acid Dehydration.
**Geet Gupta** and Brandon Bukowski, *Johns Hopkins University, USA*.

**Short Summary:**
Selective catalytic dehydration of biomass-derived lactic acid is a sustainable approach to producing valorized products like acrylic acid, that faces selectivity-activity challenges in porous solids. We develop a microkinetic model with accurate and efficient entropic and diffusion coefficients of species using machine learning force fields (MLFF) trained 'on-the-fly AIMD'.

9:00 AM **Fri-552AB-0900** Mechanistic Study of Dehydra-Decyclization of THF to Butadiene on $ZrO_2$ and $Al_2O_3$.
**Sai Praneet Batchu**, Stavros Caratzoulas and Dionysios Vlachos, *University of Delaware, USA*.

**Short Summary:**
We investigate the mechanism of the reaction of THF to butadiene and retro-Prins products on dry and hydroxylated surfaces of t-$ZrO_2$ (101) and γ-$Al_2O_3$(110) and explain the selectivity differences observed across these surfaces. The local topology around the active site plays a key role in guiding the product selectivities.

## Design and Synthesis of 2D Materials & Thin Films

Session Chairs: Theodore (Ted) Walker, *Syracuse University, USA* and Madelyn Ball, *West Virginia University, USA*.

9:40 AM **Fri-552AB-0940** Nanometric-Thick Metal-Free h-Boron Nitride/Graphene Films As Base Catalyst for the Synthesis of Benzoxazoles.
Sabina Ion[1], Ana Primo[2], Bogdan Cojocaru[1], Camelia Bala[1], Dana Popescu3, **Vasile Parvulescu**[1] and Hermenegildo Garcia[2], *(1)University of Bucharest, Romania, (2)Universitat Politècnica de València, Spain, (3)The National Institute of Materials Physics, Romania*.

**Short Summary:**
The superlattice configuration of h-BN corresponded to the exact overlapping of the hexagonal lattice with the defective graphene as an effect of the templating action of the pre-formed h-BN sheets controlling the epitaxial growth. The resulted defects acted as as base catalyst for the synthesis of benzoxazoles.

10:00 AM **Fri-552AB-1000** Selective Acetylene Hydrogenation over Pd and Bimetallic PdAu 2D Thin Film Catalysts.
Zehua Li[1], Eylül Öztuna[1,2], Christian Rohner[1], Alexander Steigert[2], Martin Muske[2], Matus Stredansky[1], Manuela Arztmann[2], Sabine Wrabetz[1], Jutta Kröhnert[1], Maria Dimitrakopoulou[1], Lukas Thum[1], Wiebke Frandsen[1], Adnan Hammud[1], Frank Girgsdies[1], Daniel Delgado Munoz[1], Johannes Frisch[2], Tathiana M. Kokumai[2], Marcus Bär[2], Simone Raoux[2,3], Thomas Schmidt[1], Mauricio Prieto[1], Arno Bergmann[1], Helmut Kuhlenbeck[1], Olga Vinogradova[1], Vanessa J. Bukas[1], Thomas Lunkenbein[1], Annette Trunschke[1], Axel Knop-Gericke[1], Rutger Schlatmann[2], Karsten Reuter[1], Beatriz Roldán Cuenya[1], Robert Schlögl[1], Daniel Amkreutz[2] and **Katarzyna Skorupska**[1], *(1)Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany, (2)Helmholtz-Zentrum Berlin für Materialien und Energie, Germany, (3)Humboldt-Universität zu Berlin, Germany*.

**Short Summary:**
This work proves the applicability of novel 2D film system where the properties of catalyst are influence by incorporation of second metal. The addition of Au to Pd catalyst results in homogenous dispersion and shows the beneficial catalytical performance.

10:20 AM **Fri-552AB-1020** Stability and Activity of Supported Pd and Pt Thin-Film Catalysts in Dependence of the Barrier Layers.
**Manuela Arztmann**, *Helmholtz-Zentrum Berlin für Materialien und Energie, Germany*.

**Short Summary:**
Influence of various barrier layer materials on the stability and apparent activity of silicon supported Pd and Pt thin-film catalysts.

10:40 AM **Fri-552AB-1040** Electrostatic Manipulation of Lewis Acidity in Ultrathin Oxides Via Catalytic Condensers.
**Sallye R. Gathmann**, Tzia Ming Onn, C. Daniel Frisbie and Paul Dauenhauer, *University of Minnesota, USA*.

**Short Summary:**
Herein, we describe the synthesis, characterization, and catalytic performance of an oxide-based catalytic condenser, a type of programmable catalyst in which the electron density of the active site can be modulated via electrical bias. Specifically, we demonstrate this device reversibly enhances the Lewis acidity of ultrathin alumina films.

11:00 AM **Fri-552AB-1100** Enhanced $NH_3$-SCR Activity at Low Temperatures over MnOx Supported on Two-Dimensional $TiO_2$ Derived from ZIF-8.
**Hyunsub Kim** and Do Heui Kim, *Seoul National University, Korea, Republic of (South)*.

**Short Summary:**
In this study, anatase $TiO_2$ was synthesized via ZIF-8 as a sacrificial template, which showed a unique structure with a high external surface area. After impregnation of Mn, the catalyst showed excellent catalytic performance at low temperatures (~150°C), resulting from the formation of reactive bridged nitrate species.

11:20 AM **Fri-552AB-1120** Functionalized Copper-Based Graphite Nanoplatelets for Ullman-Type C-O Coupling.
**Vincenzo Ruta**, Mark Bajada and Gianvito Vile, *Politecnico di Milano, Italy*.

**Short Summary:**
This works presents a novel family of catalysts obtained via integration ligand engineering and metal single-atom materials, for the efficient conduction of Ullman-type C-O coupling.

11:40 AM **Fri-552AB-1140** Thermodynamic and Electronic Properties of $MoSi_2N_4$ Edges.
**Atharva Burte**[1], Omar Abdelrahman[2], Andre Muniz[3] and Ashwin Ramasubramaniam[1], *(1)University of Massachusetts, Amherst, USA, (2)University of Massachusetts Amherst, USA, (3)Universidade of Federal do Rio Grande do Sul, Brazil*.

**Short Summary:**
The study aims to put forth an outlook on the utility of $MoSi_2N_4$ edges for catalysis. We establish a phase diagram for the stability of $MoSi_2N_4$ and determine thermodynamically stable edge structures. The lowest-energy armchair edge is found to be potentially useful for HER.

## 555 AB

### Electrochemica $CO_2$ Conversion III

Session Chairs: Feng Jiao, *University of Delaware, USA* and Qing Zhao, *Northeastern University, .*

8:00 AM **Fri-555AB-0800** Continuum Model of $CO_2$ Reduction and (Bi)Carbonate Crossover in Membrane Electrode Assemblies.
**Eric Lees**[1], Oyinkansola Romiluyi[1,2], Adam Z. Weber[1] and Alexis Bell[1,2], *(1)Lawrence Berkeley National Laboratory, USA, (2)University of California, Berkeley, USA*.

**Short Summary:**
We report here a continuum model of electrochemical $CO_2$ reduction in a membrane electrode assembly. The maximum product formation rate was shown to be constrained by the kinetics of (bi)carbonate formation reactions that consume $CO_2$ in the ionomer. This insight pointed us to ionomer chemistries that enhance $CO_2$ reduction.

8:20 AM **Fri-555AB-0820** $CO_2$ Conversion to Ethylene in a Protonic Ceramic Electrochemical Membrane Reactor.
Min Wang[1,2], Lucun Wang[2], **Yingchao Yang**[1] and Dong Ding[2], *(1)The University of Maine, USA, (2)Idaho National Laboratory, USA*.

**Short Summary:**
A new electrocatalytic process is demonstrated for direct conversion of $CO_2$ to ethylene at intermediate temperatures (350-500°C) in an electrochemical membrane reactor. This process is based on high-performance protonic ceramic electrochemical cells integrated with highly active and selective catalysts for $CO_2$ to ethylene conversion.

8:40 AM **Fri-555AB-0840** Benchmarking Anion-Exchange Membranes for Electrocatalytic Carbon Monoxide Reduction.
**Luke Cherniack**, Bjorn Hasa and Feng Jiao, *University of Delaware, USA*.

**Short Summary:**
Multi-carbon products can be economically produced from $CO_2$ at high selectivity through a tandem $CO_2$ to carbon monoxide coupled with carbon monoxide to C2+ process. In this study, state-of-the-art anion exchange membranes for carbon monoxide electroreduction to multi-carbon products are compared based on selectivity, overpotential, and stability of the electrolyzer.

9:00 AM **Fri-555AB-0900** Using Membrane Electrode Assemblies to Compare Thermal and Electrochemical Carbon Dioxide Hydrogenation.
**Samantha Roenigk**, James McKone and Manjodh Kaur, *University of Pittsburgh, USA*.

**Short Summary:**
Our reaction of focus is carbon dioxide hydration but with an emphasis on the benefits and drawbacks of both thermochemistry and electrochemistry. Our initial work focused on building our own reactor and simplifying the coating method. We are working on combining heat and electricity in carbon dioxide hydration.

### Electrochemical $CO_2$ Conversion IV

Session Chairs: Fanglin Che, *University of Massachusetts Lowell, USA* and Max Hulsey, *Massachusetts Institute of Technology, USA*.

9:40 AM **Fri-555AB-0940** CuZn-Based Electrodes for Selective Electrochemical $CO_2$ Reduction.
**Matt Peerlings**, Kai Han, Petra E. de Jongh and Peter Ngene, *Utrecht University, Netherlands*.

**Short Summary:**
Electrochemical $CO_2$ reduction is promising to close the carbon cycle. However, suitable electrocatalysts are required. In this work, we show a CuZn-based electrocatalyst that can produce CO with high selectivity and stability. Surprisingly, no hydrocarbon products were detected. Extensive *ex-situ* and *in-situ* characterization reveal $Cu/ZnO_x$ as the active phase.

10:00 AM **Fri-555AB-1000** Understanding the Dynamic Evolution of Atomically Dispersed Cu Catalyst for $CO_2$ Electrochemical Reduction Using Integrated XANES Analysis and Mechanistic Studies.
**Cong Liu** and Xu Jason, *Argonne National Laboratory, USA*.

**Short Summary:**
We demonstrate a computational investigation combining X-ray absorption near edge structure (XANES) simulations and density function theory (DFT) mechanistic study to understand the catalyst structures during $CO_2$ electrocatalysis and the reaction pathways. The integrated study depicted the dynamic evolution of the catalytic site during electrocatalysis.

10:20 AM **Fri-555AB-1020** Navigating the Selectivity and Productivity Toward a Single C2 Product in $CO_2$ Electroreduction.
**Jingjie Wu**, *University of Cincinnati, USA*.

**Short Summary:**
This presentation demonstrates the promise of collectively controlling rate-determining and selectivity-determining steps through electrode engineering and catalyst rational design, respectively, to direct $CO_2$ conversion toward a specific C2 product (e.g., ethylene and ethanol) at high production rates and high selectivity.

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10:40 AM **Fri-555AB-1040** Enabling Selective Kw Scale Tandem Carbon Dioxide Electroreduction to Multi-Carbons.
**Bradie Crandall** and Feng Jiao, *University of Delaware, USA*.

**Short Summary:**
A tandem $CO_2$ electrolyzer system was scaled from a laboratory concept (technological readiness 2) to a more industrially relevant laboratory prototype (technological readiness 4) allowing key scaling challenges to be elucidated and resolved. Stack operation up to 0.38 kW was achieved while maintaining relatively high Faradaic efficiency towards multi-carbons (>80%).

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11:00 AM **Fri-555AB-1100** Atomically Dispersed Platinum in OMS-2 Cation Vacancy for the Conversion of $CO_2$ to CO and $CH_3OH$.
**Scott Bamonte**[1], Harshul Khanna[1], Inosh Perera[1], Meilin Li[1], Chao Li[1], Luisa Posada[1], Ryuichi Shimogawa[2], Mahdin Mahboob[2], Amelia Figueroa[3], Nicholas Eddy[1], Pu-Xian Gao[1], Ashley Head[4], Dmitri Zakharov[4], Anatoly Frenkel[2] and Steven Suib[1], *(1)University of Connecticut, USA, (2)Stony Brook University, USA, (3)Nova Southeastern University, USA, (4)Brookhaven National Laboratory, USA*.

**Short Summary:**
We synthesized atomically dispersed platinum atoms inside a cation vacancy of $MnO_2$. This catalyst was tested for $CO_2$ hydrogenation to understand how atomically dispersed platinum atoms' local environment affects the activity and selectivity. From our experiments, we show that platinum atoms in cation vacancies go through a methanol synthesis pathway.

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11:20 AM **Fri-555AB-1120** Temperature Effects on the Population of Surface Species for $CO_2$ Reduction Reaction over Cu Electrocatalysts.
**Victor Brandão** and Carsten Sievers, *Georgia Institute of Technology, USA*.

**Short Summary:**
In situ IR spectroscopy was used to understand the temperature effect on the population of surface CO during the electrochemical reduction of $CO_2$. A more even distribution of this intermediate on catalytic sites suggests that CO migration might be the mechanistic pathway by which temperature increases lead to faster conversion.

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11:40 AM **Fri-555AB-1140** $CO_2$ Conversion on Graphene Supported Single Atom Catalysts with a 2D Ferroelectric $In_2Se_3$ Substrate.
**Mo Li** and Joshua Young, *New Jersey Institute of Technology, USA*.

**Short Summary:**
Graphene supported single atomic catalysts (Graphene-SACs) were verified as promising method in $CO_2$ reduction reaction. In this computational study, DFT calculations were performed to investigate the $CO_2RR$ mechanism on a ferroelectric subtract $In_2Se_3$ covered with a Graphene-SAC.

## 556 AB

### Hydroprocessing

Session Chairs: Eswar Iyyamperumal, *Albemarle Corporation, USA* and Steven Crossley, *University of Oklahoma, USA*.

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8:00 AM **Fri-556AB-0800** Palladium Catalysts for Selective Hydrogenation of Aromatic Hydrocarbons to Cycloolefins.
Ziyu Tang, Fangliang Huo, Yue Qi and **Simon G. Podkolzin**, *Stevens Institute of Technology, USA*.

**Short Summary:**
Efficient palladium catalysts for selective hydrogenation of aromatic hydrocarbons into cycloolefins were developed. Adsorption sites and hydrocarbon surface species were determined. Selectivity improvements were attributed to changes in relative adsorption energies between the initial aromatic hydrocarbon and the cycloolefin product.

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8:20 AM **Fri-556AB-0820** Analysis of the Catalytic Performance of Ni Supported in Hydrotreating.
Rodrigo Valderrama-Zapata[1], Omar Vargas[1], Julieth T. García-Sánchez[1], Sergio A. Rincón-Ortiz[2], Iván D. Mora-Vergara[1], **Luisa Acevedo**[1], David Pérez-Martínez[3], Edgar M. Morales-Valencia[1] and Victor Baldovino Medrano[1,2], *(1)Centro de Investigaciones en Catálisis (CICAT), Universidad Industrial de Santander, Colombia, (2)Universidad Industrial de Santander, Colombia, (3)ECOPETROL S.A., Colombia*.

**Short Summary:**
This work shows that Ni is catalytically active in hydrotreating when it is supported over a zeolite carrier. Its performance can be improved when it is impregnated by strong electrostatic adsorption and when mesoporosity in introduced to zeolite.

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8:40 AM **Fri-556AB-0840** New Insights in the Reactivity of 3-Methylthiophene and Benzothiophene Depending on the Bulk NiMoS Synthesis: Experimental and Kinetic Modeling Study..
Alexandre Carvalho[1], Valentin Hetier[2], Julie Rousseau[1], Etienne Girard[3], Denis Uzio[3], Patrick Lacroix-desmazes[2], Annie Pradel[2], Laurence Courtheoux[2] and **Brunet Sylvette**[1], *(1)University of Poitiers, France, (2)University of Montpellier, France, (3)IFP Energies Nouvelles, France*.

**Short Summary:**
Differencies of reactivity of two model molecules, 3-methylthiophene and benzothiophene, were showed depending on the synthesis method used for NiMoS bulk preparation. Kinetic modeling indicated a modification of the adsorption constants taking into account of differences of catalyst properties and mechanisms involved in the transformation of both sulfur molecules.

9:00 AM **Fri-556AB-0900** Refining of Biosyngas-Derived Paraffin Wax into Low-Carbon Lubricating Oil over Mesoporous Pt/Al-TUD-1 Dewaxing Catalyst.
**Sundaramurthy Vedachalam** and Ajay Dalai, *University of Saskatchewan, Canada*.

**Short Summary:**
Lubricating oil that can reduce the carbon footprint of the lubricants industry was produced from biomass-derived hydrocarbon wax by hydroisomerization. Mesoporous Pt/Al-TUD-1 dewaxing catalyst resulted in a clean drop-in substitute for mineral-based lubricating oil.

## Insights into Catalysis II

Session Chairs: Siddarth Krishna, *University of Wisconsin, Madison, USA* and Líney Árnadóttir, *Oregon State University, USA*.

9:40 AM **Fri-556AB-0940** Active, Selective, and Stable COPROX Using Cu/$CeO_2$ and Cu/Gd-Substituted $CeO_2$ Aerogels.
**Travis Novak**[1], Paul DeSario[2], Todd Brintlinger[2], Ryan DeBlock[1], Jeffrey Long[2] and Debra Rolison[2], *(1)US Naval Research Laboratory (NRC Postdoc), USA, (2)U.S. Naval Research Laboratory, USA*.

**Short Summary:**
Cu photodeposited onto $CeO_2$ or Gd-doped $CeO_2$ aerogels are active, stable, and selective catalysts for the COPROX reaction, achieving >95% CO conversion with >95% selectivity even in humidified feedstreams. Interfacial Cu/aerogel intimacy stabilizes the more active low-valent Cu, but when Cu is photodeposited over commercial nanoparticulate ceria, significant $Cu^{2+}$ forms.

10:00 AM **Fri-556AB-1000** Quantifying the Influence of Surface and Subsurface H Species on Selective C-O Bond Scission Rates over $MoO_x$ Catalysts.
**Laura Alejandra Gomez**, Caleb Q. Bavlnka, Tianhao E. Zhang and Steven Crossley, *University of Oklahoma, USA*.

**Short Summary:**
$MoO_3$ catalysts are both promising and incredibly complex for selective C-O bond scission. This work uses a combination of carbon nanotube bridges with controlled doses of reducing and oxidizing species to evaluate the kinetic relevance of oxygen vacancies from surface and subsurface H species on selective deoxygenation chemistry.

10:20 AM **Fri-556AB-1020** Unraveling Soot Oxidation Evolution and Water Promotion Mechanism on 3D Nanoarray Structured Catalysts.
**Chunxiang Zhu**, Shoucheng Du, Xingxu Lu, Bo Zhang, Fangyuan Liu, Sibo Wang, Binchao Zhao, Jiyu Sun, Yunjiang Ding and Pu-Xian Gao, *University of Connecticut, USA*.

**Short Summary:**
This work offers a novel and rational 3D nanoarray catalyst surface platform to increase catalyst-soot close contact for low temperature soot oxidation. Furthermore, the work unravels the mesoscopic illustration of soot oxidation evolution.

10:40 AM **Fri-556AB-1040** Hydrogen Reduction Reaction (HRR).
**Hai-Xu Wang** and Yogesh Surendranath, *Massachusetts Institute of Technology, USA*.

**Short Summary:**
We report a conceptually novel electrocatalytic hydrogen reduction reaction which in net reduces $H_2$ to hydrides. The reaction proceeds by $H_2$ dissociative adsorption on a metal electrode to form surface M−H species, which are then negatively polarized to drive hydride transfer to molecular hydride acceptors with tunable surface hydricity.

11:00 AM **Fri-556AB-1100** Effect of Metal Nuclearity and Support Oxygen Vacancy on Reactivity of Pt/$CeO_2$ Catalysts for Ethylene Hydrogenation.
**Md Raian Yousuf**[1], Kristin Knight[1], Stephen Porter[2], Eli Stavitski[3], Adam Hoffman[4], Simon Bare[4], Abhaya Datye[2], John Morris[1] and Ayman M. Karim[1], *(1)Virginia Polytechnic Institute and State University, USA, (2)University of New Mexico, USA, (3)Brookhaven National Laboratory, USA, (4)SLAC National Accelerator Laboratory, USA*.

**Short Summary:**
We demonstrate, utilizing $C_2H_4$ hydrogenation, kinetic measurements, IR and X-ray spectroscopy, and AC-STEM, that support oxygen-vacancy can be tuned to alter electron density of supported metal for the same particle size and in turn affect the catalytic reactivity. Effect of metal particle size on this phenomenon will also be discussed.

11:20 AM **Fri-556AB-1120** Impact of Feed Temperature and Composition on the Steady State Performance and Spatial Features of Catalytic Oxidation of Methane.
**Jonathan Ratcliff**, Pak Wing Chen, Lars Grabow and Michael P. Harold, *University of Houston, USA*.

**Short Summary:**
This study is focused on the effect of operating conditions on rich methane oxidation for both overall performance as well as spatial temperature and concentration profiles. These experiments reveal a strong impact of inlet oxygen concentration on kinetic inhibition, spatial profiles, and the presence of multiple steady states.

11:40 AM **Fri-556AB-1140** Catching Elusive Reaction Intermediates By Photoionization.
**Zihao Zhang**, Patrick Hemberger and Andras Bodi, *Paul Scherrer Institute, Switzerland*.

**Short Summary:**
The short-lived reaction intermediates, e.g., radicals and ketenes, can be detected by *operando* photoelectron photoion coincidence spectroscopy, notably in methanol(chloromethane)-to-olefins and oxidative dehydrogenation of propane processes. This provides the mechanistic insights with molecular resolution to guide viable process optimization pathways.

# Ballroom A

## C1 Chemistry

Session Chairs: John Kuhn, *University of South Florida, USA* and Michael Lanci, *ExxonMobil Technology and Engineering Company, USA*.

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8:00 AM **Fri-BLRMA-0800** Support Effects for the Water-Gas-Shift Reaction over Cu.
**Jian Chang**, Zhuoming Feng, John M. Vohs and Raymond J. Gorte, *University of Pennsylvania, USA*.

**Short Summary:**
The water-gas-shift (WGS) reaction was studied on a series of supported Cu catalysts in which the $MgAl_2O_4$ (MAO) support was modified by depositing ZnO, $CeO_2$, $Mn_2O_3$ and CoO using Atomic Layer Deposition (ALD). The implications of the results for the development of better WGS catalysts are discussed.

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8:20 AM **Fri-BLRMA-0820** Catalytic Involvement of Interfacial Oxygen of Vanadium Oxide and Support in Methanol Oxidative Dehydrogenation.
**William Broomhead**[1], Lili Zhang[1], Wei Tian[2], Jose Herrera[2] and Cathy Chin[1], *(1)University of Toronto, Canada, (2)Western University, Canada*.

**Short Summary:**
This study correlates Gibbs free energies of the kinetically consequential steps with changing oxygen content in supported vanadium oxides catalyzing methanol ODH reactions. Most notably, we find these energies compensate with each other and this compensation is a function of the lattice oxygen content in VOx domains.

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8:40 AM **Fri-BLRMA-0840** Conversion of Methane to Acetonitrile over Supported GaN Catalysts: A Spectroscopic Observation of GaN Reduction and Surface CN Formation.
**Korawich Trangwachirachai**[1], Ai-Lin Huang[1], Chia-Hsin Wang[2], Hong-Kang Tian[1] and Yu-Chuan Lin[1], *(1)National Cheng Kung University, Taiwan, (2)National Synchrotron Radiation Research Center, Taiwan*.

**Short Summary:**
ACN can be produced from methane over supported GaN catalysts, in which 5GaN/HZ showed the best performance. The amount of reducible-N is correlated with ACN productivity. The operando NAPXPS and DRIFTS suggested that CN species are the key intermediates in ACN formation.

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9:00 AM **Fri-BLRMA-0900** Computational Design of Supported Amorphous Metal Oxide Nanoclusters for Methane Activation.
**Xijun Wang**, Kaihang Shi, Anyang Peng and Randall Q. Snurr, *Northwestern University, USA*.

**Short Summary:**
We leveraged DFT calculations combined with machine learning (ML) to predict and screen promising candidate metal oxide nanoclusters (MeO-NCs) for methane activation. Exploiting an unsupervised ML protocol, we achieved a quick distinction between high and low performing nanoclusters, opening a window for future rapid screening and prediction of advanced Me-NCs.

## Methane Dehydroaromatization

Session Chairs: Aditya Bhan, *University of Minnesota, Twin Cities, USA* and Gustavo A. Fuentes, *Universidad A. Metropolitana-Iztapalapa Mexico City, Mexico*.

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9:40 AM **Fri-BLRMA-0940** Partially Overcoated Molybdenum Supported Catalysts Under Methane Dehydroaromatization Conditions.
**Jordy Ramos-Yataco** and Justin Notestein, *Northwestern University, USA*.

**Short Summary:**
This work evaluates the effect of oxide overcoat on supported molybdenum oxide catalysts. It has shown that overcoat redispersed the MoOx species and impact MDA performance. Also, regeneration evaluations shows that $Al_2O_3$ overcoat slow down the loss of MDA activity under different number of regeneration cycles under isothermal oxidative conditions.

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10:00 AM **Fri-BLRMA-1000** Low-Temperature Production of Aromatics from Non-Thermal Plasma Stimulation of Methane over Mo/H-ZSM-5.
**Gerardo Rivera-Castro**, Ibukunoluwa Akintola, David Go and Jason C. Hicks, *University of Notre Dame, USA*.

**Short Summary:**
In this work, we studied the influence of a non-thermal plasma for methane activation over Mo/H-ZSM-5, and shown that the plasma can enhance the conversion of methane at 700 °C. Furthermore, we studied decreasing the temperature of the reaction under plasma stimulation for the production of aromatics.

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10:20 AM **Fri-BLRMA-1020** Reaction Pathways, Site Requirements, and Thermodynamic Barriers of $CH_4$ Dehydroaromatization on MoCx/H-ZSM-5 Catalysts.
**Neil Kanth Razdan**[1], Anurag Kumar[2], Brandon Foley[2] and Aditya Bhan[2], *(1)Massachusetts Institute of Technology, USA, (2)University of Minnesota, Twin Cities, USA*.

**Short Summary:**
In this work, we identify the key reactive intermediate to $CH_4$ dehydroaromatization (i.e. acetylene) and the catalytic active center for responsible for its dehydrogenative production and subsequent aromatization (i.e. carbidic Mo centers), and develop polyfunctional strategies to overcome equilibrium limitations without detriment to aromatic selectivity.

10:40 AM **Fri-BLRMA-1040** Uncovering the Effects on a Mo/ZSM-5 Catalyst When Co-Feeding Steam during Methane Dehydroaromatization.
**Joyce Kromwijk**, Matteo Monai, Ward van der Stam and Bert M. Weckhuysen, *Utrecht University, Netherlands*.

**Short Summary:**
The effect of steam as co-reactant on the MDA activity and selectivity as well as of the structural and compositional effects on a Mo/ZSM-5 catalyst were investigated using various techniques. Co-feeding 4% steam results in more stable benzene yields, but adding 10% is detrimental to the MDA activity.

11:00 AM **Fri-BLRMA-1100** Improved Benzene Selectivity for Methane Dehydroaromatization *via* Modifying the Zeolitic Pores by Dual Templating Approach.
**Deepti Mishra**[1], Kamal Pant[2] and Muxina Konarova[3], *(1)The University of Queensland, Australia, Australia, (2)Indian Institute of Technology Delhi, India, (3)University of Queensland, Australia*.

**Short Summary:**
Soft templating strategy was applied for the fabrication of hierarchical HZSM-5 via hydrothermal approach. Later, Mo was impregnated in HZSM-5 and Mo/HZSM-5(H) performs better in MDA reaction than Mo/ZSM-5(C). Mo/HZSM-5(H) contributes to higher benzene production with reduced carbon deposition at the catalyst surface, due to the presence of hierarchical micro/mesoporous structure.

11:20 AM **Fri-BLRMA-1120** On the Reactivity of Metastable Active Sites Encapsulated in ZSM-5 in Methane Activation and C-C Coupling and Kinetic Modelling of Methane Dehydroaromatization Chemistry.
**Iqra Ahangar** and M. Ali Haider, *Indian Institute of Technology Delhi, India*.

**Short Summary:**
MDA is an energy-efficient route that will decrease the production cost of transportation fuels and chemicals as it eliminates the energy-intensive step, i.e., syngas production. The mechanistic insights obtained from DFT calculations provides a molecular level design strategy for the active sites.

11:40 AM **Fri-BLRMA-1140** Light Alkane Dehydroaromatization with ppm Pt Loading in Zinc-Exchanged HZSM-5 Zeolite.
Genwei Chen, Hossein Toghiani and **Yizhi Xiang**, *Mississippi State University, USA*.

**Short Summary:**
We show that the bimetallic Pt/Zn-HZSM-5 catalysts, with Pt loading below 10 ppm, are highly active and stable for light alkanes dehydroaromatization. Specifically, the turnover frequency at 550oC is up to 150 s-1, and the deactivation constant obtained from the first order power law equation model is only 0.01 h-1.

## Ballroom BC

### Modeling and Fundamentals of Catalyst Synthesis

Session Chairs: Silvina Tomassone, *Rutgers University, USA* and Helena Hagelin-Weaver, *University of Florida, USA*.

8:00 AM **Fri-BLRMBC-0800** Theoretical Model for Predicting the Catalytic Properties of Complex Surface Alloys.
Shikha Saini[1,2], Joakim Stenlid[1,2], Shyam Deo[1,2], Philipp N. Plessow[3] and **Frank Abild-Pedersen**[1], *(1)SLAC National Accelerator Laboratory, USA, (2)Stanford University, USA, (3)Karlsruhe Institute of Technology, Germany*.

**Short Summary:**
We introduce a simple and general theoretical framework for predicting the site stability of multi-metallic surfaces and nanoparticles spanning a wide-ranging combinatorial space. The model requires only a small set of density functional theory calculations of metal atom adsorption energies on clean and dilute surface slabs.

8:20 AM **Fri-BLRMBC-0820** Modeling Distribution Tendencies of Noble Metals on Fe(100).
**Isaac Onyango**[1], Greg Collinge[1,2], Yong Wang[1,2] and Jean-Sabin McEwen[1,2], *(1)Washington State University, USA, (2)Pacific Northwest National Laboratory, USA*.

**Short Summary:**
Promotion of Fe-based catalysts with noble metals is shown to protect them from oxidation and improve HDO activity. Understanding condition-dependent variations in dispersion/agglomeration tendency of noble metals within Fe requires sampling an enormous configuration space inaccessible using DFT models. This study bypasses this challenge by using DFT-parameterized cluster expansions.

8:40 AM **Fri-BLRMBC-0840** Enabling Electrocatalyst Discovery at Unprecedented Throughput with Nanoparticle Megalibraries.
**Jordan Swisher**, *Mattiq, USA*.

**Short Summary:**
Stoicheia is developing the world's highest throughput technology for electrocatalyst discovery using nanomaterial Megalibraries. In one experiment, 90,000 unique and monodisperse polyelemental electrocatalysts can be synthesized and screened for various applications. Using this technology, we accelerate the discovery and design of enabling electrocatalysts for a myriad of applications.

9:00 AM **Fri-BLRMBC-0900** Activating Nanoglue-Confined, Atomically Dispersed Pt Species for Low-Temperature Carbon Monoxide Oxidation.
Yiwei Yu and **Jingyue Liu**, *Arizona State University, USA*.

**Short Summary:**
Use of functional nanoglues to localize atomically dispersed metal species enables activation of these active metal centers by reductive treatment. The carbon monoxide activated Pt molecular species, confined by $CeO_x$ nanoglue islands on $SiO_2$, enhanced their activity by more than two orders of magnitude for low temperature carbon monoxide oxidation.

## Carbon-Carbon Bond Formation Among Biomass-Derived Oxygenates

Session Chairs: Alan Allgeier, *University of Kansas, USA* and Jimmy Faria, *University of Twente, Netherlands*.

9:40 AM **Fri-BLRMBC-0940** Intensification of 5,5'-Dimethyl-2,2'-Bifuran Synthesis from 2-Methylfuran Via Oxidative Coupling.
**Charles Fields**, Mi Jen Kuo, Raul Lobo and Dionysios Vlachos, *University of Delaware, USA*.

**Short Summary:**
Renewable synthesis of the platform chemical 4,4'-dimethylbiphenyl requires the oxidative coupling of 2-methylfuran to 5,5'-dimethylbifuran followed by tandem Diels-Alder and dehydration reactions yielding 4,4'-dimethylbiphenyl. Achieving a 139% increase in the 5,5'-dimethylbifuran space-time yield for the homocoupling of 2-methylfuran provides an effective and scalable pathway to renewable 4,4'-dimethylbiphenyl for sustainable materials.

10:00 AM **Fri-BLRMBC-1000** Tailoring the Reactivity of Acid Sites for C-O Cleavage and C-C Coupling Reaction over Zeolites in Water and Decalin.
**Sungmin Kim**, Oliver Y. Gutierrez, Donald M. Camaioni and Johannes A. Lercher, *Pacific Northwest National Laboratory, USA*.

**Short Summary:**
We elucidate how solvents and steric constraints direct self-organization of molecules within zeolite pores. Our study aims to predict the effect of confined environments on a variety of reactions by correlating the nature of acid sites and intrapore solvation environments with C-O cleavage and C-C coupling reaction rates.

10:20 AM **Fri-BLRMBC-1020** Investigating the Prins Mechanism As a Sustainable Pathway for the Production of Renewable Liquid Fuels.
**Laura Paz Herrera**[1], Randy Cortright[2] and Will Medlin[1], *(1)University of Colorado Boulder, USA, (2)NREL, USA*.

**Short Summary:**
The Prins reaction between propionaldehyde and ethylene to 1,3-pentadiene over aluminosilicates (H-ZSM-4, H-Al-MCM-41, $SiO_2$-$Al_2O_3$) was investigated. Results showed propionaldehyde self-aldol condensation as the most prominent pathway over all catalysts, whereas the Prins product was only observed with H-Al-MCM-41 and $SiO_2$-$Al_2O_3$. Effects of feed ratio, temperature, and residence time were studied.

10:40 AM **Fri-BLRMBC-1040** Shape Selectivity-Controlled Cross Aldol Reactions.
**Isaac O. Ogabiela** and Friederike C. Jentoft, *University of Massachusetts Amherst, USA*.

**Short Summary:**
Aldol reactions pose a difficulty with respect to selectivity control since various products, including fission products, may form. Microporous solid acid catalysts (zeolites) of different frameworks are tested for the aldol reaction between benzaldehyde and diverse ketones to explore the potential of porosity for controlling selectivity in cross aldol reactions.

11:00 AM **Fri-BLRMBC-1100** Mechanisms and Selectivity in Acid-Catalyzed Aldol Reactions.
**Shubham Malviya**, Isaac O. Ogabiela, Friederike C. Jentoft and Peng Bai, *University of Massachusetts Amherst, USA*.

**Short Summary:**
Aldol reactions find applications with their potential to generate diverse products via competing condensation and fission pathways. Our research shows that condensation favors E1 mechanism whereas fission favors Grob-like fragmentation. Substitutions to the reactant to tune the transition-state stability provides an effective way to control the selectivity of the reactions.

11:20 AM **Fri-BLRMBC-1120** Consequence of Altering Acid Strength in MFI Zeolites Via Phosphorus Modification and Their Effects on Acylation Reaction.
**Ismaeel Alalq** and Steven Crossley, *University of Oklahoma, USA*.

**Short Summary:**
This work presents the advantage of adding phosphorous to aluminosilicate zeolite to use for upgrading biomass derived chemicals. This catalyst modification reduces the acidity and changes confinements within zeolite pores. Consequently, improved catalyst life and selectivity has been observed during acylation of 2-methylfruan with acetic acid.

11:40 AM **Fri-BLRMBC-1140** Confinement of Dual Lewis Acid Centers in CeSndeAlBeta for the Conversion of Acetone-to-Isobutene.
**Vannessa Caballero**[1], Houquian Li[1], Wenda Hu[1,2], Konstantin Khivantsev[2], Jian Zhi Hu[1,2] and Yong Wang[1,2], *(1)Washington State University, USA, (2)Pacific Northwest National Laboratory, USA*.

**Short Summary:**
This work presents the remarkable catalytic activity of CeSndeAlBeta which catalyzes the acetone-to-isobutene reaction with a high selectivity and stability in the absence of water. The study of the chemical nature of this material provides understanding on the mechanisms of Lewis acid-base pairs for selective C-C coupling and self-deoxygenation reactions.

## Ballroom DE

### Selective Catalytic Reduction of NO$_x$ II

Session Chairs: Haiying Chen, *Oak Ridge National Laboratory, USA* and Unmesh Menon, *Cummins Inc., USA*.

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8:00 AM **Fri-BLRMDE-0800** Monomeric Fe Species in Square Planar Geometry Active for Low Temperature NH$_3$-SCR of NO.
**Dominik Wierzbicki**[1,2], Oliver Kröcher[3], Davide Ferri[3] and Maarten Nachtegaal[2], *(1)Brookhaven National Laboratory, USA, (2)Paul Scherrer Institute, Switzerland, (3)Paul Scherrer Institut, Switzerland*.

**Short Summary:**
New synthesis route of Fe/zeolites, using a bulky Fe complex, resulted in formation of exclusively isolated Fe species. Such homogenous speciation may provide mechanistic insight in the role of active species with spectroscopy (XAS) that goes beyond current knowledge due to heterogeneous Fe speciation in the samples reported so far.

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8:20 AM **Fri-BLRMDE-0820** Mechanistic Insights into Hysteresis Phenomena during NH$_3$ Oxidation on Pt/Al$_2$O$_3$ Catalysts for NH$_3$ Slip Applications.
**Brandon K. Bolton**[1], Hanyu Ma[2], Amish Chovatiya[2], Rohil Daya[3], Dylan Trandal[3], Krishna Gunugunuri[3], Krishna Kamasamudram[3], William Schneider[2] and Raj Gounder[1], *(1)Purdue University, USA, (2)University of Notre Dame, USA, (3)Cummins Inc., USA*.

**Short Summary:**
Model Pt/$\gamma$-Al$_2$O$_3$ samples were synthesized with different Pt particle size and used to study the kinetics of NH$_3$ oxidation, combined with XAS measurements and microkinetic modeling, in order to determine the factors that give rise to a hysteresis in oxidation behavior in NH$_3$ slip catalysts (ASC).

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8:40 AM **Fri-BLRMDE-0840** Tailoring the Mechanochemical Interaction between Vanadium Oxidesand Zeolite for Sulfur-Resistant DeNOx Catalysts.
Se Won Jeon, Inhak Song, Hwangho Lee and **Do Heui Kim**, *Seoul National University, Korea, Republic of (South)*.

**Short Summary:**
The surface modification of the Al-rich zeolite with Octadecyltrichlorosilane(OTS) coating allows us to suppress the chemical and physical poisoning in V-based catalysts physically mixed with zeolite, which is promising catalyst for the selective catalytic reduction of NO with NH$_3$ reaction.

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9:00 AM **Fri-BLRMDE-0900** The Role and Structure of Ce and Mn for NOx Reduction in Application-Relevant Catalysts.
**Javier Ruiz-Martinez**, *King Abdullah University of Science and Technology (KAUST), Saudi Arabia*.

**Short Summary:**
The role of Ce one Mn-based catalysts for the selective catalytic reduction of NOx at low temperature is an ongoing debate. We havedemonstrate that Ce has a structural promoting effect but impacts negatively on the intrinsic catalytic activity of Mn.

### Selective Catalytic Reduction of NO$_x$ III

Session Chairs: Dhruba Deka, *Oak Ridge National Laboratory, USA* and Kun Wang, *ExxonMobil Technology and Engineering Company, USA*.

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9:40 AM **Fri-BLRMDE-0940** Low-Temperature NH$_3$-SCR over Copper-Exchanged Small-Pore Zeolites: An Interplay between Copper Redox and Transfer, and Support Acidity and Topology.
**Feng Gao**, Eric Walter, Ying Chen, Yilin Wang, Kenneth Rappe and Yong Wang, *Pacific Northwest National Laboratory, USA*.

**Short Summary:**
This work for the first time reveals detailed interplays between Cu-amine active species and support Bronsted acid sites at a molecular level during low-temperature selective NOx reduction over Cu-zeolite catalysts, and is thus highly important for our interpretation of low temperature SCR mechanisms.

10:00 AM **Fri-BLRMDE-1000** Reaction Hysteresis and Cu Sites Variations Detected By in-Situ UV-Vis Spectroscopy during NH$_3$-SCR f NO$_x$ over Cu/SSZ-13 and Cu/SSZ-39.
Gustavo A. Fuentes[1] and **Gabriela I. Hernandez-Salgado**[2], *(1)Universidad A. Metropolitana-Iztapalapa Mexico City, Mexico, (2)Autonomous Metropolitan University-Iztapalapa, Mexico*.

**Short Summary:**
The reaction hysteresis observed during NH$_3$-SCR of NOx over Cu/SSZ-13 and Cu/SSZ-39 is reported for the first time. In-situ DRS UV-Vis spectroscopy evidences parallel structural changes in Cu moieties upon heating and cooling that appear to be responsible for the reaction hysteresis. The mechanistic implications are clear.

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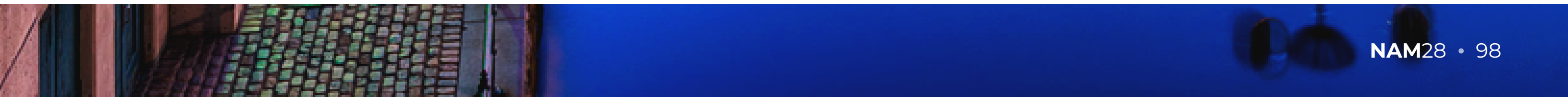
10:20 AM **Fri-BLRMDE-1020** Quantifying the Monomeric and Dimeric Cu Species in Hydrothermal and Sulfur Aged Cu-CHA for NH$_3$-SCR.
**Unmesh Menon**[1], Mi-Young Kim[1], Rohil Daya[1], Lai Wei[2], Feng Gao[3], Kenneth Rappe[3], Yong Wang[4] and Krishna Kamasamudram[1], *(1)Cummins Inc., USA, (2)University of Virginia, USA, (3)Pacific Northwest National Laboratory, USA, (4)Washington State University, USA*.

**Short Summary:**
In this presentation reactor-based titration methods are developed to quantify the speciation of Cu ions in Cu-CHA catalysts. Specific probe molecules such as NO+NH$_3$, NO$_2$, CO, NO are used in a specific test sequence to quantify the chemically distinct Cu configurations. Tests were performed over hydrothermally-aged and sulfur exposed catalysts.



10:40 AM **Fri-BLRMDE-1040** Experimental and Modelling Study of SAR and $H_2O$ Effects on the RHC and OHC of STD-SCR over Cu-CHA Catalysts.
Nicola Usberti[1], Nicole Daniela Nasello[1], Umberto Iacobone[1], Roberta Villamaina[2], Maria Pia Ruggeri[2], Djamela Bounechada[2], Andrew York[2], Jillian Collier[2], Isabella Nova[1] and **Enrico Tronconi**[1], *(1)Politecnico di Milano, Italy, (2)Johnson Matthey Technology Centre, United Kingdom*.

**Short Summary:**
We apply transient response methods and transient kinetic analysis to close the Standard SCR redox cycle over Cu-CHA catalysts and shed light on the controversial effects of $H_2O$ and SAR. We show for the first time that both wet conditions and high SAR inhibit RHC but promote “NO silent” OHC.

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11:00 AM **Fri-BLRMDE-1100** Mechanism for so2 Poisoning of Cu-CHA during Low Temperature $NH_3$-SCR.
**Joachim Bjerregaard**[1], Martin Votsmeier[2] and Henrik Grönbeck[1], *(1)Chalmers University of Technology, Sweden, (2)Umicore AG & Co. KG, Germany*.

**Short Summary:**
Density functional theory (DFT) calculations are performed to investigate the deactivation of Cu-CHA by SO2 during low-temperature $NH_3$-SCR. We propose a mechanism involving the reaction of SO2 with $[Cu_2(NH_3)4O_2]^{2+}$, a critical intermediate in low-temperature $NH_3$-SCR. We suggest that the loss in SCR activity originates from destabilization of paired $[Cu(NH_3)_2]$+ complexes.

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11:20 AM **Fri-BLRMDE-1120** Poisoning of Cu-CHA Catalyst for $NH_3$-SCR By $SO_2$ Monitored By X-Ray Absorption Spectroscopy.
Anastasia Molokova[1,2], **Kirill Lomachenko**[1], Gloria Berlier[2], Elisa Borfecchia[2], Silvia Bordiga[2], Fei Wen[3], Peter N.R. Vennestrøm[4] and Ton V.W. Janssens[4], *(1)European Synchrotron Radiation Facility, France, (2)University of Turin, Italy, (3)Umicore AG & Co, Germany, (4)Umicore Denmark ApS, Denmark*.

**Short Summary:**
Well-defined Cu species in Cu-CHA catalysts have been exposed to $SO_2$ at 200 °C, and the X-ray absorption spectra were recorded in-situ. $SO_2$ reacts with the $[Cu^{II}(NH_3)_4O_2]^{2+}$ complex, a key intermediate in the $NH_3$-SCR reaction cycle. This provides an explanation for the sensitivity of Cu-CHA catalysts for $NH_3$-SCR.

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11:40 AM **Fri-BLRMDE-1140** Reactor-Based Temperature-Cycled Sulfur Exposure over a Cu-SSZ-13 Catalyst for $NH_3$-SCR.
**Lai Wei**[1], Dylan Trandal[1], Unmesh Menon[1], Rohil Daya[1], Hongmei An[1], Poonam Rani[2], William Epling[2] and Yuhui Zha[1], *(1)Cummins Inc., USA, (2)University of Virginia, USA*.

**Short Summary:**
A reactor-based temperature-cycled sulfur exposure method was developed for Cu-SSZ-13 SCR catalysts to mimic the real-world sulfur exposure. The impact of reactor-based temperature-cycled sulfur exposure on both the active Cu sites and zeolite framework of the Cu-SSZ-13 catalyst was also investigated.

## Rotunda

### Electrocatalytic Hydrogen and Oxygen Activation

Session Chairs: Astrid Mueller, *University of Rochester, USA* and Omar Abdelrahman, *University of Massachusetts Amherst, USA*.

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8:00 AM **Fri-RTND-0800** Fast Oxygen Reduction and Evolution Kinetics Enabled By $LaNi_{0.5}Co_{0.5}O_3$ Perovskite Cathode for a Molten Salt Li-$O_2$ Battery.
Qianyuan Qiu, Zhengze Pan, Penghui Yao and **Yongdan Li**, *Aalto University, Finland*.

**Short Summary:**
We report a reversible lithium oxygen battery with bulk perovskite oxide as both the substrate and catalyst working at 160 oC. The LOB delivers charge-discharge overpotential 50 mV and energy efficiency as high as 98.2% in 100 cycles. A porous and fluffy $Li_2O$ is the discharge product without remaining $Li_2O_2$.

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8:20 AM **Fri-RTND-0820** Hydrogen Peroxide, an Oxidant, or a Potential Fuel for Next Generation Batteries.
**Samira Siahrostami**, *University of Calgary, Canada; Simon Fraser University, Canada*.

**Short Summary:**
Metal-air batteries are one of the most promising next generation energy technologies. However, the challenges associated with the air electrode such as slow kinetic of oxygen redox reactions hinders their widespread application. This talk will discuss the concept of a novel rechargeable battery based on hydrogen peroxide redox chemistry.

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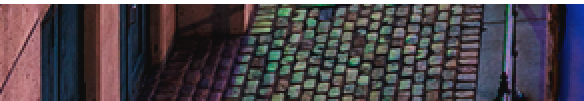
8:40 AM **Fri-RTND-0840** Novel NiFe Based Catalysts for Hydrogen Production By Water Electrolysis in Alkaline Medium.
**Victor Raud**[1] and Laurence Pirault-Roy[2], *(1)IC2MP/Université de Poitiers, France, (2)IC2MP, Institute of Chemistry of Poitiers: Materials and Natural Resources/University of Poitiers, France*.

**Short Summary:**
A new synthesis pathway of novel corosion resistant and conductive support for OER in alkaline media was studied using ball milling. NiFe catalysts were developed using this new support and the performances of this new catalysts are promising. The importance of the catalysts loading and metal ratio was then investigated.



9:00 AM **Fri-RTND-0900** Role of Palladium Hydride on the Electrocatalytic Hydrogenation of *Cis,Cis*-Muconic Acid to Biobased Adipic Acid.
**Prathamesh T. Prabhu**[1,2], Deep M. Patel[1,2], Samantha Kling[1,2], Luke Roling[1,2] and Jean-Phillippe Tessonnier[1,2], *(1)Iowa State University, USA, (2)Center for Biorenewable Chemicals (CBiRC), USA*.

**Short Summary:**
Biobased muconic acid can be electrocatalytically hydrogenated to adipic acid, a Nylon 6,6 building block, using carbon-supported noble metal catalysts. While the reaction follows a similar pathway on all metal surfaces, Pd/C showed a much higher activity, which may be attributed to the presence of a Pd hydride phase.

## Characterization of Electrocatalysts and Supports

Session Chairs: Christopher Williams, *University of South Carolina, USA* and Eli Stavitski, *Brookhaven National Laboratory, USA*.

9:40 AM **Fri-RTND-0940** Identifying and Alleviating the Durability Challenges in the Membrane-Electrode-Assembly for High-Rate CO Electrolysis.
**Qiucheng Xu** and Brian Seger, *Technical University of Denmark, Denmark*.

**Short Summary:**
By utilizing the *operando* wide-angle X-ray scattering (WAXS) technique and monitoring the dynamic change of electrolyte and components, we identified several degradation mechanisms of the membrane-electrode-assembly (MEA) during the high-rate and long-term CO electrolysis, *e.g.*, the GDEs flooding and metal contaminant at cathode cause the predomination of competitive HER.

10:00 AM **Fri-RTND-1000** Characterizing Acidic Electrolyte Effects on Degradation of Non-Precious PEM Fuel Cell Cathode Catalysts with On-Line ICP-MS.
**Gaurav Kamat**[1,2], Sanzeeda Shuchi[1], Melissa Kreider[1,2], Ashton Aleman[1,2], Michaela Burke Stevens[2] and Thomas F. Jaramillo[1,2], *(1)Stanford University, USA, (2)SLAC National Accelerator Laboratory, USA*.

**Short Summary:**
We use an electrochemical flow cell coupled to on-line ICP-MS to provide specific mechanistic insights into degradation phenomena occurring during oxygen electroreduction on non-Pt transition metals in acidic environments. This approach in general accelerates the identification of conditions where low-cost materials are stable during catalysis in various microenvironments.

10:20 AM **Fri-RTND-1020** Modeling of Copper Nanoparticles Sintering during $CO_2$RR Using Kinetic Monte Carlo Approach.
**Hori Pada Sarker** and Frank Abild-Pedersen, *SLAC National Accelerator Laboratory, USA*.

**Short Summary:**
Cu-based electrocatalysts have shown drastic changes in morphology and crystal structure during $CO_2$RR which limits durability. To gain insights into the dynamic phenomena of degradation, herein, a Kinetic Monte Carlo approach is used to simulate sintering of Cu nanoparticles supported on a graphene layer.

10:40 AM **Fri-RTND-1040** Near-Surface X-Ray Characterization of Titanium Electrode Evolution Under Electrochemical Nitrate Reduction Reaction Conditions.
**Jinyu Guo**[1], Matthew Liu[1], Adam Hoffman[2], Joakim Stenlid[1,2], Michael Tang[1,2], Kristen Abels[1], Sarah Blair[1], Elizabeth Corson[1], Alessandro Gallo[2], Dean Miller[1], Kindle Williams[1], Jose Zamora Zeledon[1], Thomas F. Jaramillo[1,2], Kevin Stone[2], Frank Abild-Pedersen[2], Simon Bare[2] and William Tarpeh[1,2], *(1)Stanford University, USA, (2)SLAC National Accelerator Laboratory, USA*.

**Short Summary:**
We combined GIXRD and XAS measurements of Ti electrodes with electrochemical testing to quantitatively link near-surface structure with $NO_3$RR performance. Ti hydride was observed and found to be enriched with increasing $NO_3$RR applied potential and duration. *In situ* XAS demonstrated the time evolution and electrolyte effects on the hydride formation.

11:00 AM **Fri-RTND-1100** Unraveling Hierarchical Pore Networks Using Differential High-Resolution Mercury Intrusion.
**Anthony Thornton**[1], Luca Lucarelli[2] and Jeffrey Kenvin[1], *(1)Micromeritics Instrument Corporation, USA, (2)Micromeritics Instrument Corporation, Italy*.

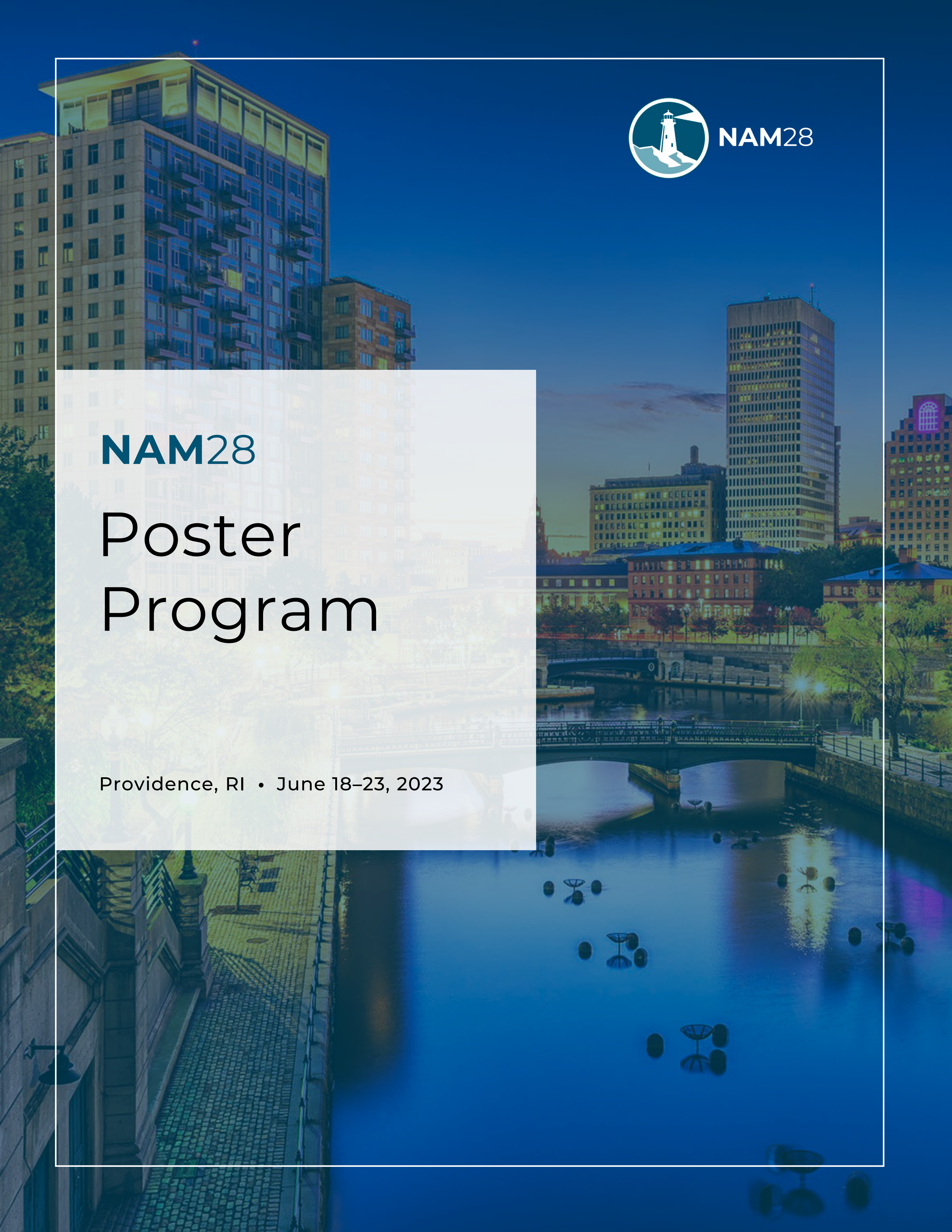
**Short Summary:**
A new method for determining pore cavity volume filled through pore throats is presented along with results for eight different alumina and titania catalyst supports.

11:20 AM **Fri-RTND-1120** Tuning the Functionality and Reactivity of Carbon Surfaces.
**Jiahua Zhou**, Piaoping Yang, Pavel Kots, Maximilian Cohen, Stavros Caratzoulas, Weiqing Zheng and Dionysios Vlachos, *University of Delaware, USA*.

**Short Summary:**
Our work not only provides novel insights into the nature of the oxygen species on carbon surfaces but also open an opportunity to develop analytical approaches by combining nutimodal characterizations and machine learning in identifying active centers in heterogeneous. The methodology we introduce can be applied to other materials.

11:40 AM **Fri-RTND-1140** Liquid-Phase Adsorption Isotherms of Formate Species on Platinum Via MSD Analysis of Active Particle Dynamics.
**Ezra Baghdady**, J. Will Medlin and Daniel K. Schwartz, *University of Colorado, USA*.

**Short Summary:**
The attenuation of peroxide-fueled active particle drift velocity in the presence of adsorbates is used to determine liquid-phase adsorption parameters of formate species on metal catalysts. The results demonstrate a method for obtaining quantitative adsorption parameters in the liquid phase for the development of liquid phase catalysis.



NAM28

# NAM28

# Poster Program

Providence, RI • June 18–23, 2023

# Monday Poster Sessions

## Exhibit Hall CD

### Conversion of Hydrocarbon Feedstocks Poster Session

**Mon-P-87**
**Advances in Catalyst Testing for Hydroprocessing Applications**
Benjamin Mutz and Ioan-Teodor Trotus, *hte GmbH, Germany*.

**Short Summary:**
An efficient choice of catalysts for any application, requires many experiments to be performed. For this, high throughput technology, is an indispensable tool. Our work utilizes this tool in hydroprocessing applications to develop sustainable solutions toward reducing material waste and $CO_2$ emission abatement via the upgrading of renewable raw materials.

### Catalysis for Chemical Synthesis and Functionalization Poster Session

**Mon-P-17**
**Dynamic Perturbation of Catalyst-Adsorbed Surface Species for Selective Acrylonitrile Formation Via Propylene Ammoxidation**
Debtanu Maiti[1], M. Ross Kunz[1], Kai Wu[2], Kenneth L. Kusima[2], Rebecca Fushimi[1] and Lars Grabow[2], *(1)Idaho National Laboratory, USA, (2)University of Houston, USA*.

**Short Summary:**
Dynamic ammoxidation of propylene over industrial bismuth molybdate catalysts can allow for on-demand flexible and distributed manufacturing of high-value hydrocarbons. This investigation using the Temporal Analysis of Products (TAP) reactor demonstrates the importance and ways of controlling catalyst surface states, and adsorbate coverages for flexible manufacturing of acrylonitrile and acrolein.

### Catalyst Design, Synthesis and Manufacturing Poster Session

**Mon-P-51**
**Bimetallic Single-Atom Catalysts Demonstrate Synergistic Interactions Enhancing Reactivity for CO Oxidation**
Kayla Eudy[1], Zayne Weber[1], Michael Janik[2] and Rob Rioux[1], *(1)Pennsylvania State University, USA, (2)The Pennsylvania State University, USA*.

**Short Summary:**
A Pd-Pt single atom catalyst (SAC) is more active on a per atom basis with a lower apparent activation energy than monometallic SACs of Pd(or Pt) for CO oxidation. This unique kinetic behavior suggests Pd and Pt influence the reaction mechanism through non-bonding interactions mediated by the reducible ceria support.

### Catalysis for Environmental Applications and Sustainable Nitrogen Chemistry Poster Session 1

**Mon-P-36**
**Revised Nitrogen Reduction Scaling Relations from Potential-Dependent Modeling of Chemical and Electrochemical Steps**
Cooper Tezak[1], Nicholas Singstock[1] and Charles Musgrave[2], *(1)University of Colorado, Boulder, USA, (2)University of Colorado, USA*.

**Short Summary:**
The electrochemical nitrogen reduction reaction was modeled on (111), (211), and (110) facets of metal surfaces with Grand Canonical Density Functional Theory using a composite mechanism. The first protonation and chemical desorption steps were identified as potential determining steps, which should be the focus of future catalyst discovery studies.

## Carbon Dioxide Conversion Poster Session 1

**Mon-P-1**

**Low Contents of Zn on Cu/$SiO_2$ Modify the Surface and the Mechanism of $CO_2$ Hydrogenation to Methanol**

Tomás Vergara Senociain[1], Daviel Gomez[1], Sebastian Collins[2], Romel Jiménez[1] and Alejandro Karelovic[1], *(1)Universidad de Concepción, Chile, (2)Instituto de Desarrollo Tecnológico para a Industria Química, Argentina*.

**Short Summary:**

The ultra-low Zn content addition increases the TOF of methanol by more than an order of magnitude and forms heterogeneous surface sites with strong affinity for CO. On catalysts with a higher Zn content, the surface is homogeneous, stabilizes the formates and reduces the $E_{app}$ of methanol.

## Catalyst Design, Synthesis and Manufacturing Poster Session

**Mon-P-52**

**Ni Nanoparticle Exsolution from the $NiAl_2O_4$ Spinel Catalyst for Dry Reforming of Methane**

Min-Jae Kim, Jeongmin Kim, Bon-Jun Ku and Kyubock Lee, *Chungnam National University, Korea, Republic of (South)*.

**Short Summary:**

The exsolution was mainly investigated with perovskite structure. In this study, we report the exsolution phenomenon happened in spinel catalyst, which combined with the various characterization technique and complementary density functional theory calculations.

## Catalysis for Environmental Applications and Sustainable Nitrogen Chemistry Poster Session 1

**Mon-P-37**

**Low-Temperature Methane Oxidation Catalysts to Reduce GHG Emissions from Lean-Burn Natural Gas Engines**

Melanie Moses-DeBusk, *Oak Ridge National Laboratory, USA*.

**Short Summary:**

New methane oxidation catalyst formulations are needed to reduce GHG emissions from lean-burn natural gas engines used in hard-to-electrify sectors. State-of-the-art catalysts are not effective for methane oxidation in the low exhaust temperatures of these high-efficiency engines. Modified-Pd supported catalysts are presented that improve low temperature activity and hydrothermal durability.

## Carbon Dioxide Conversion Poster Session 1

**Mon-P-2**

**$CO_2$-to-Value Including Rwgs As Crucial Step for Fast Process Integration, Fully Supported By High Throughput Experimentation**

Benjamin Mutz, Peter Kolb and Marius Weber, *hte GmbH, Germany*.

**Short Summary:**

This presentation describes the $CO_2$-to-value path with focus on CO production via rWGS supported by performance results using hte's most advanced 16-fold high throughput experimentation setup. Cu and Ni catalysts were used to gain insights into the rWGS process while optimizing the process parameters toward >98% CO selectivity.

## Conversion of Hydrocarbon Feedstocks Poster Session

### Mon-P-88

### Highly Selective and Coke-Resistant Ga/SUZ-4 Zeolites for Ethane Dehydrogenation

Sunkyu Kim, Jian Pan and Raul Lobo, *University of Delaware, USA*.

**Short Summary:**

A Ga supported on SUZ-4 zeolite catalyzes the ethane dehydrogenation reaction with high $C_2H_4$ selectivity and high resistance to coking. Extraframework Ga species exchanged with Brønsted acid sites on the SUZ-4 can contribute to high activity and stability without carbon formation during the reaction.

## Catalysis for Chemical Synthesis and Functionalization Poster Session

### Mon-P-18

### Precious Metal-Free $LaMnO_3$ Perovskite Catalyst with an Optimized Nanostructure for Aerobic C–H Bond Activation Reactions: Alkylarene Oxidation and Naphthol Dimerization

Emrah Ozensoy, *Bilkent University, Turkey*.

**Short Summary:**

In this work, we developed a highly effective precious metal-free $LaMnO_3$-based perovskite catalyst for C–H bond activation in alkylarene oxidation and naphthol dimerization and unraveled various relevant catalytic structure-functionality relationships.

## Carbon Dioxide Conversion Poster Session 1

### Mon-P-3

### Identification of Active Phase of Copper-Based Nanocatalysts Under Reverse Water-Gas Shift Reaction Conditions

Sundaram Bhardwaj Ramakrishnan, Ravi Teja Addanki Tirumala and Marimuthu Andiappan, *Oklahoma State University, USA*.

**Short Summary:**

This work aims to study the active phase of Cu-based nanomaterials during $CO_2$ reduction under Reverse-Water-Gas-Shift reaction conditions

## Conversion of Hydrocarbon Feedstocks Poster Session

### Mon-P-89

### Plastic Waste Upgrade to Olefins Via Microwave Pyrolysis over Solid Acids

Esun Selvam[1], Pavel Kots[1], Borja Hernandez[1], Abhinav Malhotra[1], José Catalá-Civera[2], Jesús Santamaría[3], Marianthi Ierapetritou[1] and Dionysios Vlachos[1], *(1)University of Delaware, USA, (2)Universitat Politècnica de València, Spain, (3)Universidad de Zaragoza, Spain*.

**Short Summary:**

Catalytic pyrolysis is a very promising chemical upcycling strategy as it is feedstock agnostic. However, the high energy demand associated with pyrolysis is a significant drawback. This work demonstrates a single-pot, microwave-assisted catalytic approach to selectively convert polyethylene to medium-sized olefins ($C_4$-$C_{12}$) at low reaction temperatures in seconds.

## Catalysis for Chemical Synthesis and Functionalization Poster Session

**Mon-P-19**

### Ce and Au Promoted Nanostructured Manganese Tungstate Catalysts for Selective Oxidation of Cyclohexane

Senpei Peng and David Chadwick, *Imperial College London, United Kingdom*.

**Short Summary:**

The effect of preparation pH on the catalyst activity of nanostructured $MnWO_4$ in the cyclohexane selective oxidation was studied. Different functionalities of the Mn and W oxides suggested a possible synergistic effect of two species on the catalyst surface. Ce and Au promotion further improved catalyst activity and selectivity, respectively.

## Catalyst Design, Synthesis and Manufacturing Poster Session

**Mon-P-53**

### Design of Multi-Component Alloy Metal Catalyst Based on the Exsolution Method for Efficient Dry Reforming of Methane

Dong Hyun Kim[1], Beom-Jun Kim[2], Min-Jae Kim[1], Yong Jun Kim[1], Jeong-Cheol Seo[3], Hyun-Seog Roh[2] and Kyubock Lee[1], *(1)Chungnam National University, Korea, Republic of (South), (2)Yonsei University, Korea, Republic of (South), (3)Korea Research Institute of Chemical Technology, Korea, Republic of (South).*

**Short Summary:**

In this study, we propose Ni+M(Co, Cu, and Fe)/$Al_2O_3$ catalyst with a well-defined mesoporous structure, robust thermal stability, and high specific surface area, which could be synthesized based on a spinel structure by exsolution process.

## Catalysis for Environmental Applications and Sustainable Nitrogen Chemistry Poster Session 1

**Mon-P-38**

### Kinetic Modeling of Site Transformations in a Cu/SSZ-13 SCR Catalyst during Aging

Tetyana Zheleznyak[1], Petr Koci[1], Poonam Rani[2], Lai Wei[2,3] and William Epling[2], *(1)University of Chemistry and Technology, Czech Republic, (2)University of Virginia, USA, (3)Cummins Inc., USA*.

**Short Summary:**

Migration of Cu species during hydrothermal aging, as well as the change in Cu distribution on low-temperature and high-temperature $NH_3$ oxidation and SCR reaction mechanisms are considered. Transformation of $Z_2Cu$ and ZCuOH is described, but also agglomeration of Cu atoms into clusters and further into CuO nanoparticles.

## Catalysis for Chemical Synthesis and Functionalization Poster Session

**Mon-P-20**

### Exploring Regimes during Plasma Catalytic Ammonia Synthesis

Fnu Gorky and Maria Carreon, *University of Massachusetts Lowell, USA*.

**Short Summary:**

We identify two possible regimes during plasma catalytic ammonia synthesis, a metal and a surface-plasma driven in mesoporous silica. At lower plasma densities, the addition of metal is beneficial, while at higher power and plasma density, the best performance is achieved without the aid of a metal catalyst.

## Catalyst Design, Synthesis and Manufacturing Poster Session

**Mon-P-54**

### Mapping the Evolution of Atomically Dispersed Transition Metal Catalysts from Surface to Subsurface Sites on MgO Support

Rachita Rana[1], Ambarish Kulkarni[2], Simon Bare[3], Coleman Kronawitter[2], Yizhen Chen[2], Sam Holton[2], Ty Sours[2] and Bruce Gates[2], *(1)University of California, USA, (2)University of California - Davis, USA, (3)SLAC National Accelerator Laboratory, USA*.

**Short Summary:**

Screening of TMs to understand the nature of atomically dispersed sites was successfully accomplished and the trends for the most commonly used TMs– Ni, Pd, and Pt on MgO were experimentally studied. This experiment-theory integrated synthesis creates a pathway towards predictive and well-defined site synthesis for targeted stability and activity.

## Catalysis for Environmental Applications and Sustainable Nitrogen Chemistry Poster Session 1

**Mon-P-39**

### Dielectric Barrier Discharge Plasma Catalysis to Produce Ammonia from Seawater Gathered in Massachusetts

Shelby Guthrie and Maria Carreon, *University of Massachusetts Lowell, USA*.

**Short Summary:**

This work utilizes seawater vapor to synthesize ammonia through non-thermal plasma catalysis, with a dielectric barrier discharge reactor. We employed different catalysts, among them the highest ammonia production rates occurred at a high plasma power and with the $CoSiO_2$ catalyst.

## Carbon Dioxide Conversion Poster Session 1

**Mon-P-4**

### $ZrO_2/CeO_2$ supported Niga Alloy for $CO_2$ Hydrogenation to Methanol

Laura Proaño and Christopher Jones, *Georgia Institute of Technology, USA*.

**Short Summary:**

$ZrO_2$-$CeO_2$ mixed oxides were evaluated as supports of NiGa alloy during $CO_2$ hydrogenation to methanol. The creation of oxygen vacancies in the support resulted in enhanced methanol yield. Different Zr:Ce molar ratios were employed to tune Ov concentration of the support, and the $Zr_7Ce_3$ exhibit the highest productivity.

## Conversion of Hydrocarbon Feedstocks Poster Session

**Mon-P-90**

### Effects Zeolite Acidity and Pore Structure on Polyolefin Cracking

Leilei Dai, Ozlem Karakas, Yanling Cheng, Paul Chen and Roger Ruan, *University of Minnesota, USA*.

**Short Summary:**

The relationship between catalyst lifetime and zeolite acidity/pore structure during catalytic cracking of polyolefins was clearly demonstrated, which will enable us to formulate catalyst design rules, and synthesize better catalysts, with the aim to maximize lifetime.

## Catalysis for Environmental Applications and Sustainable Nitrogen Chemistry Poster Session 1

**Mon-P-40**

**Nano-Sized Ru/$MgAl_2O_4$ Catalyst for $CO_x$-Free Hydrogen Production Via Ammonia Decomposition Reaction**

Kyoung Deok Kim[1], Jiyu Kim[2], Unho Jung[3], Yongha Park[3], Kwang Bok Yi[4] and Kee Young Koo[5], *(1)Korea Institute of Energy Research/Chungnam National University, Korea, Republic of (South), (2)Korea Institute of Energy Research/Korea University, Korea, Republic of (South), (3)Korea Institute of Energy Research, Korea, Republic of (South), (4)Chungnam National University, Korea, Republic of (South), (5)Korea Institute of Energy Research/University of Science and Technology, Korea, Republic of (South).*

**Short Summary:**

Ru/$MgAl_2O_4$ catalyst (polyol) showed the best catalytic activity at low temperature of 450 °C and 30,000 mL/$g_{cat}$·h in $NH_3$ decomposition reaction. It is due to the fact that the polyol method improves the formation of the B5 site, the main active site of Ru.

## Carbon Dioxide Conversion Poster Session 1

**Mon-P-5**

**Perovskite Oxide Composites for Thermochemical $CO_2$ Conversion**

Bryan Hare, Hanzhong Shi, Debtanu Maiti, Jeremy Brower, Venkat R. Bhethanabotla and John Kuhn, *University of South Florida, USA.*

**Short Summary:**

Perovskite oxide face materials design challenges for use as catalysts. The current effort details advances made to exploit materials oxygen shuttling abilities for thermochemical $CO_2$ conversion.

## Conversion of Hydrocarbon Feedstocks Poster Session

**Mon-P-91**

**Direct Conversion of Ethylene to Propylene through Simultaneous Ethylene Dimerization and Olefin Metathesis with Dual-Site 8%$NiSO_4$/8%$ReO_4$/γ-$Al_2O_3$ Catalyst**

Eli Ream[1], Shuting Xiang[2] and Israel Wachs[1], *(1)Lehigh University, USA, (2)Stony Brook University, USA.*

**Short Summary:**

A supported 8%$NiSO_4$/8%$ReO_4$/γ-$Al_2O_3$ dual-site catalyst was synthesized for the direct conversion of ethylene to propylene, in which $NiSO_4$ performs ethylene dimerization to butenes and $ReO_4$ performs olefin metathesis to propylene. The catalyst was extensively characterized at the molecular level, revealing new insights about the structure-function relationship.

## Catalysis for Chemical Synthesis and Functionalization Poster Session

**Mon-P-21**

**Impact of Heat Treatment and Thiol Modifiers on the Selective Oxidation of Glutaraldehyde Using Pd/$Al_2O_3$**

Faysal Al Khulaifi[1,2], Yousef Alsunni[1,2], Charles Musgrave[1], Adam Holewinski[1] and J. Will Medlin[1], *(1)University of Colorado Boulder, USA, (2)King Fahd University of Petroleum and Minerals, Saudi Arabia.*

**Short Summary:**

In the partial oxidation reaction of glutaraldehyde using Pd/$Al_2O_3$, heat pretreatment of the catalyst enhances activity and reduces induction period. Using hydrophilic thiolate surface modifiers, such as thioglycerol, induces selectivity promotion. DFT calculations indicate that hydrogen-bonding interactions between reaction species and thiol ligands are the dominant effect in influencing selectivity.

## Catalyst Design, Synthesis and Manufacturing Poster Session

**Mon-P-55**

### Effect of the Acidic, Alkali, Ion Exchange and Tandem Modification over Textural Properties of Mexican Clinoptilolite

Francisco Javier Sanabria Pérez[1], Carolina Solis Maldonado[1], María Rebeca Rojas Ronquillo[1], Rodrigo Cuervo[1], Ladislao Sandoval-Rangel[2], Lucía Atehortua[3], Gloria Dimas Rivera[4] and Javier Rivera De la Rosa[4], *(1)Universidad Veracruzana, Mexico, (2)Tecnológico de Monterrey, Mexico, (3)Universidad de Antioquia, Colombia, (4)Universidad Autónoma de Nuevo León, Mexico*.

**Short Summary:**

Clinoptilolite was modified with individual, tandem impregnations (combined) and calcination procedures. We design a hierarchical catalyst for use in pyrolysis with bulky molecules of biomass (seaweed and synthetic polymers). Tandem modification achieved a superior hierarchical catalyst due to increases the surface area, the pore volume and the mesopore size.

## Conversion of Hydrocarbon Feedstocks Poster Session

**Mon-P-92**

### Cross-Metathesis of Acetylene-Ethylene over Supported $WO_3/SiO_2$ Catalysts: Alternative Approach for Acetylene Removal in Ethylene Feedstock

Pratya Promchana[1], Tawan Sooknoi[1,2] and Kittisak Choojun[1,2], *(1)King Mongkut's Institute of Technology Ladkrabang, Thailand, (2)King Mongkut's Institute of Technology Ladkrabang, Thailand*.

**Short Summary:**

Alternative approach for ethylene purification via cross-metathesis between acetylene impurity with ethylene feed could be achieved over $WO_3/SiO_2$ catalysts. The active W=O species can be obtained depending on $WO_3$ loading and types of $SiO_2$ supports. The isolated $W=CH_2$ species obtained in 5%$WO_3$/MCM-41 and 5%$WO_3$/SBA-15 are more active and coke resistance.

## Catalysis for Chemical Synthesis and Functionalization Poster Session

**Mon-P-22**

### Precise Control of Electron Hole Density for Surface Chemistry Regulation Using a Platinum Catalytic Condenser

Benjamin Page[1] and Omar Abdelrahman[2,3], *(1)University of Massachusetts, Amherst, USA, (2)University of Massachusetts Amherst, USA, (3)University of Minnesota, USA*.

**Short Summary:**

The authors utilized a platinum catalytic condenser and temperature-programmed desorption (TPD) to demonstrate how different applied catalytic voltages can alter the binding energy of CO onto the catalyst surface at a frequency range permitting catalytic resonance, which has shown to enhance the rate of reaction.

## Catalysis for Environmental Applications and Sustainable Nitrogen Chemistry Poster Session 1

**Mon-P-56**

### Rational Design of Well-Dispersed Single Fe Sites in Hierarchical ZSM-5

Peeranat Chaipornchalerm[1] and Chularat Wattanakit[2], *(1)Vidyasirimedhi Institute of Science and Technology, Thailand, (2)Vidyasirimedhi Institute of Science and Technology (VISTEC), Thailand*.

**Short Summary:**

The single Fe species on hierarchical zeolite was successful synthesized via atomic layer deposition procedure. The EXAFS and TEM-EDS characterization revealed the existence of highly dispersed Fe atoms as a single-site stabilized by the oxygen framework. This catalyst is expected to apply in both of chemical production and material synthesis.

## Catalysis for Environmental Applications and Sustainable Nitrogen Chemistry Poster Session 1

**Mon-P-41**

**CO Interaction over CuNi Supported on Nanostructured Ceria: An Experimental-Theoretical Approach.**

Mishai Avila[1], Christian A. Celaya[2], Diana G. Arcos[1], Jesús Muñiz Soria[2] and Gabriela Díaz[1], *(1)Instituto de Física, Universidad Nacional Autónoma de México, Mexico, (2)Universidad Nacional Autónoma de México (UNAM), Mexico.*

**Short Summary:**

Support effects (ceria cubes and polyhedra) on reactivity of CO with $O_2$ over CuNi catalysts was evaluated. Synergistic effects were observed but reactivity was lower over ceria cubes. DFT calculation showed the proposed sites for CO adsorption over optimized $Cu_n$-$Ni_m$/$CeO_2$ (111) systems and their role in the CO oxidation mechanism.

## Carbon Dioxide Conversion Poster Session 1

**Mon-P-6**

**Kinetic Modeling for Direct Conversion of $CO_2$ Via Fischer-Tropsch Synthesis**

Yubeen Jung[1], Yesol Woo[1], Hyeon Park[1], Hae-Gu Park[2], Jeong-Rang Kim[2], Ki-Won Jun[2] and Myung-June Park[1], *(1)Ajou University, Korea, Republic of (South), (2)KRICT(Korea Research Institute of Chemical Technology), Korea, Republic of (South).*

**Short Summary:**

A kinetic model for detailed hydrocarbon distribution of $CO_2$-FTS was developed on the basis of two parallel pathways (direct $CO_2$ conversion and RWGS followed by CO-FTS). The CFD model for a mini-pilot scale $CO_2$-FTS reactor was developed.

## Catalyst Design, Synthesis and Manufacturing Poster Session

**Mon-P-57**

**Hierarchical Zeolites Synthesized from Recycled Al and Si Resources for Friedel-Crafts Alkylation**

Jesús Eduardo García Rodríguez, Jorge G. Huerta and Brent E. Handy, *Universidad Autónoma de San Luis Potosí, Mexico.*

**Short Summary:**

Synthesis of zeolite ZSM-5 from recycled resources and it's hierarchization, characterization and evaluation on benzyl alcohol benzylation reaction and it's polymerization.

## Catalysis for Environmental Applications and Sustainable Nitrogen Chemistry Poster Session 1

**Mon-P-42**

**Impact of Amorphous Silica Alumina Physical Properties As a Pt/Pd Support for Environmental Catalysts.**

Jeremy Madynski[1], David Shepard[1,2] and Ashwin Sankaran[1], *(1)Pacific Industrial Development Inc, USA, (2)PIDC, USA.*

**Short Summary:**

The physical properties of different amorphous silica alumina as supports for precious metal-based catalysts impacted the light off temperatures for conversion of both carbon monoxide and hydrocarbons. The data showed a strong correlation between larger volume of mesopores and catalytic activity.

## Carbon Dioxide Conversion Poster Session 1

**Mon-P-7**

**High $C_2$-$C_4$ Selectivity in $CO_2$ Hydrogenation By Particle Size Control of Co-Fe Alloy Nanoparticles Wrapped on N-Doped Graphitic Carbon**

Vasile Parvulescu[1], Lu Peng[2], Ana Primo[2], Bogdan Jurca[1], Octavian D. Pavel[1], Alvaro Gordillo[3] and Hermenegildo Garcia[2], *(1)University of Bucharest, Romania, (2)Universitat Politècnica de València, Spain, (3)BASF SE, Germany.*

**Short Summary:**

This study shows the importance of the size control in Co-Fe NPs wrapped on N-doped graphitic carbon hydrogenation of $CO_2$ to hydrocarbons with more than one carbon. Experimental and theoretical calculations demonstrated that a size window around 10 nm of the Co-Fe favors the formation of C2-C4 hydrocarbons.

## Conversion of Hydrocarbon Feedstocks Poster Session

**Mon-P-93**

**Catalytic Production of $H_2$ from $H_2S$: Challenges and Opportunities**

Hassan Aljama, Zainab Alaithan and Ali Almofleh, *Aramco, Saudi Arabia*.

**Short Summary:**

$H_2S$ is currently treated by converting it to sulfur and water. Ideally, $H_2S$ is converted to $H_2$. We shed light on the role of adsorbates and transition states in $H_2S$ splitting using DFT. We identify the limitations of the catalysts and outline the ideal catalyst properties to overcome these limitations.

## Catalysis for Chemical Synthesis and Functionalization Poster Session

**Mon-P-23**

**Modeling of Hydrolysis/Alcoholysis of Tris(pentafluorophenyl)Borane (BCF) in Epoxide Ring-Opening Reactions**

Guanhua Wang[1], Hiyab Mekonnen[1], Carlos Villa[2], Arjun Raghuraman[2], Varinia Bernales[2], Sukaran Arora[2], Saket Bhargava[2], Justin Notestein[1] and Linda Broadbelt[1], *(1)Northwestern University, USA, (2)The Dow Chemical Company, USA*.

**Short Summary:**

Uncovering this catalyst's decomposition could be critical to the understanding of the ring-opening of epoxides and lead to proposals of new catalysts that perform the regioselective reaction towards P1. Incorporating reaction kinetics from the DFT calculations into a microkinetic model offers perspectives on a larger scale.

## Carbon Dioxide Conversion Poster Session 1

**Mon-P-8**

**Hydrogenation of $CO_2$ over Supported Ni Catalysts**

Dipesh Adhikari and Robert Davis, *University of Virginia, USA*.

**Short Summary:**

The product distribution from $CO_2$ hydrogenation by $H_2$ over supported Ni nanoparticles depends on the support composition whereby $Ni/CeO_2$ is selective to $CH_4$ formation and $Ni/SiO_2$ is selective to CO formation.

## Conversion of Hydrocarbon Feedstocks Poster Session

**Mon-P-94**

**Boron-Stabilized Platinum-Copper Single Atom Alloy for Stable Non-Oxidative Light Alkane Dehydrogenation Reaction**

Kang Hui Lim, Anupam Samanta and Sibudjing Kawi, *National University of Singapore, Singapore*.

**Short Summary:**

An optimal boron doping in platinum-copper single-atom alloy catalyst effectively limits severe copper agglomeration at elevated temperatures, and boron synergistically enhances $C_3H_8$ activation and $C_3H_6$ desorption through modifying the catalyst support's properties and single atomic Pt in PtCu alloy design, thereby giving the superb stability required for commercial applications.

## Catalysis for Chemical Synthesis and Functionalization Poster Session

**Mon-P-24**

**Identification of Reaction Pathways of Chromium Species Formation in Crox/Al2O3 Dehydrogenation Catalysts**

Danielle Covelli[1], Vladimir Fridman[1], Rong Xing[1], Renqin Zhang[1] and Matthew Greaney[2], *(1)Clariant Corporation, USA, (2)Clariant, USA*.

**Short Summary:**

Growth in propylene demand has increased the need for $CrOx/Al_2O_3$ dehydrogenation catalysts. This work provides evidence regarding the reaction pathway and nature of $Cr^{6+}$ and $Cr^{3+}$ species formation in $CrOx/Al_2O_3$ dehydrogenation catalysts. This provides an opportunity to tune the catalyst to minimize the formation of hazardous species.

## Catalyst Design, Synthesis and Manufacturing Poster Session

**Mon-P-58**

**Ordered 3D Mesoporous Graphene Materials with Well-Defined and Tunable Pore Size and Shape**

Kelly J.H. Brouwer, Evert M.E. Simons and Alfons van Blaaderen, *Utrecht University, Netherlands*.

**Short Summary:**

Using well-defined $Fe_3O_4$ nanoparticles, highly ordered 3D mesoporous graphene materials were prepared. Conversion of ligand molecules resulted in graphene materials with ordered mesopores, high surface area, large pore volume and adjustable pore symmetry. The pore size could be tuned from 8–20 nm and pore shape from spherical to cubic.

## Catalysis for Environmental Applications and Sustainable Nitrogen Chemistry Poster Session 1

**Mon-P-43**

**A Study on the Ammonia Slip Catalysts for Improving N2-Selectivity in Ammonia Fueled Marine Engines**

Minseo Chun, *Eco and Dream, Korea, Republic of (South)*.

**Short Summary:**

In this study, we increased N2-selectivity(that is, NH3 conversion to N2) in ammonia fueled marine engines by coating V-SCR or Cu-CHA zeolite on ASC(Ammonia Slip Catalyst) and observed the effect of enhancing DeNOx performance and preventing ammonia slip.

## Catalysis for Chemical Synthesis and Functionalization Poster Session

**Mon-P-25**

**Using Aminosilica Catalysts to Produce Bio-Derived Surfactants: Investigating the Activity and Selectivity for Aldol Chemistry**

Hannah Pineault and Nick Brunelli, *The Ohio State University, USA*.

**Short Summary:**

Aminosilica catalysts are investigated for the production of bio-derived surfactants through aldol chemistry. Work is ongoing to improve the activity and selectivity of aminosilica by tuning the amine type, temperature, and solvation environment.

## Catalyst Design, Synthesis and Manufacturing Poster Session

**Mon-P-59**

**One-Pot Synthesis of Bulk NiMoS Catalysts: Influence of pH and Addition of Pluronic®P123. HDS of FCC Gasoline**

Laurence Courtheoux[1], Alexandre Carvalho[2], Valentin Hetier[1], Julie Rousseau[2], Etienne Girard[3], Denis Uzio[3], Patrick Lacroix-desmazes[1], Annie Pradel[1] and Brunet Sylvette[2], *(1)University of Montpellier, France, (2)University of Poitiers, France, (3)IFP Energies Nouvelles, France*.

**Short Summary:**

A novel one-pot synthesis of NiMoS bulk catalysts has been carried out. This procedure involving the reduction of a thiomolybdate followed by an *in-situ* Ni promotion in the liquid reaction medium, led to a remarkable amount of mixed NiMoS phase when it was conducted at pH 7.

## Catalysis for Environmental Applications and Sustainable Nitrogen Chemistry Poster Session 1

**Mon-P-44**

**Novel Explosion-Proof Catalytic Methane Destruction Unit for the Oil and Gas Industry’s Fugitive Emissions**

Jarek Szynkarczuk, *Thermon Canada Inc., Canada*.

**Short Summary:**

The oil and gas industry often lacks electricity while exploring for natural resources and are forced to use pneumatic equipment. Compressed natural gas is often the driving force of this equipment. We have developed an explosion-proof catalytic methane destruction unit to convert methane and other hydrocarbons to carbon dioxide.

## Carbon Dioxide Conversion Poster Session 1

**Mon-P-9**

### Quantum Mechanical Modeling of Electrocatalytic Carbon Dioxide Reduction Reactions on Copper-Doped Two-Dimensional Materials

Hongshan Bi[1], Zhihao Liu[2], Jun Yi[3], Guo Ling[4] and Zhou Lin[1], *(1)University of Massachusetts Amherst, USA, (2)University of Oxford, United Kingdom, (3)University of Massachusetts, USA, (4)University of Massachusetts, Amherst, USA.*

**Short Summary:**

This work is motivated by the need to convert CO2 with the help of catalysts into fuels and feedstocks. Our goal is to propose a transition metal-doped two-dimensional material as an alternative electrocatalyst for the electrocatalytic reduction of carbon dioxide and the mechanism is studied by means of computational chemistry.

## Conversion of Hydrocarbon Feedstocks Poster Session

**Mon-P-95**

### Tuning Ru/C Properties for Polypropylene Waste Hydrogenolysis

Jessie Sun and Dionysios Vlachos, *University of Delaware, USA.*

**Short Summary:**

Investigating the effects of catalyst particle size, structure, and metal-support interactions on Polypropylene hydrogenolysis to further advance catalyst design for applications in plastic waste upcycling.

## Catalysis for Environmental Applications and Sustainable Nitrogen Chemistry Poster Session 1

**Mon-P-45**

### Speciation of Fe Ions in Fe/CHA Catalysts Determined By Transient Response Methods

Maria Elena Azzoni[1], Isabella Nova[1], Enrico Tronconi[1], Roberta Villamaina[2], Maria Pia Ruggeri[2], Veselina Georgieva[2], Loredana Mantarosie[2] and Jillian Collier[2], *(1)Politecnico di Milano, Italy, (2)Johnson Matthey Technology Centre, United Kingdom.*

**Short Summary:**

We innovatively use transient response methods to investigate the active species of Fe/CHA catalysts for $NH_3$-SCR. NO+$NH_3$ do not reduce all the available Fe, while $NO_2$ titrates also the iron species which are not oxidized by $O_2$ alone.

## Carbon Dioxide Conversion Poster Session 1

**Mon-P-10**

### Eutectic Mixture-Promoted MgO Sorbents for $CO_2$ Capture at Low-Temperature: Kinetic Study and Pretreatment Optimization

You Seok Kang, Monica Louise Triviño and Jeong Gil Seo, *Hanyang University, Korea, Republic of (South).*

**Short Summary:**

A series of alkali nitrate eutectic mixture-promoted MgO sorbents were investigated for $CO_2$ capture at low-temperature. The kinetics of sorption behavior were calculated to find out the relationship with the EM melting point. Adsorption performance was compared by varying pretreatment conditions.

## Conversion of Hydrocarbon Feedstocks Poster Session

**Mon-P-96**

### Effects of Hollow Sphere Macroporous MCM-22 on Aromatization of Acetylene

Hee Hwan Kim, Jin Ju Hong, Jonghyun Jeon and Kyoung-Su Ha, *Sogang University, Korea, Republic of (South).*

**Short Summary:**

MWW-type zeolite with hollow sphere morphology was prepared by hard-templating method. By introducing macroporosity to the zeolite, mass transfer limitation was appreciably reduced, resulting in higher BTX yield, lower deactivation rate, and improved regeneration capability.

## Catalysis for Chemical Synthesis and Functionalization Poster Session

**Mon-P-26**

**Selective Vapor-Phase Formation of Dimethylformamide Via Oxidative Coupling of Methanol and Dimethylamine over Bimetallic Catalysts**

Alexander Minne, Tristan Maxson, Tibor Szilvasi and James Harris, *The University of Alabama, USA*.

**Short Summary:**

By combining late transition group metals, catalytic synergy is unlocked which allows for oxidative coupling chemistry over supported bimetallic nanoparticle catalysts. As the dilute metal ratio increases, the rate and selectivity of methanol and dimethylamine oxidative coupling to dimethylformamide increases.

## Catalyst Design, Synthesis and Manufacturing Poster Session

**Mon-P-60**

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

Tania Class Martínez[1], Subramanian Prasad[2], Ahmad Moini[2] and Raj Gounder[1], *(1)Purdue University, USA, (2)BASF Corporation, USA*.

**Short Summary:**

Proton-form chabazite (CHA) zeolites were synthesized with varying amounts of framework Al and percentages of 6-MR paired Al site arrangements, and used to quantify the influence of zeolite material properties on the kinetics of dealumination under hydrothermal aging conditions and gain fundamental insights into the mechanisms of dealumination.

## Catalysis for Chemical Synthesis and Functionalization Poster Session

**Mon-P-27**

**Acid Catalyst for the Dehydration of Polyols**

Anne Boehme, Hans-Joerg Woelk, Sean Hunt and David Weiner, *Solugen, Inc., USA*.

**Short Summary:**

As Solugen expands its chemical manufacturing footprint, it is also developing new chemistries. Within this study, numerous acid catalysts were studied for the dehydration of glucose to the formation FDCA, which is a promising substitute for widely used acids in the production of polyesters, using an acid catalyst.

## Catalyst Design, Synthesis and Manufacturing Poster Session

**Mon-P-61**

**Sequentially and Co-Deposited Palladium-Rhenium Supported Oxide Catalysts for Selective Hydrogenation**

Christopher Heaton[1,2], Gopinathan Sankar[1] and Armando Borgna[3], *(1)University College London, United Kingdom, (2)A*STAR, Singapore, (3)Agency for Science, Technology and Research in Singapore (A*STAR), Singapore*.

**Short Summary:**

It is believed that supported rhenium oxides are reduced at markedly lower temperatures when in a bimetallic system compared to monometallic analogues. This work has investigated the possible room temperature partial reduction of rhenium oxide promoted by the presumed hydrogen spillover mechanism from nearby supported palladium.

## Catalysis for Environmental Applications and Sustainable Nitrogen Chemistry Poster Session 1

**Mon-P-46**

### Highly Active Pd/$Al_2O_3$ Catalysts for Total Propane Oxidation Synthesised By Chemical Vapour Impregnation

Liam Bailey[1], Thomas Davies[2], David Morgan[3] and Stuart Taylor[3], *(1)Cardiff Catalysis Institute, United Kingdom, (2)Cardiff University, United Kingdom, (3)Cardiff Catalysis Institute, Cardiff University, United Kingdom*.

**Short Summary:**

Chemical vapour impregnation (CVI) was found to produce more active catalysts for the total oxidation of propane than wet impregnation. This was due to increased metal dispersion and number of active sites. CVI was studied in depth finding activity scaled with weighloading with activity per site consistent throughout.

## Carbon Dioxide Conversion Poster Session 1

**Mon-P-11**

### Photo-Excited Electrons Drive the $CO_2$ Reduction on $Cu_2o$

Tien Le, Taha Salavati Fard and Bin Wang, *University of Oklahoma, USA*.

**Short Summary:**

Excited electrons, in the presence of oxygen vacancies, can change both the thermodynamic and kinetic of the $CO_2$ (photo) reduction reaction on $Cu_2O$, then make this reaction is favorable on this low cost catalyst. Our results also show that oxygen vacancy is easy to form via photocatalytic hydrogenation process.

## Conversion of Hydrocarbon Feedstocks Poster Session

**Mon-P-97**

### Effect of Methane on Butane Aromatization over Metal-Modified ZSM-5

Yeseul Hwang[1,2], Yong Hyun Lim[2], Sunhwan Hwang[1], Kyong Yong Cha[1], Dong Hyun Ko[1] and Do Heui Kim[2], *(1)LG Chem, Korea, Republic of (South), (2)Seoul National University, Korea, Republic of (South)*.

**Short Summary:**

This study investigated the catalytic aromatization of n-butane, the main component of C4 raffinate. Also we introduce a scheme of the reaction in the case of adding methane which can be produced by thermal cracking of n-butane and recycled from final product of the aromatization process.

## Catalyst Design, Synthesis and Manufacturing Poster Session

**Mon-P-62**

### Au@Co Core-Shell Bimetallic Catalyst Supported on SBA-15 (Au@Co/SBA-15) for Atmospheric Pressure CO Hydrogenation

Preeti Jain[1] and Vinod C. Prabhakaran[2], *(1)University of Kansas, USA, (2)CSIR-NCL Pune, India*.

**Short Summary:**

The deactivation of the catalyst is a significant drawback in CO hydrogenation (syngas conversion/FT synthesis), and the present study provides the design of a new material, which resists the surface cobalt oxide formation and inactive coke formation and gives efficient CO conversion with high stability.

## Catalysis for Environmental Applications and Sustainable Nitrogen Chemistry Poster Session 1

**Mon-P-47**

**Efficient Technology for Catalytic Virus Inactivation**

Ana Serrano-Lotina[1], Angela Vazquez-Calvo[2], Paula Llanos[1], Alicia Gómez-López[1], Rocío Martin[2], Victor Alcolea-Rodríguez[1], Antonio Alcamí[2] and Miguel A. Bañares[1], *(1)Institute of Catalysis and Petrochemistry/ CSIC, Spain, (2)Center of Molecular Biology Severo Ochoa (CBMSO)/ CSIC, Spain*.

**Short Summary:**

Very effective catalytic filters have been prepared (being patented) and will provide an efficient technology which prevents airborne transmission of viruses. A new methodology to facilitate the pre-screening of catalytic filter has been established.

## Carbon Dioxide Conversion Poster Session 1

**Mon-P-12**

**$CO_2$ Hydrogenation to $C_2$/$C_3$ Olefins at Atmospheric Pressure Using Fe-Ce-Zr Catalysts: Effect of Potassium Incorporation**

Ananda Vallezi Paladino Lino[1], Elisabete M. Assaf[2] and José Mansur Assaf[1], *(1)Federal University of São Carlos, Brazil, (2)University of São Paulo, Brazil*.

**Short Summary:**

Fe, Ce, Zr-based catalyst was promoted with potassium, with four nominal weight contents (0,5; 1; 2 and 4%- FCZ-K0.5, FCZ-K1, FCZ-K2 e FCZ-K4, respectively),and applied to the catalytic $CO_2$ hydrogenation at atmospheric pressure, aiming to produce light olefins.

## Conversion of Hydrocarbon Feedstocks Poster Session

**Mon-P-98**

**Insights into Size Effect of $Pt/Al_2O_3$ on Hydrogen Production from Methylcyclohexane Dehydrogenation**

Yiqing Wu and Zili Wu, *Oak Ridge National Laboratory, USA.*

**Short Summary:**

Methylcyclohexane (MCH)/toluene pair is a promising liquid organic hydrogen carrier for hydrogen storage and release. As one of the most active catalysts for the MCH dehydrogenation, the performance of $Pt/Al_2O_3$ was found to be strongly dependent on Pt size with the medium Pt size showing the highest atomic efficiency.

## Catalysis for Chemical Synthesis and Functionalization Poster Session

**Mon-P-28**

**Sonogashira Synthesis of New Pafs-Embedded Palladium Nanoparticles As Heterogeneous Catalysts in Suzuki-Miyaura Cross-Coupling**

Vasile Parvulescu[1], Lidia Cata[2], Natalia Terenti[2], Cristina Cociug[2], Niculina Daniela Hadade[2], Ion Grosu[2], Simona Coman[1], MIchal Mazur[3] and Jiri Cjeka[3], *(1)University of Bucharest, Romania, (2)Babes-Bolyai University, Romania, (3)Charles University, Czech Republic*.

**Short Summary:**

This contribution demonstrates the synthesis and catalytic properties of PAFs materials self-incorporating Pd nanoparticles also unveiling their catalytic activity in C-C cross-coupling reactions of brominated derivatives and boronic acids or pinacol boronic esters. To the best our knowledge these were the first examples of POFs incorporating *in situ* generated NPS.

## Carbon Dioxide Conversion Poster Session 1

**Mon-P-13**

**Scale up Factors for Dual-Function Materials (DFM) for $CO_2$ Direct Air Capture (DAC) and Catalytic Conversion to Renewable Methane**

Monica Abdallah and Robert J. Farrauto, *Columbia University, USA*.

**Short Summary:**

Feasibility of combined $CO_2$ direct air capture (DAC) and catalytic conversion to renewable methane using the dual function material (DFM) has been shown. This presentation focuses on recent work adapting the DFM to a washcoated monolith and performing simulated long-term aging tests in accordance with scale up objectives.

## Conversion of Hydrocarbon Feedstocks Poster Session

**Mon-P-99**

**Microwave Co-Gasification of Mixed Plastics and Biomass to Produce $H_2$ Using Fe-SiC Catalyst**

Ashraf Abedin, Xinwei Bai, Mark Smith and Pranjali D. Muley, *National Energy Technology Laboratory, USA*.

**Short Summary:**

Plastic-biomass cogasification was ran using Fe-SiC catalyst while varying parameters like Fe loading, temperature and heating technique. Compared to conventional, microwave gasification required lower energy input(1.168kWh in conventional vs 0.0064kWh in microwave) to produce 5 times more hydrogen, suggesting that generated carbon may couple with microwave to produce additional hydrogen.

## Catalysis for Chemical Synthesis and Functionalization Poster Session

**Mon-P-29**

**Two-Dimensional Bimetallic Hydroxide Nanostructures for Catalyzing Low-Temperature Aerobic C–H Bond Activation in Alkylarene and Alcohol Partial Oxidation**

Emrah Ozensoy, *Bilkent University, Turkey*.

**Short Summary:**

We developed a highly efficient LDH-based noble metal-free heterogeneous catalyst for partial oxidation of alkylarenes and alcohols. Using very low catalyst loadings and by utilizing only molecular oxygen (i.e., without other additives) at mild temperatures, we were able to obtain efficient C-H activation in challenging organic substrates.

## Catalyst Design, Synthesis and Manufacturing Poster Session

**Mon-P-63**

**Synthesis and Structural Characterization of Gallium and Zinc Modified ZSM-5 Zeolites**

Luis Faith Aguilar, *UNIVERSIDAD AUTONOMA METROPOLITANA, Mexico*.

**Short Summary:**

In the present work, structural characterization studies of ZSM-5 zeolites synthesized and modified with gallium and zinc of medium and nanometric pore size, respectively, were carried out; through the isomerization/disproportionation reaction of xylenes to determine the influence of chemical and structural parameters on the activity and selectivity of said materials.

## Catalysis for Environmental Applications and Sustainable Nitrogen Chemistry Poster Session 1

**Mon-P-48**

**Nano Oxide Surface Coatings on Cu-SSZ-13 for High Temperature Selectivity SCR Applications**

David Shepard, Ashwin Sankaran, Jeremy Madynski and Geng Zhang, *Pacific Industrial Development Inc, USA*.

**Short Summary:**

The investigation of nano-oxide surface coatings onto Cu-SSZ-13 found that utilizing an optimal nano particle size alumina loading and crystallite size onto the surface of the Cu-SSZ-13 could maintain low temperature activity while boosting high temperature selectivity towards NOx reduction. These findings were consistent for both fresh and aged catalysts.

## Catalysis for Chemical Synthesis and Functionalization Poster Session

**Mon-P-30**

**Mechanistic Insights into Role of the Electrode Surface in the Selective Oxidation of Benzyl Alcohols**

Kaida Liu[1], Mayank Tanwar[1], Matthew Neurock[1], Qiwei Jing[2], Enqi Feng[2] and Kevin Moeller[2], *(1)University of Minnesota, Twin Cities, USA, (2)Washington University, USA*.

**Short Summary:**

A strikingly different performance was observed between Pt and RVC electrode during the selective oxidation of 4-methoxybenzyl alcohol over 4-nitrobenzyl alcohol (1:1 selectivity on Pt while 19:1 on RVC). Constant-potential DFT calculations along with AIMD simulations were carried out to examine the complex solid-liquid interface and elucidate the mechanistic features.

## Catalyst Design, Synthesis and Manufacturing Poster Session

**Mon-P-64**

**Synthesis of Benzaldehyde from Styrene Oxidation Catalyzed by MOF-74**

Gabriel Flores[1], Julia Aguilar Pliego[2], Jose Antonio de los Reyes[3] and Nancy Martín[3], *(1)Universidad Autónoma Metropolitana, Mexico, (2)Universidad Autonoma Metropolitana-Azcapotzalco, Mexico, (3)Universidad Autónoma Metropolitana-Iztapalapa, Mexico*.

**Short Summary:**

The synthesis of benzaldehyde will be carried out by oxidation of styrene using three M-MOF-74, The Cu catalyst was the most active and selective, followed by Co and finally Zn-MOF-74. The optimal conditions for benzaldehyde yield were: TBHP as oxidant, 75 °C, 3 hours, and Cu-MOF-74 as catalyst.

## Catalysis for Environmental Applications and Sustainable Nitrogen Chemistry Poster Session 1

**Mon-P-49**

**Nitrous Oxide As Secondary Emission from Interaction of Hydrocarbons and Nitric Oxide over Pt-Pd Oxidation Catalysts**

Patrick Lott[1], Simon Bastian[1], Heike Többen[2], Lisa Zimmermann[2] and Olaf Deutschmann[1], *(1)Karlsruhe Institute of Technology (KIT), Germany, (2)Purem GmbH, Germany*.

**Short Summary:**

The interaction of hydrocarbons and NOx over Pt-Pd oxidation catalysts can lead to the formation of the strong greenhouse gas $N_2O$. Systematic kinetic tests comprising a broad variety of relevant catalyst operation regimes identify critical parameters governing $N_2O$ formation and provide guidance in designing strategies that minimize $N_2O$ emissions.

## Carbon Dioxide Conversion Poster Session 1

**Mon-P-14**

### Monolith Supported Multifunctional Catalysts for the Direct Conversion of $CO_2$ to Dimethyl Ether

Haiying Chen, Josh Pihl, Todd Toops and Sreshtha Sinha Majumdar, *Oak Ridge National Laboratory, USA*.

**Short Summary:**

A novel monolith catalyst concept with different catalytic components coated on metallic monolith substrates as separate layers was demonstrated. This layered configuration enhances the synergistic effects while minimizing the detrimental interactions among the components. The monolith catalyst showed excellent on-steam durability for the direct conversion of $CO_2$ to DME.

## Conversion of Hydrocarbon Feedstocks Poster Session

**Mon-P-100**

### Kinetics of Propylene Oxidation over Extracrystalline Gold on Au/TS-1 Catalysts

Jeremy Arvay[1], Wei Hong[1], Christina Li[1], W. Nicholas Delgass[1], Fabio Ribeiro[1] and James Harris[1,2], *(1)Purdue University, USA, (2)The University of Alabama, USA*.

**Short Summary:**

Kinetics of propylene epoxidation are identical over intra- and extracrystalline Au on Au/TS-1, while reaction orders but not activation energies are identical for hydrogen oxidation over these catalysts. Geometric models suggest epoxidation occurs through both a simultaneous mechanism and kinetically relevant diffusion of $H_2O_2$ from Au to distant Ti sites.

## Catalysis for Environmental Applications and Sustainable Nitrogen Chemistry Poster Session 1

**Mon-P-50**

### Remarkable Promotional Effect of Tungsten on NOx Reduction By Ethanol over $Ag/Al_2O_3$

Jungseob So[1], Seung Jun Lee[2], Hyeonwoo Shin[3], Wo Bin Bae[3], Minkyu Kim[2], Sung Bong Kang[3] and Young Jin Kim[1], *(1)Korea Research Institute of Chemical Technology, Korea, Republic of (South), (2)Yeungnam University, Korea, Republic of (South), (3)Gwangju Institute of Science and Technology, Korea, Republic of (South)*.

**Short Summary:**

We will present the promotional effect of W NOx reduction activity over $Ag/Al_2O_3$ during ethanol-SCR. The designed catalyst was rich with metallic Ag species and Brønsted acid sites from $WO_x$, leading to improving deNOx activity compared to the conventional $Ag/Al_2O_3$ catalyst.

## Carbon Dioxide Conversion Poster Session 1

**Mon-P-15**

### Low Temperature Plasma-Assisted Conversion of Greenhouse Gases into Oxygenates over Ordered Macroporous Catalysts

Dong Hyeon Kim, Juchan Kim and Kyoung-Su Ha, *Sogang University, Korea, Republic of (South)*.

**Short Summary:**

Utilizing greenhouse gases, industrially valuable oxygenates could be directly and successfully synthesized over ordered macroporous catalyst in a DBD plasma reactor at room temperature and atmospheric pressure. Employing the ordered macroporous catalyst in the plasma bed, selectivity of alcohols including methanol and ethanol dramatically increased, while coke selectivity decreased.

## Conversion of Hydrocarbon Feedstocks Poster Session

**Mon-P-101**

### Closed-Loop Optimization of Catalyst for Oxidative Propane Dehydrogenation with $CO_2$ Using Artificial Intelligence

Jin-Soo Kim[1], Iljun Chung[2], Jisu Park[2], Hyeonjun Jung[2], Dongmin Lee[2], Jung Ho Shin[1], Hyunju Chang[1] and Yongju Yun[2], *(1)Korea Research Institute of Chemical Technology, Korea, Republic of (South), (2)Pohang University of Science and Technology, Korea, Republic of (South).*

**Short Summary:**

We optimize the catalyst composition for oxidative propane dehydrogenation with $CO_2$ using machine learning (ML) and metaheuristics. The ML model is trained on our experimental dataset to predict propylene yield and $CO_2$ conversion. The metaheuristics optimize the composition to maximize the targets. $Co_{0.5}Cr_{7.0}Ni_{1.7}$ catalyst mixed with $ZrO_2$ exhibits enhanced performance.

## Catalysis for Chemical Synthesis and Functionalization Poster Session

**Mon-P-31**

### Metal – Metal Oxide Catalysts for the Ring Opening Hydrogenolysis of Furanic Compounds

Samir Castilla[1], Ben Auer[1], Titus Szobody[2], Cameron Boydston[1], Jacob St. John[1], Ray Carter[3] and Alan Allgeier[1], *(1)The University of Kansas, USA, (2)University of North Carolina, USA, (3)University of Kansas, USA*.

**Short Summary:**

We studied the HDO Pt-$MO_x$/& of tetrahydrofuran 2,5'-dicarboxylic acid, Furan 2,5-dicarboxylic acid to obtain adipic acid, and 2,2'-bifuran 5,5'-dicarboxylic acid to obtain sebacic acid. By tuning the type and amount of metal oxide supported, temperature and pressure of reaction, the selectivity towards the ring opening products could be enhanced.

## Catalyst Design, Synthesis and Manufacturing Poster Session

**Mon-P-65**

### Acidity of $MoO_3/Ta_2O_5$ as Characterized by $NH_3$-TPD and Pyridine DRIFTS

Jhonattan Manosalvas Mora, A.K.M. Kazi Aurnob and James J. Spivey, *Louisiana State University, USA*.

**Short Summary:**

This study shows the different effects produced by varied weight loading impregnation of $MoO_3$ on various forms of $Ta_2O_5$ support, and how the formation of Brønsted acid sites is related to the weight loading of Mo. We demonstrate that Mo loading can increase the acidity and acid thermostability of $MoO_3/\gamma\text{-}Al_2O_3\text{-}Ta_2O_5$

## Catalysis for Chemical Synthesis and Functionalization Poster Session

**Mon-P-32**

### Cu-Ni/Bentonite Catalysts for Transfer Hydrogenation of Levulinic Acid for the Synthesis of Alkyl Levulinate Biofuel Additives.

Gloria Dimas Rivera[1], David De Haro Del Rio[1], Carlos Lucio Ortiz[1], Javier Rivera De la Rosa[1], Ladislao Sandoval-Rangel[2] and Carolina Solis Maldonado[3], *(1)Universidad Autónoma de Nuevo León, Mexico, (2)Tecnológico de Monterrey, Mexico, (3)Universidad Veracruzana, Mexico*.

**Short Summary:**

In this work was performed conversion and selectivity of LA to VA or valeric acid esters by a Cu-Ni/Bentonite catalyst under catalytic transfer hydrogenation whit 2-propanol as a hydrogen donor. Cu and Ni-based catalysts supported on bentonite were synthesized using the Poliol method; these catalysts were characterized using different techniques.

## Catalyst Design, Synthesis and Manufacturing Poster Session

**Mon-P-66**

### Surface Chemistry of 1st-Row Transition Metal Boride, Aluminide, and Silicide IMC and Their Synthesis as Phase-Pure Supported Nanoparticles

Sijie Guo and Siris Laursen, *University of Tennessee, USA*.

**Short Summary:**

This study has focused upon developing reactive support methods to synthesize supported IMCs as nanoparticles.This approach combines deposited metal precursors with p-block elements from the surface of the support to produce strongly bound, phase-pure IMC nanoparticles with high surface area.

## Carbon Dioxide Conversion Poster Session 1

**Mon-P-16**

### Characterization of $CO_2$ Binding on Alkaline Metal Oxide Sorbents and Interaction with Hydrogenation Catalysts for Reactive Carbon Capture

Chae Jeong-Potter and Dan Ruddy, *National Renewable Energy Laboratory, USA*.

**Short Summary:**

DFM are composed of co-supported sorbents and catalysts and allows capture and conversion of $CO_2$ to occur in a single reactor. We describe in this work the $CO_2$ binding characteristics of established and/or new DFM and their sorbent-only counterparts to deepen fundamental understanding of some critical features of these materials.

## Conversion of Hydrocarbon Feedstocks Poster Session

**Mon-P-102**

### Comparison of Iron-Based Catalysts to Utilize Nitrous Oxide As a Selective Green Oxidant

Alexander Simon and Justin Notestein, *Northwestern University, USA*.

**Short Summary:**

Iron-based catalysts were studied for oxidative dehydrogenation of propane using $N_2O$ recovered from wastewater streams as an oxidant. A rare head-to-head comparison of the metal-organic framework MIL-100(Fe) and zeolite Fe-ZSM-5 was performed, including differences in catalytic activity and stability, and resistance to residual water vapor present in recycled $N_2O$ streams.

## Catalyst Design, Synthesis and Manufacturing Poster Session

**Mon-P-67**

### KIT-5 Structural and Textural Changes in Response to Different Methods of Functionalization with Sulfonic Groups

Agata Wawrzyńczak, Sylwia Chałupniczak and Izabela Nowak, *Adam Mickiewicz University, Poznan, Poland*.

**Short Summary:**

KIT-5 was effectively functionalized with sulfonic groups by grafting and co-condensation method and used as a heterogeneous solid acid catalyst. Co-condensation proce-dure leading to the stable, $-SO_3H$ functionalized KIT-5 materials was successfully established.

## Conversion of Hydrocarbon Feedstocks Poster Session

**Mon-P-103**

### Olefin Intermediate Process: Effect of the Dehydrogenation Catalyst on Rate, Reaction Selectivity, and Yield in Tandem Catalysis for Polyolefin Depolymerization

Selena Moore[1], Lucas Ellis[1], Andreas Palmateer[1], Joel Miscall[2], Yuriy Roman[3] and Gregg T. Beckham[2], *(1)Oregon State University, USA, (2)Center for Bioenergy Innovation, USA, (3)Massachusetts Institute of Technology, USA*.

**Short Summary:**

We investigated the role of the dehydrogenation catalyst as it impacts tandem dehydrogenation and olefin metathesis, a low-temperature means to depolymerize polyolefin plastics to alkanes or alkenes. Our top performing catalyst was not the expected Pt (or SnPt) catalyst, even though dehydrogenation is the rate-limiting reaction.

## Catalysis for Chemical Synthesis and Functionalization Poster Session

**Mon-P-33**

### Structure-Reactivity Relationships and Periodic Trend of C-H Activation and C-O Formation in Alkanol and Alkane on Transition Metal Oxides

Guangming Cai, Qiuyu Shi, Xinyu (Bella) Zhang and Cathy Chin, *University of Toronto, Canada*.

**Short Summary:**

We interrogate the catalytic consequences of the oxygen contents $x$ and metal identity of doped MMoO$x$ oxides (M = Fe, Co, or Ni) and establish the common mechanistic traits for the C-H activation of alkanols and alkanes with $O_2$ or $CO_2$ and for the C-O formation of alkanols with $O_2$.

## Conversion of Hydrocarbon Feedstocks Poster Session

**Mon-P-104**

### Impact of Diluents on Non-Oxidative Dehydrogenation of Ethane

Jeffrey Weissman[1], Abhaya Datye[2], Erik Spoerke[3], Christopher Riley[3], Alexander Brown[3], Andrew De La Riva[2] and Andre DeCarmine[1], *(1)Precision Combustion, Inc., USA, (2)University of New Mexico, USA, (3)Sandia National Laboratories, USA*.

**Short Summary:**

We report on reaction mechanisms involved in a potentially lower energy low carbon approach to ethylene production, non-oxidative dehydrogenation, an alternative to energy intensive steam cracking. Understanding how reactants and diluents impact ethylene selectivity can led to optimization of the process to maximize ethylene yields will minimizing side product formation.

## Catalysis for Chemical Synthesis and Functionalization Poster Session

**Mon-P-34**

### Synthesis of Isobenzofuranones Using La Promoted Mg-Al Hydrotalcites

Daniel Hernández López, Victoria Eugenia Tamaño Galván, Amaay De Jesús Ñani Epitacio García, Tómas Viveros García, Juan Carlos Piña Victoria and Jose Francisco Ramirez, *Universidad Autónoma Metropolitana, Mexico*.

**Short Summary:**

In the present work, the use of acetophenone as a reactive solvent and a hydrotalcite catalyst. The reaction results showed the best catalyst with was the 2.5:1 ratio, Mg:Al. The catalysts were characterized by FTIR, TG-DTA, physisorption, EDX, while the products obtained were identified by NMR and FTIR.

## Catalyst Design, Synthesis and Manufacturing Poster Session

**Mon-P-68**

### Synthesis and Characterization of Cu-Doped & Films as Photocatalyst in the Oxidation of Benzyl Alcohol.

Zaira Humphreys Salas[1], Carolina Solis Maldonado[1], Raúl Luna[1], María Rebeca Rojas Ronquillo[1], Nayely Pineda Aguilar[2], Ladislao Sandoval-Rangel[3] and Carlos Lucio Ortiz[4], *(1)Universidad Veracruzana, Mexico, (2)Centro de Investigación en Materiales Avanzados S.C., Mexico, (3)Tecnológico de Monterrey, Mexico, (4)Universidad Autónoma de Nuevo León, Mexico*.

**Short Summary:**

The development of technologies for obtaining industrial molecules aims to replace conventional processes with more sustainable options. There is interest in improving the processes for producing benzoic acid from benzyl alcohol. Photocatalysis with & favors sustainability by using a radiation source to promote the activation of the photocatalyst.

## Catalysis for Chemical Synthesis and Functionalization Poster Session

**Mon-P-35**

### Identification of Catalytically Active Oxygen Structures on Silver

Ziyu Tang, Yue Qi and Simon G. Podkolzin, *Stevens Institute of Technology, USA*.

**Short Summary:**

Catalytically active oxygen structure on silver were identified with in situ Raman spectroscopic measurements and DFT calculations as O-O atomic-molecular hybrid structures, which form when one adsorbed O atom reacts with one lattice O atom by forming an O-O bond.

## Catalyst Design, Synthesis and Manufacturing Poster Session

**Mon-P-69**

### Investigation of the Formation and Thermal Stability of Pd-Zn Alloys

Ahmed Maged Aly Hamed and Rob Rioux, *Pennsylvania State University, USA*.

**Short Summary:**

In-situ characterization is utilized to examine the role of synthetic parameters on the formation and thermal stability of bulk Pd-Zn intermetallic structures. Intermetallic catalysts synthesized in different gas atmospheres display the same bulk structure, but impact the composition of the surface region.

## Conversion of Hydrocarbon Feedstocks Poster Session

**Mon-P-105**

### Hydrogenolysis of Polyethylene into Naphtha-like Products Using Ni-Based Catalysts

Gokhan Celik[1], Hamdiye Ece[1], Arzum Ceren Aydogdu[1], Ali Süerkan[2], Berrak Erkmen[2] and Ayhan Ezdesir[2], *(1)Middle East Technical University, Turkey, (2)SOCAR Turkey R&D and Innovation Inc., Turkey*.

**Short Summary:**

Hydrogenolysis of PE for producing naphtha-like products was demonstrated using Ni-based catalysts with a performance similar to its precious metal containing counterparts.

**Mon-P-106**

### The Role of Directed Energy and Transport in the Catalyst Design for Low-Temperature Up-Cycling of Polyolefin Plastics Waste

Max Mortensen and Siris Laursen, *University of Tennessee, USA*.

**Short Summary:**

Improved understanding of fundamental catalytic surface chemistry and reactor design in an environment with detrimental mass transport issues that promote over cleavage and uncatalyzed thermal radical side reactions to then promote more efficient upcycling of polyolefins.

## Catalyst Design, Synthesis and Manufacturing Poster Session

### Mon-P-70

### Synthesis of Si-LTA Zeolites with Controllable Defects in Presence of Ammonia Fluoride

Taras Nagornyy, *University of Massachusetts Amherst, USA*.

**Short Summary:**

Successful exclusion of HF from the synthesis of zeolites including Si-LTA can lead to a relatively safe method to synthesize siliceous and high-silica zeolites. Replacing HF with $NH_4F$ in the synthesis allows the zeolites to be formed in a basic solution which can result in different defect densities and structures.

### Mon-P-71

### Delicate Synthesis of Uniform Palladium Species in Chabazite for Passive $NO_x$ Adsorption and $CH_4$ Combustion

Yongwoo Kim[1], Jongbaek Sung[2], Jungwon Park[3] and Do Heui Kim[3], *(1)University of Illinois at Urbana-Champaign, USA, (2)Institute for Basic Science (IBS), Korea, Republic of (South), (3)Seoul National University, Korea, Republic of (South)*.

**Short Summary:**

We achieved synthesizing Pd/SSZ-13 with fully isolated $Pd^{2+}$ ions based on understanding of ion-exchange process and thermal treatment. Furthermore, through understanding nucleation and growth of Pd clusters in zeolite, we could prepare the Pd/SSZ-13 having uniformly nano-sized PdO clusters. It emphasizes the significance of the delicate synthesis of metal-incorporated zeolites.

## Conversion of Hydrocarbon Feedstocks Poster Session

### Mon-P-107

### Upgrading of Disposable Face Masks via Low-$CO_2$ Emissions Thermal Catalytic Conversion: A TGA-FTIR Study

Ladislao Sandoval-Rangel[1], Cinthia J. Ramírez-Murillo[1], Gloria Lourdes Dimas-Rivera[2], Carolina Solis Maldonado[3], Javier Rivera De la Rosa[2], Carlos Lucio Ortiz[2] and Alejandro Montesinos Castellanos[1], *(1)Tecnológico de Monterrey, Mexico, (2)Universidad Autónoma de Nuevo León, Mexico, (3)Universidad Veracruzana, Mexico*.

**Short Summary:**

The results reported in this work show the high potential of an economic natural mineral (clinoptilolite) in the catalytic pyrolysis of disposable face masks. This technology may be able to help in the reduction of municipal solid waste volume, and avoid sources of pollution such as landfills and incinerators.

## Catalyst Design, Synthesis and Manufacturing Poster Session

### Mon-P-72

### Synthesis of Sub-Nanometer-Sized Catalytically Active Ligand-Stabilized Ruthenium Nanoparticles

Sayed Abu Sufyan, Brian van Devener and Michael Nigra, *University of Utah, USA*.

**Short Summary:**

Sub-nanometer ruthenium nanoparticles are synthesized with bulky phosphine and thiol ligands. Catalytic activity is demonstrated in $H_2O_2$ decomposition and CO oxidation. Notably, in both reactions, the reactions are performed without ligand removal. The bulky nature of the ligand enables open sites for catalytic reactions on the Ru nanoparticles' surfaces.

## Conversion of Hydrocarbon Feedstocks Poster Session

### Mon-P-108

#### Comparison and Characterization of Thermal Hydrocracking of Heavy Fuel Oil and Heavy Fuel Oil-Castor Oil Products

Martin Martinez Ruiz, Felipe Sanchez and Gilberto Alonso Ramirez, *UCyEH, Instituto Politecnico Nacional-ESIQIE, Mexico*.

**Short Summary:**

Thermal hydrocracking of 75 wt% fuel oil- 25 wt% castor oil mixture was carried at 1000 psi of hydrogen and at different reaction temperatures (360, 380, and 400 °C). The presence of 25 wt% castor oil reduced density, viscosity, sulfur, and asphaltenes concentration and increased 57.57 % gasoil production.

### Mon-P-109

#### Catalytic Upcycling of Polymer Wastes: Efficient Conversion of Polymer Waste to Aromatic Monomers

Yuxin Wang, Kaushal Parmar, Vishal Tuli, Thang Luong and Jianli Hu, *West Virginia University, USA*.

**Short Summary:**

Most single-use polymers, such as LDPE, PP, and PS, are not recycled and end up in landfill, affecting the environment. In this study, the microwave catalytic upcycling technology devloped for convrting these single-use polymers to valuable aromatics products like benzene, toluene, and xylene (BTX).

## Catalyst Design, Synthesis and Manufacturing Poster Session

### Mon-P-73

#### Green Methanol from Renewable Feeds – Towards Scalable Catalyst Synthesis and Improved Stability

Lucas Warmuth, David Guse, Matthias Kind, Dieter Schild, Gabriela Rodrigues Niquini, Moritz Herfet, Matthias Steurer, Anna Zimina, Jan-Dierk Grunwaldt, Thomas Zevaco and Stephan Pitter, *Karlsruhe Institute of Technology (KIT), Germany*.

**Short Summary:**

High quality control and the possibility of scale-up is enabled by analysis of precatalyst formation. Additionally, a reduction of the catalyst's ageing time could be achieved. Deactivation processes are investigated for pure gases in this work as a base for further examinations regarding renewable feeds and their impurities.

### Mon-P-74

#### Development of Highly Active and Stable Ni Supported on Porous Yolk Shell Catalysts

Hyun-Seog Roh[1], Beom-Jun Kim[1], Won-Jun Jang[2], Kyung-Won Jeon[2] and Yun-Chan Kang[3], *(1)Yonsei University, Korea, Republic of (South), (2)Kyungnam University, Korea, Republic of (South), (3)Korea University, Korea, Republic of (South)*.

**Short Summary:**

Yolk-shell-structured catalyst was designed for hydrogen production from renewable sources or in the DIR-MCFC (direct internal reforming in molten carbonate fuel cells). The developed catalyst exhibited remarkable resistance for alkali poisoning and coke deposition.

### Mon-P-75

#### Mechanistic Insights into the Solid-State Crystallization of High-Density Zeolite

Debkrishna Dey[1] and Manjesh Kumar[2], *(1)Indian Institute of Technology, Delhi, India, (2)Indian Institute of Technology Delhi, India*.

**Short Summary:**

This work established mechanistic insights into the crystallization of zeolite in solid-state synthesis. A hybrid pathway of non-classical growth was observed where nanoparticles tend to form nano-domains having features of oriented attachment through a common crystal plane, whereas these nano-domains combine randomly to form bulk crystals of the CAN phase.

### Mon-P-76

#### Understanding Titania Crystallization to Generate Engineered Anatase Particle Architecture

Anusha Jain and Manjesh Kumar, *Indian Institute of Technology, Delhi, India*.

**Short Summary:**

Understanding the growth mechanism pathways of titania helps to develop designer crystals that directly improve structure-property-performance matrix. We controlled three aspects of particle: (i) size, (ii) dimensionality, and (iii) morphology. Overall, we established various precursors that participate in crystallization that presents a complex blueprint of crystal growth.

### Mon-P-77
### Controlling Intrinsic Defects in Hierarchical Zeolite ZSM-5 Catalysts and Their Impact on Methanol to Hydrocarbons
Kumari Shilpa and Jeffrey D. Rimer, *University of Houston, USA*.

**Short Summary:**

We report a novel approach to tune “defects” in zeolites: a process called annealing. We have tested this technique for MFI, MEL and BEA and it’s shown to yield catalysts with high turnover numbers and low rate of deactivation.

### Mon-P-78
### Directing Reaction Pathways on Supported Metal Catalysts with Low-Density Self-Assembled Monolayers
Zachary Blanchette[1], Daniel K. Schwartz[1] and J. Will Medlin[2], *(1)University of Colorado at Boulder, USA, (2)University of Colorado Boulder, USA*.

**Short Summary:**

$Pt/Al_2O_3$ was modified with a full monolayer of thiols and a low-density monolayer to investigate the effect of SAM density on catalyst behavior. Both showed improvement in hydrodeoxygenation selectivity via steric effects while the low-density SAM catalyst exhibited improved activity compared to the full monolayer attributed to reduced site blocking.

### Mon-P-79
### Effect of Strong Support Interaction in Modulating the Catalytic Activity of Mo Nitrides Species in Ammonia Synthesis
Said Laassiri[1], Amanda Sfeir[2], Jean-philippe Dacquin[2], Herve Vezin[3] and Sébastien Royer[2], *(1)Mohammed VI Polytechnic University, Morocco, (2)Univ. Lille, CNRS, ENSCL, Centrale Lille, Univ. Artois, UMR 8181 - UCCS - Unité de Catalyse et Chimie du Solide, F-59000 Lille, France, France, (3)Laboratoire de Spectrochimie Infrarouge et Raman, France*.

**Short Summary:**

Modulating the interaction between molybdenum and the support was found to be decisive in controlling the catalytic activity in ammonia synthesis. Amongst the studied supports, SBA-15 was found to be the most appropriate for Mo dispersion. In comparison, when supported on reducible oxide (&), Mo species showed poor catalytic activity.

### Mon-P-80
### Activated Carbon Monoliths for Oleochemical Hydrogenation
Benjamin Egelske, Hunter Brown, Robert Gulotty and Myranda Jackson, *Applied Ceramics, USA*.

**Short Summary:**

Activated carbon monolith catalysts (ACMC) are a class of materials whereby carbon and ceramic are co-extruded to form a stable honeycomb structure with high physical strength an tunable properties. In this work, ACMC technology has been compared to state-of-the-art hydrogenation catalysts to selectively hydrogenate 2500 pounds of proprietary oleochemical derivative.

### Mon-P-81
### Aqueous Synthesis of Uniform Pt Nanocrystals
Pin-Hung Chung[1], An-Chih Yang[1], Chengshuang Zhou[1], Carlos Lizandara[2], Yuejin Li[2] and Matteo Cargnello[1], *(1)Stanford University, USA, (2)BASF Corporation, USA*.

**Short Summary:**

This work reports aqueous methods for synthesizing uniform Pt nanocrystals, making it possible to reduce costs and avoid toxic solvents/reagents during industrial production. The results suggest that this aqueous-synthesized Pt NP possesses comparable catalytic performance to that of organic-synthesized Pt and is a promising candidate for emission control catalyst.

### Mon-P-82
### Novel Microwave-Assisted Synthesis of Finned-FER and Its Effect on Methyl-Oleate Isomerization
Alexandre F. Young, Leandro Alves de Sousa, Pedro Nothaft Romano, Donato Aranda and João M.A.R. de Almeida, *Universidade Federal do Rio de Janeiro, Brazil*.

**Short Summary:**

This work describes the unprecedented microwave-assisted synthesis of finned zeolite, its thorough characterization and its application on FAME isomerization. The accelerated crystallization of zeolites and the production of more active catalysts due to the higher surface acidity and area has great significance for the fuel and energy industries.

**Mon-P-83**

### Optimization of a Ru-Catalyst for Ammonia Cracking

Santiago Casu, Konrad Krois, Christian Breuer and Hendrik Spod, *Heraeus Deutschland GmbH & Co. KG, Germany*.

**Short Summary:**

Ammonia is a promising hydrogen carrier and will play an important role in the hydrogen economy. Hydrogen can be released from ammonia using the ammonia cracking reaction. In this paper, a series of Ru based catalysts were tested for ammonia cracking. Incorporation of promoters significantly improved the catalytic activity.

**Mon-P-84**

### Hierarchical ZSM-5/TNT Nanocomposites: Synthesis, Characterization, and Friedel-Crafts Alkylation

Jorge G. Huerta, Brent E. Handy and María-Guadalupe Cárdenas-Galindo, *Universidad Autónoma de San Luis Potosí, Mexico*.

**Short Summary:**

Depolymerization of a synthesized zeolite from $Al(OH)_3$ is possible using glycerol at high temperatures, developing better textural properties and higher conversion rate. A nanocomposite of ZSM-5/TNTs is a suitable catalyst for FC alkylation.

**Mon-P-85**

### Development of a Method to Produce Technical Catalysts Based on Mechanochemistry and Using Water for Extrusion

Luisa Acevedo[1], Omar Vargas[1], Edwing Velasco[1], Edgar M. Morales-Valencia[1,2] and Victor Baldovino Medrano[1], *(1)Centro de Investigaciones en Catálisis (CICAT), Universidad Industrial de Santander, Colombia, (2)Grupo GREIP, Instituto Universitario de la Paz-UNIPAZ, Colombia*.

**Short Summary:**

This work shows how it is possible to use mechanochemistry and water to produce extrudates of supported Ni-$MoO_x$/H-Y-alumina to be employed in a hydrocracking process and contributes to the development of an initial methodology for mechanochemical impregnation for a green alternative to produce industrial prototype catalysts.

**Mon-P-86**

### Novel Catalyst Synthesis Monitoring System of Emission Spectroscopy Techniques with Advanced Machine Learning Algorithms

Can Wang, Ben Ko, Musa Najimu and Erdem Sasmaz, *University of California, Irvine, USA*.

**Short Summary:**

Combining in-situ laser-induced breakdown spectroscopy with flame spray pyrolysis can monitor nanoparticles' chemical properties through their emission spectra. Using advanced machine learning models can successfully predict the chemical properties of same-type compounds without requiring further post-characterization, which can speed up the discovery of novel functional catalysts.

# Tuesday Poster Sessions

## Exhibit Hall CD

### Conversion of Oxygenated Feedstocks Poster Session 1

**Tue-P-69**

**Thermal and Catalytic Pathways in the Deconstruction of Ethylene Vinyl Alcohol**

Christine Oberhausen, Brandon Vance and Dionysios Vlachos, *University of Delaware, USA*.

**Short Summary:**
Hydroconversion is a promising approach to deconstructing multilayer film plastic packaging. However, the deconstruction of non-polyolefin components of these films has not been thoroughly addressed. This work establishes thermal and catalytic routes to deconstruct ethylene vinyl alcohol copolymer with tunable product selectivities and elucidates reaction mechanisms for both process chemistries.

### Catalysis for Environmental Applications and Sustainable Nitrogen Chemistry Poster Session 2

**Tue-P-32**

**Analysis of the Adsorption Rate on Catalysts for Ammonia Synthesis**

Simon Ingeman Hansen, Jakob M. Christensen and Anker D. Jensen, *Technical University of Denmark, Denmark*.

**Short Summary:**
A kinetic model to describe the rate of nitrogen adsorption relevant for ammonia synthesis has been constructed in this study. Moreover, this study also includes adsorption with hydrogen in the adsorption gas, which indicate that the adsorption rate is increased when hydrogen is present.

### New and Advanced Methods in Catalyst Characterization Poster Session

**Tue-P-88**

**A Comprehensive Characterization of Catalytic Active Sites in Sodium-Modified Zirconia**

Han Chen[1], Zhexi Lin[2], Sai Praneet Batchu[3], Mengjie Fan[4], Stavros Caratzoulas[3], Jingguang Chen[2,3], Dionysios Vlachos[3], Raymond J. Gorte[3,4], John M. Vohs[3,4] and Omar Abdelrahman[1,3], *(1)University of Massachusetts Amherst, USA, (2)Columbia University, USA, (3)University of Delaware, USA, (4)University of Pennsylvania, USA*.

**Short Summary:**
Sodium-modified zirconia, as potential biomass upgrading catalyst, were synthesized and investigated using surface characterizations and kinetic measurement. With increasing Na content, higher selectivity towards dehydrogenation against dehydration was observed when using isopropanol as probe molecule for catalytic activity analysis. Effect of water on isopropanol catalytic conversion was also examined.

### Conversion of Methane, Methanol and Syngas Poster Session 1

**Tue-P-51**

**Effect of Pre-Treatment Conditions on the Kinetic Character and Carbon Accumulation for Mo/HZSM-5 Catalysts**

Erin Sobchinsky[1,2], Debtanu Maiti[2], M. Ross Kunz[2], Md Sifat Hossain[3,4], Gagandeep Singh Dhillon[4,5], Sheima Khatib[3,4] and Rebecca Fushimi[2], *(1)Lehigh University, USA, (2)Idaho National Laboratory, USA, (3)Virginia Tech, USA, (4)Texas Tech University, USA, (5)Lydian Labs Inc., USA*.

**Short Summary:**
Molecular probe experiments were performed in a Temporal Analysis of Products (TAP) reactor, to elucidate the effect of pretreatment on 4Mo/HZSM-5 catalysts for methane dehydroaromatization. Insights are provided for the time-evolution of reactant conversion, product formation, and the kinetics of carbon accumulation and removal for prolonged sustainable dehydroaromatization chemistry.

## Carbon Dioxide Conversion Poster Session 2

**Tue-P-1**

### Optimization and Understanding of ZnO Nanoarray Supported $Cu\text{-}ZnO\text{-}Al_2O_3$ Catalyst for Enhanced $CO_2$ -Methanol Conversion at Low Temperature and Pressure

Jiyu Sun, Usman Salahuddin, Chunxiang Zhu, Xingxu Lu and Pu-Xian Gao, *University of Connecticut, USA*.

**Short Summary:**

A highly improved $Cu\text{-}ZnO\text{-}Al_2O_3$ catalysts supported on ZnO nanorod arrays was prepared by tuning the processing factors, such as precursor solution, loading amount and annealing temperature. At 200 °C and 1 bar conditions, the optimized catalyst achieved a methanol yield of 2.1 mol $h^{-1}$ $kg^{-1}$ with a selectivity of 56%.

## Homogeneous, Molecular and Supramolecular Catalysis Poster Session

**Tue-P-85**

### Mechanistic Insight into Tris(pentafluorophenyl)Borane Speciation during Ring Opening of Epoxides

Hiyab Mekonnen[1], Guanhua Wang[1], Carlos Villa[2], Arjun Raghuraman[2], Varinia Bernales[2], Sukaran Arora[2], Saket Bhargava[2], Linda Broadbelt[1] and Justin Notestein[1], *(1)Northwestern University, USA, (2)The Dow Chemical Company, USA*.

**Short Summary:**

*In situ* VT NMR sheds light on catalyst decomposition and catalyst speciation during epoxide ring opening reactions by BCF. Understanding these effects are especially important to building overall microkinetic models that captures the behavior of the catalyst at low loadings and high temperatures relevant to industrial conditions.

## Conversion of Oxygenated Feedstocks Poster Session 1

**Tue-P-70**

### Insights into the Noble Metal Catalyzed Simultaneous Hydrodeoxygenation and Hydrodenitrogenation of Amides

Emma Verkama[1], Sylvia Albersberger[2], Aitor Arandia[1], Marja Tiitta[2], Reetta Karinen[1] and Riikka L. Puurunen[1], *(1)Aalto University, Finland, (2)Neste Corporation, Finland*.

**Short Summary:**

This work provides insights into the simultaneous hydrodeoxygenation and hydrodenitrogenation of amides over supported noble metal catalysts. A reaction network is proposed, and active catalyst compositions are identified. The implications of the catalyst composition on the activity and selectivity are discussed.

## Catalysis for Environmental Applications and Sustainable Nitrogen Chemistry Poster Session 2

**Tue-P-33**

### Transient CO Oxidation to Ascertain Multinuclear $Cu^{2+}$ Structure Formation from $ZCu^{2+}(OH)^-$ Cations over a Cu-SSZ-13 Catalyst

Umberto Iacobone[1], William Epling[2], Isabella Nova[1] and Enrico Tronconi[1], *(1)Politecnico di Milano, Italy, (2)University of Virginia, USA*.

**Short Summary:**

Transient CO oxidation has been proposed as an effective probe reaction for Cu-dimers, originating from isolated $ZCu^{2+}(OH)^-$ sites, over Cu-CHA catalysts under low-temperature $NH_3$-SCR conditions. A 24hrs. CO exposure led to a complete conversion, and the overall $CO_2$ production matched the expected cations population, supporting the underlying mechanistic theory.

## New and Advanced Methods in Catalyst Characterization Poster Session

**Tue-P-89**

**Reaction Calorimetry for Adsorption Thermodynamics in Zeolite**

Ajibola Lawal and Omar Abdelrahman, *University of Massachusetts Amherst, USA*.

**Short Summary:**

Reactive calorimetry as a technique affords us the ability to expand our understanding of adsorption thermodynamics, particularly for adsorbates strongly bound to Brønsted acid sites in solid acid catalysts. The entire method is carried out within a gas chromatograph, serving both as an automated reactor and a quantification tool.

## Conversion of Methane, Methanol and Syngas Poster Session 1

**Tue-P-52**

**Selective and Stable In-Promoted Fe Catalyst for Syngas Conversion to Light Olefins**

Yang He[1,2], Hanzhong Shi[2], Olusola Johnson[2], Babu Joseph[2] and John Kuhn[2], *(1)Oak Ridge National Laboratory, USA, (2)University of South Florida, USA*.

**Short Summary:**

A stable and selective In-promoted iron catalyst controls surface chemistry and promotes C-C coupling toward olefin products during high-temperature (400 °C) and moderate pressure (5 bar) FTS reactions.

## Carbon Dioxide Conversion Poster Session 2

**Tue-P-2**

**Direct Air Capture (DAC) of $CO_2$ over Na-Cation Exchanged Zeolites**

Do Yeong Kim[1], Wo Bin Bae[1], Hyeonwoo Shin[1], Bogyung Kim[1], Sungjoon Kweon[2], Min Bum Park[2] and Sung Bong Kang[1], *(1)Gwangju Institute of Science and Technology, Korea, Republic of (South), (2)Incheon National University, Korea, Republic of (South)*.

**Short Summary:**

The DAC performance of H-form zeolites was improved by exchanging Na cation into the channel. The Na-ZSM-5 showed the highest capacity of the DAC and, we found that the presence of Na cation causes Lewis-acid sites in the ZSM-5, resulting in the acido-basic pairing sites for active capture of $CO_2$.

## Homogeneous, Molecular and Supramolecular Catalysis Poster Session

**Tue-P-86**

**Silver Catalyzed H/D Exchange for Deuteration of Aryl Bromides**

Honghai Zhang, *Oak Ridge National Laboratory, USA*.

**Short Summary:**

We developed a silver-catalyzed H/D exchange reaction for valuable muti-deuterated aryl bromides, which are important synthetic building blocks in pharmaceutical industrial and materials science.

**Tue-P-87**

**Kinetic Study for Polygalacturonic Acid Decomposition As a Model for Pectin-Rich Biomass Upgrading Via Hydrolysis**

Eva E. Rivera-Cedillo, María Fernanda Quintana Olivera, Brent E. Handy, Marco Martín González Chávez and María-Guadalupe Cárdenas-Galindo, *Universidad Autónoma de San Luis Potosí, Mexico*.

**Short Summary:**

A kinetic model for depolymerizing D-polygalacturonic acid to D-Galacturonic acid and its consecutive dehydration to furfural under hydrolysis conditions is developed. This kind of models are required to design a biorefinery process for upgrading waste biomass rich in pectin.

## Conversion of Oxygenated Feedstocks Poster Session 1

**Tue-P-71**

### Electrochemical Oxidation of Hydroxymethylfurfural (HMF) to Furandicarboxylic Acid (FDCA) over Metal Nanoparticles/Carbon Nanotubes Derived from $CO_2$

Anousha Sohail and Chularat Wattanakit, *Vidhyasirimmedhi Institute of Science and Technology, Thailand*.

**Short Summary:**

Electrochemical oxidation using non-noble metals of 5-hydroxymethylfurfural (HMF) is highly demanded. This work reports the successful synthesis of Iron Nickel-carbon nanotubes; (FeNi-MWCNT) aiding in almost 100% HMF conversion and 94% FDCA yield. The promising synergetic effect of this bimetallic composite enlightens the use of non-noble metals for further developmental perspectives.

## Catalysis for Environmental Applications and Sustainable Nitrogen Chemistry Poster Session 2

**Tue-P-34**

### An Investigation of the Effect of Oxygen Storage Capacity Material with Spaci-MS over a Pd/Rh-Based Three-Way Catalyst

Aldo Lanza[1], Steven Raphy[1], Djamela Bounechada[1], Amy Kolpin[1], Andrew York[1] and Donna Liu[2], *(1)Johnson Matthey Technology Centre, United Kingdom, (2)Johnson Matthey, USA*.

**Short Summary:**

In this work the role of the OSC material of a Three Way Catalyst was spatiotemporally resolved by SPACI-MS to identify where the different reactions occur during lean to rich conditions and give feed back into the improvement of emission control catalysts for Gasoline.

## New and Advanced Methods in Catalyst Characterization Poster Session

**Tue-P-90**

### Characterizing Meso- and Microporous Catalyst Supports with Gas Adsorption

Katie Cychosz and Alyssa Henderson, *Anton Paar Quantatec, USA*.

**Short Summary:**

Gas adsorption was used to determine structural parameters such as BET surface area, pore size distribution, and total pore volume of micro- and mesoporous catalyst supports. For the complete micro-mesopore size distribution, the pore size distribution from $CO_2$ (273 K) were merged with that from an $N_2$ (77 K) measurement.

## Conversion of Methane, Methanol and Syngas Poster Session 1

**Tue-P-53**

### Tandem Catalytic Synthesis of Liquid Fuel and Chemicals from Biogas

Olusola Johnson, Babu Joseph and John Kuhn, *University of South Florida, USA*.

**Short Summary:**

In this study, a tandem catalytic reactor system was developed to combine low-temperature methane reforming and high-temperature FTS reaction. This innovative biofuel manufacturing route converts biogas ($CO_2$ and $CH_4$) directly into liquid hydrocarbons and light olefins, thereby lowering cost and energy requirements.

## Carbon Dioxide Conversion Poster Session 2

**Tue-P-3**

**Development of Catalysts for Selective $CO_2$ Hydrogenation**

Marc Porosoff, *University of Rochester, USA*.

**Short Summary:**

The Porosoff Group is studying Si/Al ratio and extra-framework cations in the highly-tunable ZSM-5 topology to control hydrogenation of the mildly acidic $CO_2$ molecule. Zeolites are impregnated with Co, Fe and $Mo_2C$-based active phases to determine if the zeolite formulation has a predictable effect on hydrogenation of $CO_2$ to olefins.

## Conversion of Oxygenated Feedstocks Poster Session 1

**Tue-P-72**

**Ruthenium Catalysts for the Efficient Conversion of 5-HMF into Dff to Produce Phenolic Resins**

Hendrik Spod, Gisa Meissner and Ingo Graef, *Heraeus Deutschland GmbH & Co. KG, Germany*.

**Short Summary:**

The use of heterogeneous $Ru/Al_2O_3$ catalysts leads to full conversion of 5-HMF with molecular oxygen as well as to a selective formation of DFF. Furthermore, the recovery and recycling of Ruthenium as PM is of great importance from an ecological and economical point of view.

## Catalysis for Environmental Applications and Sustainable Nitrogen Chemistry Poster Session 2

**Tue-P-35**

**Effect of Promoters on Activity and Selectivity for Selective Catalytic Reduction (SCR) of NO with $NH_3$ By Supported $V_2O_5$-$WO_3$/& Catalysts**

Dang Nguyen, Bar Mosevitzky Lis and Israel Wachs, *Lehigh University, USA*.

**Short Summary:**

*In situ* spectroscopy techniques (Raman, IR, and TPSR) were used to investigate the effects of different promoters ($CeO_x$, $SiO_x$, and $ZrO_x$) on activity and selectivity of supported $V_2O_5$-$WO_3$/& catalysts for Selective Catalytic Reduction (SCR). The results indicate that SCR activity and selectivity are controlled by the promoter ligands.

## New and Advanced Methods in Catalyst Characterization Poster Session

**Tue-P-91**

**Surface Hydroxyl Chemistry of Titania and Alumina Supports: Quantitative Titration and Temperature Dependence of Surface Brønsted Acid-Base Parameters**

Tae Yong Yun and Bert Chandler, *The Pennsylvania State University, USA*.

**Short Summary:**

The fundamental chemistry of surface hydroxyl group is investigated using quantitative acid/base titration. This study utilized thermal gravimetric analysis and aqueous acid-base titrations to quantify the temperature dependence of surface hydroxyl Brønsted acid-base parameters for a series of metal oxides.

## Conversion of Methane, Methanol and Syngas Poster Session 1

**Tue-P-54**

### Design, Synthesis, and Catalytic Testing of 3D-Printed Fischer-Tropsch Catalysts

Luis Caballero, Joseph Brindle, Sayed Abu Sufyan, Nathan Ramey, Swomitra Mohanty and Michael Nigra, *University of Utah, USA*.

**Short Summary:**

The 3D printing of supports for Fischer-Tropsch synthesis catalysts is described in this work. These structures are designed to transport heat away from the catalytically active nanoparticles in order to control selectivity and minimize thermal gradients which cause deactivation. These 3D-printed materials are compared to catalysts that use conventional supports.

## Carbon Dioxide Conversion Poster Session 2

**Tue-P-4**

### Microkinetic Modelling of $CO_2$ Hydrogenation over α-MoC Surfaces

Thobani G. Gambu[1,2], Eric van Steen[1] and Mark Saeys[2], *(1)University of Cape Town, South Africa, (2)Ghent University, Belgium*.

**Short Summary:**

Density functional theory calculations and microkinetic simulations are conducted to study $CO_2$ hydrogenation over α-MoC surfaces. Results also include surface mobility of reaction intermediates as well as its impact on the reaction kinetics. Furthermore, oxygen removal is identified as a limiting step – bulk modification remedies are proposed and discussed.

## New and Advanced Methods in Catalyst Characterization Poster Session

**Tue-P-92**

### Bridging Surface Science to Atmospheric Pressure with Pulsed Flow: Probing CO Oxidation on Pd Catalysts

Eric High, Christopher O'Connor and Christian Reece, *Harvard University, USA*.

**Short Summary:**

We examine CO oxidation over palladium-based catalysts using a transient flow reactor at atmospheric pressure. We demonstrate that the surface science derived kinetics on planar $Pd/Al_2O_3$ can accurately model $CO_2$ production in our reactor studies. Our technique provides a new regime for studying technical catalysts under applied reaction conditions.

## Conversion of Methane, Methanol and Syngas Poster Session 1

**Tue-P-55**

### Ferrihydrite-Based Catalysts for Fischer-Tropsch Synthesis: Anomaly in Activation Behavior and Catalytic Performance

Dong Hyun Chun[1,2], Hyeon Song Lee[1], Geun Bae Rhim[1], Kwangsoo Kim[1], Kwang Young Kim[1], Byung-Hyun Kim[1] and Min Hye Youn[1], *(1)Korea Institute of Energy Research, Korea, Republic of (South), (2)University of Science and Technology, Korea, Republic of (South)*.

**Short Summary:**

Fischer-Tropsch synthesis (FTS) was carried out over ferrihydrite-based and hematite-based catalysts pre-activated by syngas with different pressures (ambient pressure–15 bar). Unlike conventional hematite-based catalysts, the ferrihydrite-based catalysts exhibited positive dependence of syngas pressure in activation on the $C_{5+}$ hydrocarbon production rate in the FTS.

## Carbon Dioxide Conversion Poster Session 2

**Tue-P-5**

### Differentiating the Impacts of $Cu_2o$ Initial Low- and High- Index Facets on Their Reconstruction and Catalytic Performance in Electrochemical $CO_2$ Reduction Reaction

Chen Han and Jian Pan, *the University of New South Wales (UNSW), Australia*.

**Short Summary:**

This study reveals that the initial facet exposure of $Cu_2O$ directly determines its transformation or reconstruction behavior under EC $CO_2RR$ conditions, which subsequently governs the catalytic selectivity. The operando SR-PD was used together with in-situ Raman to give a clear structure-transformation-performance relationship.

## Conversion of Oxygenated Feedstocks Poster Session 1

**Tue-P-73**

### Effects of Metal Dispersion and Reaction Time on the Reductive Catalytic Depolymerization of Lignin to Phenols

Aliaksandr Karnitski[1,2], Jae-Wook Choi[1], Chun-Jae Yoo[1], Dong Jin Suh[1], Chang Soo Kim[1,2], Kwang Ho Kim[1,2], Kyeongsu Kim[1,2], Hyunjoo Lee[1,2] and Jeong-Myeong Ha[1,3], *(1)Korea Institute of Science and Technology, Korea, Republic of (South), (2)Korea University of Science and Technology, Korea, Republic of (South), (3)Korea University, Korea, Republic of (South).*

**Short Summary:**

The reductive depolymerization of lignin was performed using supported noble metal catalysts. The metal dispersion and reaction time were manipulated to obtain the optimal reaction conditions, which were further discussed to understand the reaction mechanism on the catalyst surface.

## Catalysis for Environmental Applications and Sustainable Nitrogen Chemistry Poster Session 2

**Tue-P-36**

### Effect of Promoter on Ammonia Synthesis over MOF-Derived $Ru\text{-}CeO_2$

Ki Hyuk Kang[1], Pill Won Seo[1] and Sunyoung Park[1,2], *(1)Korea Research Institute of Chemical Technology, Korea, Republic of (South), (2)University of Science and Technology (UST), Korea, Republic of (South).*

**Short Summary:**

With the increasing demand for a carbon-free society, recent research is focusing on the development of catalysts with higher activity under mild conditions in ammonia synthesis. Here, a method for improving the catalytic activity was studied by confirming the promoter effect in the MOF-derived $Ru\text{-}CeO_2$ catalyst.

## Conversion of Oxygenated Feedstocks Poster Session 1

**Tue-P-74**

### Selective Hydrogenation of Aromatic Alcohol to Cyclic Ketones over Pd Based Catalysts

Jimmy Soeherman[1] and Paul Dauenhauer[2], *(1)University of Minnesota-Twin Cities, USA, (2)Låkril Technologies Corporation, USA.*

**Short Summary:**

Kinetic measurements and a stability study of selective hydrogenation of alkyl-substituted phenols over time will be presented as a function of alkyl groups, metal dispersion, and different operating conditions such as flow rates, reducing conditions, and more.

## Catalysis for Environmental Applications and Sustainable Nitrogen Chemistry Poster Session 2

**Tue-P-37**

**Kinetics for Catalytic Oxidation of Dioxins and Model Compounds**

William Gundtorp[1], Anker D. Jensen[2] and Thomas Klint Torp[1], *(1)Topsoe, Denmark, (2)Technical University of Denmark, Denmark*.

**Short Summary:**

In the literature the majority of research on catalytic oxidation of dioxins are conducted using model compounds instead. In this analysis, the kinetics for the catalytic oxidation of dioxins and commonly used model compounds are extracted and compared, using data from existing literature, to establish the potential similarities and differences.

## New and Advanced Methods in Catalyst Characterization Poster Session

**Tue-P-93**

**High-Throughput Catalyst Nanoparticle Characterization Using TEM with Automated Particle Workflow (APW)**

Lee Casalena and Mark McClendon, *Thermo Fisher Scientific, USA*.

**Short Summary:**

Achieving statistically significant nanoparticle measurements, once a tedious process, can now be massively accelerated using advances in software automation, integration and modern hardware stability. The Automated Particle Workflow (APW) integrates live TEM data directly into processing software producing immediate and reproducible particle analysis, minimizing operator and sampling bias.

## Conversion of Methane, Methanol and Syngas Poster Session 1

**Tue-P-56**

**Effect of Acidity on the Liquid Fuel Production in the Fischer-Tropsch Synthesis over Bifunctional Catalysts**

Min Hye Youn[1], Deviana Deviana[1], Geun Bae Rhim[1], Young-eun Kim[1], Kwang Young Kim[1], Kee Young Koo[2] and Dong Hyun Chun[1], *(1)Korea Institute of Energy Research, Korea, Republic of (South), (2)Korea Institute of Energy Research/University of Science and Technology, Korea, Republic of (South)*.

**Short Summary:**

Fischer-Tropsch synthesis (FTS) was performed on a bifunctional catalyst prepared by physically mixing precipitated iron-based catalyst (P-Fe) and H-ZSM-5. The correlation between hydrocarbon selectivity and BAS concentration was demonstrated in the bifunctional system of FTS and cracking, and it was found that the C5-C20 selectivity improved as the BAS increased.

## Carbon Dioxide Conversion Poster Session 2

**Tue-P-6**

**Influence of Basicity of Cs-Forms of Hierarchical Aluminosilicate Zeolites on Their Catalytic Activity in Cycloaddition Reactions of Epoxides Under Carbon Dioxide Pressure**

Oleksiy Shvets, Mykhailo Kurmach and Nataliya Shcherban, *L.V. Pisarzhevskii Institute of Physical Chemistry of the National Academy of Sciences of Ukraine, Ukraine*.

**Short Summary:**

Cs-forms of hierarchical zeolites, as well as titanosilicates, template-containing hierarchical zeolites, basic zeolite nanocomposites or mesoporous molecular sieves with anchored basic groups demonstrate high catalytic performance in the cycloaddition of styrene epoxide yielding the corresponding carbonate.

## Catalysis for Environmental Applications and Sustainable Nitrogen Chemistry Poster Session 2

**Tue-P-38**

### Non-Novel Metal-Based Supported Catalysts for Low Temperature Ammonia Decomposition Reaction

Cheol Ung Lee, Monica Louise Triviño and Jeong Gil Seo, *Hanyang University, Korea, Republic of (South)*.

**Short Summary:**

Various supports and catalysts were synthesized and their properties were evaluated. Results indicate that hydrothermally synthesized CeO2 and Co on that showed the best performance with a conversion of 75.53% at 500 . It may be concluded that cobalt supported on basic supports can be effective for the ammonia decomposition reaction.

## New and Advanced Methods in Catalyst Characterization Poster Session

**Tue-P-94**

### $NO_x$-TPD As an Original Method for the Quantitative Characterization of Oxide Surfaces

Cyril Thomas, *Sorbonne Université, France*.

**Short Summary:**

This study describes an original method, consisting in the temperature-programmed desorption of $NO_x$ ($NO_x$-TPD), aimed at quantitatively characterizing oxide surfaces. This method provides insights into complex materials that could not be obtained by the commonly used spectroscopic techniques. Structure($NO_x$-TPD)-activity(HC-SCR) correlations in environmental catalysis are also highlighted.

## Conversion of Methane, Methanol and Syngas Poster Session 1

**Tue-P-57**

### Reducing the Induction Period of Fe/ZSM-5 Catalysts for Methane Dehydroaromatization Via Facile Wet Impregnation Method

Xinrui Zhang, Amol Agarwal, Yukun Liu, Qingheng Lai, Selim Alayoglu, Tobin Marks and Justin Notestein, *Northwestern University, USA*.

**Short Summary:**

The Fe catalysts exhibit a lengthy induction period for methane dehydroaromatization reaction. We discovered that Fe catalysts prepared by the facile wet impregnation method (WI) showed a shorter induction period because they contained isolated or low-polymerized iron sites within the channels of zeolites, which are easier to activate.

## Carbon Dioxide Conversion Poster Session 2

**Tue-P-7**

### Capture and Conversion of $CO_2$ under Mild Conditions over Bifunctional Mesoporous Catalyst

Huidong Xu, Johannes A. Lercher and Andreas Jentys, *Technical University of Munich, Germany*.

**Short Summary:**

An integrated, amine-assisted $CO_2$ hydrogenation was demonstrated in a heterogeneous bifunctional (basis/metallic) catalyst system. The use of ordered mesoporous polymers allows to enhance the methanol yields over the previously studied $SiO_2$ based catalysts.

## Conversion of Oxygenated Feedstocks  Poster Session 1

### Tue-P-75
**Hydrogenolysis of Glycerol over ZSM-5 Supported Ruthenium and Copper Catalysts**
Mattheus Pires, Yutao Xing and Fabio B. Passos, *Universidade Federal Fluminense, Brazil*.

**Short Summary:**
The association of ruthenium, copper and Bronsted sites present on the HZSM-5led to improvements on glycerol hydrogenolysis. In this work these effects have been explored with the goal of reducing the formation of degradation products while maintaining good activity.

### Tue-P-76
**Kinetic Approach in the Comparison of Ru-Cu Catalysts in Hydrotreating Reactions**
Jessica Torres, Diego Duran Sanchez, Cindy Garcia and Jose Antonio de los Reyes, *Universidad Autónoma Metropolitana-Iztapalapa, Mexico*.

**Short Summary:**
The HDO of phenol and its coprocessing with the HDS of DBT on Ru-Cu/&-$ZrO_2$ catalysts were analyzed from a kinetic approach. The selectivity and inhibition of the catalysts were related to the synergy between Ru and Cu and acidity.

## Catalysis for Environmental Applications and Sustainable Nitrogen Chemistry Poster Session 2

### Tue-P-39
**Design of Ordered Mesoporous Catalyst Supports for Plasma-Assisted Ammonia Synthesis**
Sonia Arumuganainar, Stavroula Sartzetakis, Bruce E. Koel and Michele Sarazen, *Princeton University, USA*.

**Short Summary:**
Ordered mesoporous SBA-15 coated with γ-alumina demonstrated higher $N_2$ conversion in a single-stage plasma reactor than commercial, non-ordered analogs, motivating their direct use as a catalyst support and providing a basis for future work as a tunable porous model to characterize the effect of porosity on plasma-assisted ammonia synthesis.

## New and Advanced Methods in Catalyst Characterization Poster Session

### Tue-P-95
**Hydrogen Activation on Molecular Molybdenum Sulfide Clusters Encapsulated within the Pores of NaY Zeolites**
Rachit Khare[1], Roland Weindl[1], Christoph Gross[1], Andreas Jentys[1] and Johannes A. Lercher[1,2], *(1)Technical University of Munich, Germany, (2)Pacific Northwest National Laboratory, USA*.

**Short Summary:**
Transition metal sulfides (TMS) are the workhorse in industrial catalysis and are gaining major importance as replacement for noble-metals in electrocatalysis. Improving these systems will be key towards the resource-saving production of energy carriers. This study provides fundamental insights into hydrogen activation on TMS clusters encapsulated within zeolite micropores.

## Conversion of Methane, Methanol and Syngas Poster Session 1

### Tue-P-58
**Continuous Conversion of Methane into Methanol with Steam over Cu-Mordenite**
Zhenchao Xu, Jong Kyu Kang and Eun Duck Park, *Ajou University, Korea, Republic of (South)*.

**Short Summary:**
a systematical study for the Cu-mordenite catalytic performance in anaerobic and aerobic conditions was conducted. The trace amount of $O_2$ would cause significant effect for methanol productivity. Cu-mordenite with high Cu loading still showed good catalytic activity, which is of guiding significance for further improvement of methanol productivity.

## Carbon Dioxide Conversion Poster Session 2

**Tue-P-8**

### Re-Evaluating $CO_2$r Architectures with Plant Level Techno-Energetics

Tristan Gilbert[1,2] and Thomas F. Jaramillo[2], *(1)Stanford University, USA, (2)SLAC National Accelerator Laboratory, USA*.

**Short Summary:**

We conduct a combinatorial techno-energetic analysis of $CO_2$ electrolysis systems that integrates recent advances in device design and anode reactions. We calculate plant-level energy intensities from fundamental minimum energy requirements and compare to the best results in literature, identifying promising system designs for efficient $CO_2$ up-conversion.

## Conversion of Oxygenated Feedstocks Poster Session 1

**Tue-P-77**

### Effect of Ni Loading Amount of Ni/MgO-$Al_2O_3$ Catalyst on Catalytic Performance in Deoxygenation of Free Fatty Acid

I-Jeong Jeon[1], Ru-Ri Lee[1], Chang-Hyun Kim[1], Min-Jun Kim[1], Kyung-Won Jeon[2], Won-Jun Jang[2] and Jae-Oh Shim[1], *(1)Wonkwang University, Korea, Republic of (South), (2)Kyungnam University, Korea, Republic of (South)*.

**Short Summary:**

The 20% Ni/MG70 catalyst exhibited the highest performance for the deoxygenation reaction owing to its highest number of Ni active sites, easier reducibility, and appropriate acidity. In addition, the green diesel produced by the 20% Ni/MG70 catalyst showed remarkable basic fuel properties such as calorific value and viscosity.

## Catalysis for Environmental Applications and Sustainable Nitrogen Chemistry Poster Session 2

**Tue-P-40**

### Reversible Perovskite-Fluorite Phase Transition in Alumina-Supported $CeFeO_x$ and $CeMnO_x$ films

Kai Shen, Raymond J. Gorte and John M. Vohs, *University of Pennsylvania, USA*.

**Short Summary:**

Thin films with stoichiometries of $CeFeO_x$ and $CeMnO_x$ were conformally deposited on high-surface-area γ-$Al_2O_3$ by Atomic Layer Deposition. Both 2-nm-thick films exhibited perovskite phases after reduction at 1073 K but converted to fluorite phases upon oxidation. The phase transition was reversible and might make both interesting catalyst supports for metals.

## New and Advanced Methods in Catalyst Characterization Poster Session

**Tue-P-96**

### Nature of Extra-Framework Al Species in Zeolites: Solving a 60-Year-Old Mystery

Konstantin Khivantsev[1], Nicholas Jaegers[1], Libor Kovarik[1], Ja Hun Kwak[1,2] and Janos Szanyi[1], *(1)Pacific Northwest National Laboratory, USA, (2)UNIST, Korea, Republic of (South)*.

**Short Summary:**

Our findings explain the origin of enhanced activity of steamed zeolites at the molecular level and provide the missing understanding of the nature of extra-framework Al species.

## Conversion of Methane, Methanol and Syngas Poster Session 1

**Tue-P-59**

**Flame Fused Vitreous Silica Supported Iron Catalysts for Direct, Non-Oxidative Methane Conversion**

Zixiao Liu[1], Sichao Cheng[1] and Dongxia Liu[2], *(1)University of Maryland - College Park, USA, (2)University of Maryland, USA*.

**Short Summary:**

The vitreous silica-supported Fe catalysts were prepared via flame fusion for direct, non-oxidative methane conversion and exhibited better performance than the cristobalite-supported Fe catalyst. The result shows amorphous structure was obtained with a high density of defects and high coordination of Fe sites, thanks to the flame fusion.

## Carbon Dioxide Conversion Poster Session 2

**Tue-P-9**

**Inverse-Structured Cu@$ZrO_2$ Catalysts for Selective Hydrogenation of $CO_2$ to Methanol**

Junjie Chen[1], Alessandro Gallo[1,2] and Thomas F. Jaramillo[1,2], *(1)Stanford University, USA, (2)SLAC National Accelerator Laboratory, USA*.

**Short Summary:**

We engineered inversed-structured Cu@$ZrO_2$ catalysts that show > 80% MeOH selectivities under industry-relevant conditions for $CO_2$ hydrogenation. We also confirmed that the $ZrO_2$ overlayers can promote formate species formation on the interfacial sites of Cu@$ZrO_2$.

## New and Advanced Methods in Catalyst Characterization Poster Session

**Tue-P-97**

**Temperature Programmed Surface Reaction of Alcohols and Ferrierite**

Chris Gastaldo and Hoang Nguyen, *Micromeritics, USA*.

**Short Summary:**

TPSR is a rapid technique used to characterize catalysts by determining whether surface sites are acidic, basic, or redox, and to observe change in reaction types such as ethanol to olefins. Two ferrierite samples that have a SiO2/Al2O3 mole ratio of 20 and 55 are investigated with methanol and ethanol.

## Conversion of Methane, Methanol and Syngas Poster Session 1

**Tue-P-60**

**Reaction and Catalyst Optimization for the Conversion of Dimethyl Ether to Liquefied Petroleum Gas over Pd/BEA Zeolite**

Candace Eslick, *University of Cape Town, South Africa*.

**Short Summary:**

Due to stringent environmental regulations, synthesis routes that making use of captured $CO_2$ are of interest, specifically methanol-to-hydrocarbons. In this work, the influence of temperature, pressure, space velocity, $H_2$/DME ratio data is presented for the conversion of green-DME to LPG over zeolite BEA of varying hydrophobicity and mesoporosity.

## Carbon Dioxide Conversion Poster Session 2

**Tue-P-10**

### M-Bdc: A Novel Two-Dimensional Metal-Organic Framework As an Efficient CO$_2$rr Catalyst

Qiushi Ma[1,2] and Zhou Lin[1], *(1)University of Massachusetts Amherst, USA, (2)Marquette University, USA*.

**Short Summary:**

Our study not only highlights 2D MOF as a kind of promising catalyst for CO$_2$ reduction also shed light on the impact of metal centers on CO$_2$ reduction. In addition, 2D MOFs provide a new platform to study the effect of single-site atom in electrocatalyst.

## Conversion of Oxygenated Feedstocks Poster Session 1

**Tue-P-78**

### Chemical Recycling of Polyurethane Via Solvent-Free Mechanocatalytic Methanolysis/Hydrolysis with Base

Bolun Wang[1], Joel Britschgi[1], Ivana Jevtovikj[2], Stephan Andreas Schunk[2,3] and Ferdi Schüth[1], *(1)Max-Planck-Institut für Kohlenforschung, Germany, (2)Hte GmbH, the High Throughput Experimentation Company, Germany, (3)BASF SE, Germany*.

**Short Summary:**

Polyurethane (PU) is the 6th most produced plastics worldwide but its recycling is limited due to the cross-linked structure of thermoset PU. Our preliminary results show that over 50 wt% of soluble polyol can be recovered from the mechanocatalytic methanolysis/hydrolysis of commercial PU sponge with common bases under mild conditions.

## Catalysis for Environmental Applications and Sustainable Nitrogen Chemistry Poster Session 2

**Tue-P-41**

### Catalyst Ageing of Field-Returned Catalytic Diesel Particulate Filters

Samuel af Ugglas[1,2], Anders Ersson[1], Moa Sundén[1], Lars Pettersson[2] and Henrik Kusar[2], *(1)Scania CV AB, Sweden, (2)KTH Royal Institute of Technology, Sweden*.

**Short Summary:**

Activity tests of field-returned catalytic diesel particulate filters indicates lower activity of the catalyst resulting in inferior conversion of nitric oxide and hydrocarbons. Removal of ash compounds results in a slight increase in catalytic activity, indicating that ageing processes rather than ash accumulation affects the catalytic performance of the filters.

## Conversion of Oxygenated Feedstocks Poster Session 1

**Tue-P-79**

### Anisole Hydrodeoxygenation over Ni/&-ZrO$_2$. Metal Loading Effect

Reyna Rios[1], José Escobar[2], Jorge N. Díaz de León[3], Cindy Garcia[1] and Jose Antonio de los Reyes[1], *(1)Universidad Autónoma Metropolitana-Iztapalapa, Mexico, (2)Instituto Mexicano del Petróleo, Mexico, (3)Universidad Nacional Autónoma de México, Mexico*.

**Short Summary:**

The influence of metal loading on anisole HDO for Ni/&-ZrO$_2$ catalysts was explored. High activity per Ni atom and >90% deoxygenated selectivity was achieved at around 5 wt% Ni/&-ZrO$_2$ . Understanding the effect of metal loading on Ni catalysts for HDO is relevant to design materials for potential bio-oil upgrading.

## Catalysis for Environmental Applications and Sustainable Nitrogen Chemistry Poster Session 2

**Tue-P-42**

**Validation of the Iron Catalyst for Green Ammonia Application**

Cristina Pizzolitto, Alberto Biasin, Matteo Guiotto and Pierdomenico Biasi, *CASALE SA, Switzerland*.

**Short Summary:**

Ammonia is a fundamental feedstock, so its green production is crucial to support the energy transition. The goal of the work is the assessment of the Iron catalyst activity under green NH3 conditions to achieve a deep understanding on how to use it.

## New and Advanced Methods in Catalyst Characterization Poster Session

**Tue-P-98**

**How Are You Going to Affect Me? – In-Situ Deactivation Measurements on Bifunctional Catalysts for One-Step DME Synthesis**

Felix Hilfinger[1], Samuel F. Gatti[2] and Ingo Krossing[1], *(1)University of Freiburg, Germany, (2)Paul Scherrer Insitut, Switzerland*.

**Short Summary:**

An *in-situ* measurement method to detect the mutual deactivation of surface-basic $CO_2$ hydrogenation – and acidic zeolite catalysts, can be carried out by DRIFTS. It's based on the adsorption of pivalonitrile on surface silanol groups. The results can be correlated with the performance of bifunctional catalysts for one-step DME synthesis.

## Conversion of Methane, Methanol and Syngas Poster Session 1

**Tue-P-61**

**Coordination Environment of Ni Determines Catalytic Performance of Ni/$CeO_2$ Catalyst for DRM Reaction**

Fudong Liu, Shaohua Xie, Murtadha Almousawi, Daekun Kim, Kailong Ye and Xing Zhang, *University of Central Florida, USA*.

**Short Summary:**

Catalytic stability is highly essential for the catalysts in dry reforming of methane (DRM). By tuning the coordination environments of Ni on $CeO_2$, the Ni sintering can be greatly mitigated, thus significantly improving the catalytic activity and stability of Ni/$CeO_2$ catalyst in DRM reaction.

## Carbon Dioxide Conversion Poster Session 2

**Tue-P-11**

**Effect of Cadmium Addition on Tin (II) Coordination Polymers Electrocatalysts for the $CO_2$ Reduction Reaction**

Martín Daniel Trejo-Valdez and Adrián Farid Bustos-Jiménez, *Instituto Politécnico Nacional, Mexico*.

**Short Summary:**

This work describes the synthesis of MOFs structures with tin and cadmium as metal nodes and oxalate ions as organic ligands, the electrocatalytic processing of $CO_2$ in aqueous media is also presented. Organic acids derivatives were obtained from $CO_2$RR using MOF-Sn/Cd, where the cadmium content was higher than 50% mol/mol.

## Catalysis for Environmental Applications and Sustainable Nitrogen Chemistry Poster Session 2

**Tue-P-43**
**Sustainability at the Center of Novel Technologies Development**
Annalisa Sacchetti, *Casale SA, Switzerland*.

**Short Summary:**
As developer of industrial technologies, Casale SA have the sustainability as a mission to reduce the footprint of plants. An overview of a possible methods exploitable for sustainability Key performance indicators calculation will be given in the presented work, useful to monitor and continuously improve sustainability levels.

## New and Advanced Methods in Catalyst Characterization Poster Session

**Tue-P-99**
**Hierarchically Structured Rugae-like RuP$_3$–CoP Arrays for Hydrogen Generation**
Tayirjan Isimjan[1] and Xiulin Yang[2], *(1)SABIC-CRD-KAUST, Saudi Arabia, (2)Guangxi Normal University, China*.

**Short Summary:**
The rugae-like Co–Ru–P arrays exhibited NaBH$_4$ hydrolysis in alkaline media with a high turnover frequency (TOF) of 2123.6 mol$_{H2}$ min$^{-1}$ mol$_{Ru}^{-1}$ at 25 °C, which is one of the highest known so far. Additionally, the catalyst also shows a high stability with less than 8.0% lost after 5 consecutive cycles.

## Conversion of Methane, Methanol and Syngas Poster Session 1

**Tue-P-62**
**Ni-Al SHS Catalysts in Dry Reforming of Methane to Hydrogen-Enriched Fuel Mixtures**
Svetlana Tungatarova[1,2], Galina Xanthopoulou[3], Alua Manabayeva[1,4], Päivi Mäki-Arvela[5], Dmitry Murzin[5] and Tolkyn S. Baizhumanova[2], *(1)D.V. Sokolsky Institute of Fuel, Catalysis and Electrochemistry, Kazakhstan, (2)al-Faraby Kazakh National University, Kazakhstan, (3)Institute of Nanoscience and Nanotechnology, NCSR Demokritos, Greece, (4)Kazakh-British Technical University, Kazakhstan, (5)Åbo Akademi University, Finland*.

**Short Summary:**
It was developed the new catalysts for dry reforming of methane into synthesis-gas. As a result of the study, using a complex of physico-chemical methods, data were obtained for understanding the catalytic activity of catalysts, which will further promote the organization of a new environmentally friendly energy-saving production.

## Carbon Dioxide Conversion Poster Session 2

**Tue-P-12**
**Feasibility Study of Alkaline Metal Oxide Modified Cu-ZnO-Al$_2$O$_3$ for Reactive Capture of CO$_2$ to Methanol**
Martha A. Arellano-Trevino, Chae Jeong-Potter, Anh To, W. Wilson McNeary and Dan Ruddy, *National Renewable Energy Laboratory, USA*.

**Short Summary:**
We propose a Dual function material (DFM) consisting of an alkali modified Cu-ZnO-Al$_2$O$_3$ (CZA), the state-of-the-art commercial methanol synthesis catalyst, for CO$_2$ capture from a CO$_2$-rich waste gas stream and in-situ conversion to methanol. Carbon-negative methanol production could play a significant role in achieving net-carbon neutral fuels and chemicals.

## Conversion of Oxygenated Feedstocks Poster Session 1

**Tue-P-80**

**Nanocellulose-Derived Carbon Catalysts for Syngas Upgrading in Co-Pyrolysis of Plastics and Biomass**

Rongge Zou and Hanwu Lei, *Washington State University, USA*.

**Short Summary:**

One carbon catalyst derived from nanocellulose (NCBC) was developed and applied to catalytic fast pyrolysis/co-pyrolysis (CFP/co-CFP) of biomass and plastics. NCBC shows great $H_2$ promotion and wax removal ability in single pyrolysis and further promotes the $H_2$ selectivity in co-pyrolysis.

**Tue-P-81**

**Homogeneous Hydrogenation of Biomass Derivate Using Ruthenium (II) and Nickel (II) Complexes Containing Phosphorus-Nitrogen Ligands.**

Sebastian Parra Melipan and Pedro Aguirre, *Universidad de Chile, Facultad de Ciencias Químicas y Farmacéuticas, Chile*.

**Short Summary:**

In this work we have interesting results in homogeneous hydrogenation of platform compounds such as furfural and levulinic acid with nickel (II) and ruthenium (II) complexes that containing phophorus-nitrogen ligands.

## Catalysis for Environmental Applications and Sustainable Nitrogen Chemistry Poster Session 2

**Tue-P-44**

**Selectivity Modulated By Post-Plasma Species-Catalyst Interactions: Mechanism of $CH_4/N_2$ Conversion to Ammonia and Ethylene**

Sarojini Tiwari[1], Saleh Ahmat Ibrahim[2], Brandon Robinson[1], Sean Brown[1], Fanglin Che[2] and Jianli Hu[1], *(1)West Virginia University, USA, (2)University of Massachusetts Lowell, USA*.

**Short Summary:**

Methane and nitrogen are converted to methane and ammonia under microwave plasma enhanced catalysis conditions over a ceria support. Density functional theory calculations determined that the post-plasma species-induced positive charge over the Pd-Ag catalytic surface could enhance the energetics of forming ethylene but suppress the energetics of hydrogenation to ethane.

## New and Advanced Methods in Catalyst Characterization Poster Session

**Tue-P-100**

**Quantification of Hydrogen Spillover on Cu-& Catalysts and Its Effect on Alkene Hydrogenation**

Griffin Canning, Greg Barber and Rob Rioux, *Pennsylvania State University, USA*.

**Short Summary:**

Hydrogen spillover on reducible supports and the related formation of oxygen vacancies is of critical importance to many reactions, including the hydrodeoxygenation of oxygenates. An accessible and precise method for quantification of spillover hydrogen and oxygen vacancy formation is discussed, and the influence of each on hydrogenation catalysis are presented.

## Conversion of Methane, Methanol and Syngas Poster Session 1

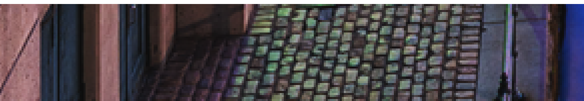
**Tue-P-63**

**Aqueous-Phase Partial Oxidation of Methane over Pd-Fe/ZSM-5 with in Situ Generated Hydrogen Peroxide**

Gunsik Yang, Jong Kyu Kang and Eun Duck Park, *Ajou University, Korea, Republic of (South)*.

**Short Summary:**

The simple one-body catalyst system (Pd-Fe/ZSM-5 with low Pd contents) was demonstrated for aqueous-phase selective oxidation of methane in the presence of $H_2$ and $O_2$.



## Carbon Dioxide Conversion Poster Session 2

### Tue-P-13

### Structural Dynamics of Cerium Oxides and Their Catalytic Consequences in Water-Gas Shift Catalytic Cycle

Guangming Cai, Siran Zhang and Cathy Chin, *University of Toronto, Canada*.

**Short Summary:**

We probe the structural dynamics of cerium oxides ($CeO_2$) and their catalytic consequences in water-gas shift catalytic cycle, in both the forward and reverse directions, and establish the overall energy landscape and kinetic consequences of the O-vacancy on $CO_2$ activation, through $H_2$-temperature programmed reduction (TPR), kinetic, and transient studies

## Conversion of Oxygenated Feedstocks Poster Session 1

### Tue-P-82

### Tunable Palladium Catalyst Using Swellable Organically Modified Silica As a Scaffold for Aqueous Phase Phenol Hydrogenation

Snehal Patil, Anagha Hunoor and Umit Ozkan, *The Ohio State University, USA*.

**Short Summary:**

Swellable organically modified silica (SOMS) support with tunable polarity/hydrophobicity was used for selective conversion of phenol to cyclohexanone and cyclohexanol. Initial activity data show that Pd supported on polar/hydrophilic SOMS support (SOMS-UD) demonstrated high selectivity towards more polar cyclohexanol while non-polar/hydrophobic SOMS support showed higher selectivity towards less polar cyclohexanone.

## Catalysis for Environmental Applications and Sustainable Nitrogen Chemistry Poster Session 2

### Tue-P-45

### Low-Temperature Oxygen Activation in Cu-CHA SCR Catalysts

Magnus Skoglundh[1], Xueting Wang[1], Lin Chen[1], Yingxin Feng[1], Peter N.R. Vennestrøm[2], Ton V.W. Janssens[2], Peter S. Hammershøi[2], Jonas Jansson[3] and Henrik Grönbeck[1], *(1)Chalmers University of Technology, Sweden, (2)Umicore Denmark ApS, Denmark, (3)Volvo Group Trucks Technology, Sweden*.

**Short Summary:**

The results show that O2 adsorption at low temperatures over Cu-CHA is more facile over Cu(NH3)2+ complexes compared to framework-bound Cu+ species. The observed differences contribute to an enhanced understanding on SCR catalysis and the underlying chemistry of partial oxidation reactions, such as direct oxidation of methane to methanol.

## New and Advanced Methods in Catalyst Characterization Poster Session

### Tue-P-101

### Reduction of $SiO_2$-Supported $WO_x$ Species Enhanced by Hydrogen Spillover

Konstantin Mamedov, Anukriti Shrestha, Chris Paolucci and Robert Davis, *University of Virginia, USA*.

**Short Summary:**

Silica-supported $WO_x$ species promoted by Pd nanoparticles are catalysts for the reduction of carboxylic acids to alcohols by $H_2$. This work demonstrates hydrogen spillover from Pd lowers the reduction temperature of $SiO_2$-supported $WO_3$ clusters.

## Conversion of Methane, Methanol and Syngas Poster Session 1

**Tue-P-64**

**Methane Carboxylation Using Electrochemically Activated Carbon Dioxide**

Yucheng Yuan, Yuhan Zhang, Haoyi Li, Muchun Fei, Hongna Zhang, John Santoro and Dunwei Wang, *Boston College, USA*.

**Short Summary:**

We developed an integrated route to synthesize $CH_3COOH$ from $CH_4$ and $CO_2$ with 100% atom economy, where $CO_2$ activation is followed by methane carbonylation. Our work is expected to inspire more carbonylation reactions utilizing preactivated $CO_2$ that take advantage of both reduction and oxidation products, thus achieving high atomic efficiency.

## Carbon Dioxide Conversion Poster Session 2

**Tue-P-14**

**The Use of Water As Boosting Agent for $CO_2$ Hydrogenation to Alcohols over Cu-Uio-67 Under Mild Conditions**

Luana de Paula, Janaina F. Gomes and José Mansur Assaf, *Federal University of São Carlos, Brazil*.

**Short Summary:**

In the present work, the hydrogenation of $CO_2$ on Cu-UiO-67 at atmospheric pressure and using $H_2$ or water as hydrogen source was investigated with the aim of producing alcohols, mainly ethanol. $H_2O$ instead of $H_2$ led to better results for alcohols production at mild conditions.

## Conversion of Methane, Methanol and Syngas Poster Session 1

**Tue-P-65**

**MeOH-Mediated Hydrogen Transfer Mechanism at Zeolitic Surface Lewis Acid Sites**

Annika E. Enss[1], Philipp N. Plessow[1] and Felix Studt[2], *(1)Karlsruhe Institute of Technology (KIT), Germany, (2)Karlsruhe Institute of Technology, Germany*.

**Short Summary:**

The reactivity of surface Lewis acid sites (LAS) of H-SSZ-13 catalyst was computationally investigated for a MeOH-mediated hydrogen transfer reaction mechanism and compared to the reactivity of a surface Brønsted acid site (BAS) and the bulk BAS. For the hydrogen transfer step, LAS showed lower free energy barriers than BAS.

## Carbon Dioxide Conversion Poster Session 2

**Tue-P-15**

**The Role of Mn in Carbon Nanosphere Encapsulated Fe-Co Core-Shell Catalyst for Carbon Dioxide Conversion to Value-Added Chemicals**

Alexa Saporita, Akash Gandotra, Sarah Forster and Cheng Zhang, *Long Island University (Post), USA*.

**Short Summary:**

We have introduced Mn to the composition of carbon nanosphere encapsulated Fe-Co core shell catalyst to determine its role in $CO_2$ hydrogenation. The value-added chemicals CO, methane, light alkanes, and light olefins were produced, showing promising results for the recycling of $CO_2$ through catalytic $CO_2$ hydrogenation.

## Conversion of Oxygenated Feedstocks Poster Session 1

### Tue-P-83

### Influence of the Metallic Charge of Ni-Pd and Ni-Pt Catalysts over Zirconium-Modified Clays in the Hydrodeoxygenation of Eugenol

Emigdio Zamora, *Autonomous Metropolitan University, Azapotzalco Campus, Mexico*.

**Short Summary:**

In this work, the activity of Ni-Pd and Ni-Pt bifunctional bimetallic catalysts was determined at different loads of noble metals supported on pillared clays with zirconium cations in the HDO reaction of eugenol as a representative molecule of a biooil at 573 K and 3 MPa.

## Catalysis for Environmental Applications and Sustainable Nitrogen Chemistry Poster Session 2

### Tue-P-46

### Promotion Effect of Thermal Treatment on the Activity of Pt/ZSM-5 for Selective Catalytic Reduction of NOx By $H_2$

Dong Chan Park, Ji Hwan Song, Sei Moon and Do Heui Kim, *Seoul National University, Korea, Republic of (South)*.

**Short Summary:**

In $H_2$-SCR reaction, when the reaction temperature increased, an undesired $H_2$-$O_2$ reaction occurs, resulting in a low de-NOx activity. Thermally treated Pt/ZSM-5 suppressed the $H_2$-$O_2$ reaction at high temperatures, thereby increasing de-NOx activity in overall temperature as compared to the Fresh catalyst. And the operating window was significantly widened.

## New and Advanced Methods in Catalyst Characterization Poster Session

### Tue-P-102

### Influence of $CeO_2$ and Au/$CeO_2$ Pretreatment on the Creation of Surface Defects That Allow Modification of the Optical Interband.

Gabriela I. Hernandez-Salgado[1], Mara Cordero-Garcia[2], Sergio Gomez Torres[2], Elizabeth Rojas-García[2], Elizabeth Salinas-Barrios[2] and Miriam Sanchez-Ordaz[2], *(1)Autonomous Metropolitan University-Iztapalapa, Mexico, (2)Universidad Autónoma Metropolitana-Iztapalapa, Mexico*.

**Short Summary:**

Cerium oxide is an interesting material because its redox properties alter the balance of surface charges causing a compensation known as oxygen vacancy (Vo). Introduction of oxygen vacancies and related defects in $CeO_2$, can modify the bandgap or other optoelectronic properties making the material suitable for visible or IR applications.

## Conversion of Oxygenated Feedstocks Poster Session 1

### Tue-P-84

### Obtaining Hydrogen By Steam Reforming of Residual Glycerol from Biodiesel Process Using Catalysts Ni/$La_2O_3$-$CeO_2$

Gabriela S. Zanelli, Alessandra F. Lucredio and Elisabete M. Assaf, *University of São Paulo, Brazil*.

**Short Summary:**

La1-XCeXNiO3 catalysts were prepared, with and without surfactant, characterized and evaluated in the glycerol steam reforming reaction. The perovskite prepared by surfactant-assisted synthesis showed the best dispersion of the active phase and the presence of Ce promoted gasification of C.

## Catalysis for Environmental Applications and Sustainable Nitrogen Chemistry Poster Session 2

**Tue-P-47**

**Simultaneous Removal of NO and $N_2o$ By $NH_3$ on Various Metal-Loaded Zeolite Catalysts**

Masaru Ogura, *The University of Tokyo, Japan*.

**Short Summary:**

NO and $N_2O$ were simultaneously removed by use of $NH_3$ at low temperatures even in excess $O_2$ and $H_2O$ coexisted on metal-loaded zeolite catalysts.

## New and Advanced Methods in Catalyst Characterization Poster Session

**Tue-P-103**

**Surface Dynamics of the Bulk Vanadium Antimony Mixed Oxide Catalyst during the Direct Selective Oxidation of Propane**

Bar Mosevitzky Lis[1], M. Olga Guerrero-Pérez[2] and Israel Wachs[1], *(1)Lehigh University, USA, (2)Universidad de Málaga, Spain*.

**Short Summary:**

The surface properties of bulk ~$VSbO_4$, used for selective propane oxidation were investigated under different conditions revealing the presence of a dynamic surface. The results help to resolve previous conflicting *ex situ* characterization results and show that surface $VO_x$ enrichment at high temperatures decreases acrolein selectivity via overoxidation.

## Conversion of Methane, Methanol and Syngas Poster Session 1

**Tue-P-66**

**Influence of the Copper Precursor of Cu Metal Organic Frameworks on the Direct Oxidation of Methane to Methanol**

Thielle Ferreira, Janaina F. Gomes and José Mansur Assaf, *Federal University of São Carlos, Brazil*.

**Short Summary:**

The influence of the metallic precursor on the catalytic properties of metal organic frameworks (MOFs) has been poorly explored in the literature. In this work we show that the copper (Cu) precursor of the Cu-MOFs impacts on the partial oxidation of methane to methanol over these materials.

## Carbon Dioxide Conversion Poster Session 2

**Tue-P-16**

**Exploring the Effects of Environment Conditions on Atomically-Dispersed Pt Catalysts in $CO_2$ Hydrogenation**

Amelia Figueroa[1], Scott Bamonte[2], Meilin Li[2] and Steven Suib[2], *(1)Nova Southeastern University, USA, (2)University of Connecticut, USA*.

**Short Summary:**

Pt was atomically-dispersed on $CeO_2$ and $WO_3$ nanoparticle supports to explore the effects of support acid-base properties on the catalytic activity of platinum active sites. Data demonstrated that the basic sites are more effective for $CO_2$ hydrogenation than acidic sites. Active sites are four-coordinated, atomically-wdispersed Pt species for both materials.

## New and Advanced Methods in Catalyst Characterization Poster Session

**Tue-P-104**

**Unraveling Acid Etching-Induced Surface Evolution of ZnO Nanorods for Boosting Catalytic CO Gas Sensing**

Fangyuan Liu, Chunxiang Zhu, Bo Zhang and Pu-Xian Gao, *University of Connecticut, USA*.

**Short Summary:**

We use *in situ* liquid cell TEM to observe the shape transformation of ZnO nanorod to pencil-shaped nanostructure during hydrochloride acid etching process. Manipulating this pencil-shaped ZnO associated with various catalytic sensitizers boost the CO sensing properties as a result of the enhanced sensitzer-semiconductor surface interactions.

## Conversion of Methane, Methanol and Syngas Poster Session 1

**Tue-P-67**
**Limiting Unselective $H_2O$ Formation in the Dry-Reforming of $CH_4$ Using Limited Hydrogenation Kinetics of Intermetallic Compounds**
Max Mortensen and Siris Laursen, *University of Tennessee, USA*.

**Short Summary:**
Improved understanding of fundamental catalytic surface chemistry to control the O/OH hydrogenation kinetics, methane and $CO_2$ activation, and promote faster C/CH oxidation kinetics. Utilization of both computation and experimental techniques to understand how to control fundamental catalytic surface chemistry.

## Carbon Dioxide Conversion Poster Session 2

**Tue-P-17**
**The Role of Dispersion Agent in the Synthesis of Carbon Nanosphere Encapsulated Fe-Co Catalyst for Carbon Dioxide Hydrogenation**
Alexa Saporita, Akash Gandotra, Sarah Forster and Cheng Zhang, *Long Island University (Post), USA*.

**Short Summary:**
In the carbon nanosphere encapsulated Fe-Co (CNS-FeCo) core shell catalyst agglomeration of the CNS can occur jeopardizing the catalytic performance. To minimize this, we introduced a dispersion agent to the synthesis of the CNS-FeCo. With addition of the dispersion agent, enhanced catalytic activity and selectivity occurred.

## Catalysis for Environmental Applications and Sustainable Nitrogen Chemistry Poster Session 2

**Tue-P-48**
**Waste-to-Energy Residuals As Catalytic Materials: $DeNO_x$ over Ash As a Starting Point**
Kaitlyn Lawrence[1] and Marco J. Castaldi[2], *(1)City College of New York, CUNY, USA, (2)The City College of New York, USA*.

**Short Summary:**
In continuation of our studies to explore beneficial uses of municipal solid waste residuals, we introduced the use of ash as a heterogeneous catalyst in several reaction systems resulting in favorable performance. Importantly, we demonstrated the high activity of ash in the reduction of nitric oxide by ammonia.

**Tue-P-49**
**Application of Metal Single-Site Zeolite Catalysts in Heterogeneous Catalysis**
Rafal Baran[1], Yannick Millot[1,2], Frederic Averseng[1] and Stanislaw Dzwigaj[1], *(1)Sorbonne-Universite, France, (2)Sorbonne Université, France*.

**Short Summary:**
V-single site zeolite catalysts containing vanadium as pseudo-tetrahedral V species have not only very high selective to desired product ($N_2$) in selective catalytic reduction of NO with ammonia but they are also very active in NO conversion at 773 K.

## New and Advanced Methods in Catalyst Characterization Poster Session

**Tue-P-105**
**An At-Line Monitoring Strategy of Sugar Isomerization via ATR-FTIR Spectroscopy for Rapid Catalyst Development**
Jakub Konkol and George Tsilomelekis, *Rutgers, The State University of New Jersey, USA*.

**Short Summary:**
The isomerization of sugars is challenging to track because of the many byproducts that can form, such as humins. The developed strategy allows the detailed estimation of kinetic parameters while can be used as a means for in-line Process Analytical Control of biomass conversion processes.

## Conversion of Methane, Methanol and Syngas Poster Session 1

**Tue-P-68**

### Influence of Rare Earth Oxides on Oxidative Coupling of Methane Towards Acetylene over Pt-Based Monolithic Catalysts

Patrick Lott, Sven Schardt, Felix Ehrlich, Jaspreet Chawla and Olaf Deutschmann, *Karlsruhe Institute of Technology (KIT), Germany*.

**Short Summary:**

Rare earth oxides were investigated for their influence in platinum-governed oxidative coupling of methane. Lanthanum, Neodymium, and Samarium oxide doped catalysts showed higher $C_2$-selectivities than pure $Pt/Al_2O_3$. Best case achieved was 11.2% $C_2$ selectivity and a $CH_4$ conversion of 88.2% with 1 wt.-% Pt/20.-% $Sm_2O_3/Al_2O_3$.

## Carbon Dioxide Conversion Poster Session 2

**Tue-P-18**

### Carbon Dioxide Hydrogenation over Physically Mixed $Fe_3O_4$-$Co_3O_4$ and $SiO_2$

Winny Chan, Allison Chan, Akash Gandotra and Cheng Zhang, *Long Island University (Post), USA*.

**Short Summary:**

This study investigates the effect of silica ($SiO_2$) as a support for $Fe_3O_4$–$Co_3O_4$ physically mixed catalysts for $CO_2$ hydrogenation. The main products from the $CO_2$ hydrogenation over the synthesized catalysts are $CH_4$ and CO and show promising results for activity and selectivity for $CO_2$ conversion to $CH_4$.

## Catalysis for Environmental Applications and Sustainable Nitrogen Chemistry Poster Session 2

**Tue-P-50**

### Enhancing Methane Oxidation Activity By Manipulating Catalysts' Structure through Flame Spray Pyrolysis

Can Wang, Musa Najimu and Erdem Sasmaz, *University of California, Irvine, USA*.

**Short Summary:**

Low-temperature methane oxidation activity can be enhanced by solid-solution catalysts with high oxygen vacancy concentration and strong metal-support interaction with highly dispersed $Pd^{2+}$ species. Flame spray pyrolysis allows to manipulate these factors and design catalysts with such desired structures by tuning the synthesis conditions.

## New and Advanced Methods in Catalyst Characterization Poster Session

**Tue-P-106**

### Studying Nanoscale Charge Transport across Interfaces Using *in Situ* Electron Holography in Photocatalyst for Solar Hydrogen Evolution

Piyush Haluai, Martha McCartney and Peter Crozier, *Arizona State University, USA*.

**Short Summary:**

Effects of rhodium (Rh) doping in strontium titanate (STO) has been studied with emphasis on visible light absorption properties and studying charge separation at nanoscale using *in situ* electron holography which would immensely benefit better design of the photocatalyst systems for renewable energy generation.

## Carbon Dioxide Conversion Poster Session 2

**Tue-P-19**

### Solvent Effects of Supercritical Carbon Dioxide on Electrocatalytic Carbon Dioxide Reduction Reaction

Guo Ling[1], Hongshan Bi[2], Qiushi Ma[3], Jun Yi[1] and Zhou Lin[2], *(1)University of Massachusetts, USA, (2)University of Massachusetts Amherst, USA, (3)Marquette University, USA*.

**Short Summary:**

The introduction of $scCO_2$ as an alternative solvent sets the stage of future modeling of $CO_2RR$ with desired products by manipulating the reaction conditions. For example, if $CO_2RR$ with $scCO_2$ produces popular industrial feedstock, like methane ($CH_4$) and methanol ($CH_3OH$), their production efficiency will be increased with $scCO_2$ suppressing HER.

**Tue-P-20**

**$CO_2$ Hydrogenation over Physically Mixed $Fe_3O_4$-$Co_3O_4$ with $MnO_2$**

Aliyah Harrison[1], Cheng Zhang[1], Winny Chan[1], Akash Gandotra[2], Allison Chan[1] and Nicole Forte[1], *(1)Long Island University (Post), USA, (2)Long Island University, USA*.

**Short Summary:**

$MnO_2$ is introduced with varying loading to the $Fe_3O_4$-$Co_3O_4$ mixture to examine the role of Mn in the catalyst's composition for $CO_2$ hydrogenation. Positive results such as olefins productions along with $CO_2$ conversions were observed at various temperatures.

## New and Advanced Methods in Catalyst Characterization Poster Session

**Tue-P-107**

**Identifying the Active Site in Catalysis: What Is the Future for X-Ray Absorption Spectroscopy?**

Simon Bare[1], Jorge Perez-Aguilar[2], Jiyun Hong[1], Adam Hoffman[1] and Fernando Vila[3], *(1)SLAC National Accelerator Laboratory, USA, (2)University of California, Davis, USA, (3)University of Washington, USA*.

**Short Summary:**

Given the significance of XAS in catalyst characterization and the need for a better understanding of catalyst structure to drive new developments it is important to ensure that the equipment and methodology available to a catalysis researcher is critically evaluated.

**Tue-P-108**

**Laboratory-Based XAFS at TU Berlin - Towards in-Situ Measurements**

Christopher Schlesiger, Sebastian Praetz, Wolfgang Malzer and Birgit Kanngießer, *Technische Universität Berlin, Germany*.

**Short Summary:**

A laboratory-based XAFS spectrometer at TU Berlin is presented, that is regularly used in catalyst characterization. The easy access gives completely new opportunities for exploiting XAFS as an analytical tool. Currently new ways for introducing in-situ capabilities are evaluated.

## Carbon Dioxide Conversion Poster Session 2

**Tue-P-21**

**The Addition of $ZrO_2$ to Highly Magnetic Mixture of $Fe_3O_4$-$Co_3O_4$ for $CO_2$ Hydrogenation to Value-Added Chemicals**

Winny Chan, Allison Chan, Akash Gandotra and Cheng Zhang, *Long Island University (Post), USA*.

**Short Summary:**

This study investigates the effect of adding zirconium dioxide ($ZrO_2$) as a support to the mixture of $Fe_3O_4$–$Co_3O_4$ catalysts for $CO_2$ hydrogenation. The main products from the $CO_2$ hydrogenation over the synthesized catalysts are $CH_4$ and CO and show promising results for activity and selectivity for $CO_2$ conversion to CH4.

## New and Advanced Methods in Catalyst Characterization Poster Session

**Tue-P-109**

**Software Developments for X-Ray Absorption Spectroscopy Characterization of Catalysts at the Stanford Synchrotron Radiation Lightsource**

Jorge Perez-Aguilar, Simon Bare and Adam Hoffman, *SLAC National Accelerator Laboratory, USA*.

**Short Summary:**

Co-ACCESS has developed software packages, CatMASS and CatXAS, to lessen the learning curve for non-specialized X-ray absorption spectroscopy (XAS) catalysis users. Additionally, we are evaluating how flow systems installed at the beamline compare from a mass transport and gas purity to lab reactors set ups.

## Carbon Dioxide Conversion Poster Session 2

### Tue-P-22
### Carbon Dioxide Hydrogenation over Physically Mixed $Fe_3O_4$-$Co_3O_4$ and &

Allison Chan, Winny Chan, Akash Gandotra and Cheng Zhang, *Long Island University (Post), USA.*

**Short Summary:**
In this current work, we introduced titanium oxide (&) to a mixture of $Fe_3O_4$–$Co_3O_4$ to investigate the effects of & as a support for $CO_2$ hydrogenation. We discovered that $CO_2$ conversion steadily increases with temperature and $CH_4$ selectivity is rather high while CO selectivity is rather low.

### Tue-P-23
### The Addition of $CeO_2$ to Carbon Nanosphere (CNS) Encapsulated Fe-Co Core-Shell Catalyst for $CO_2$ Hydrogenation to Light Olefins

Sarah Forster, *Long Island University (Post), USA.*

**Short Summary:**
Cerium oxide is added to a CNS-FeCo catalyst to increase $CO_2$ conversion and light olefin selectivity. It was found that the addition of $CeO_2$ increases the production of light olefins and CO selectivity.

### Tue-P-24
### Computational Study of Supported Pd-Cu Clusters for Electrochemical $CO_2$ Reduction

Haiying He[1], Marcus Ochsendorf[1] and Peter Zapol[2], *(1)Valparaiso University, USA, (2)Argonne National Laboratory, USA.*

**Short Summary:**
Graphene supported $Pd_{3-m}Cu_m$ ($m$=0-3) and $Pd_{4-n}Cu_n$ ($n$=0-4) clusters were investigated as potential electrocatalysts for $CO_2$ reduction using first-principles approaches and the computational hydrogen electrode model. Unique electronic structure, highly under-coordinated surface atoms of these subnanometer clusters and their interaction with the support has a profound impact on their catalytic behavior.

### Tue-P-25
### The Role of Surface Roughening in Improving the Selectivity of Copper for $CO_2$ Electroreduction

Joakim Stenlid[1,2], Joseph Gauthier[3], Alexis Bell[4], Martin Head-Gordon[5] and Frank Abild-Pedersen[2], *(1)Stanford University, USA, (2)SLAC National Accelerator Laboratory, USA, (3)Texas Tech University, USA, (4)University of California, Berkeley, USA, (5)Lawrence Berkeley National Laboratory, USA.*

**Short Summary:**
Using a combination of modeling techniques, we investigate the effect of roughening on the selectivity of Copper catalysts in electroreduction of $CO_2$. We discuss the importance of accounting for active site distribution and the limits influence of macroscopic roughness on the intrinsic catalytic properties at the atomic scale.

### Tue-P-26
### Carbon Dioxide Conversion to Value-Added Chemicals Via a Heterogeneous Pd-Pt Bimetallic Catalyst

Akash Gandotra, Nicole Forte, Daniel Weber and Cheng Zhang, *Long Island University (Post), USA.*

**Short Summary:**
Unique heterogeneous Pd-Pt bimetallic catalyst with various metal loadings supported on different iron/cobalt oxides for $CO_2$ hydrogenation to light olefins were developed. Promising catalytic performance was observed for 0.3wt%Pd-0.01wt%Pt-$Fe_2O_3$.

### Tue-P-27
### Catalytic Conversion of Carbon Dioxide Via Hydrogenation to Light Olefins over a Physically Mixed $Fe_3O_4$ and $Co_3O_4$ Catalyst

Akash Gandotra[1], Daniel Weber[1], David Levy[2] and Cheng Zhang[1], *(1)Long Island University (Post), USA, (2)William A. Shine Great Neck South High School, USA.*

**Short Summary:**
A highly magnetic mixture of $Fe_3O_4$-$Co_3O_4$ was synthesized using a novel approach. The catalytic activity of a series of $Fe_3O_4$- $Co_3O_4$ at varying molar ratios was evaluated for $CO_2$ hydrogenation. The catalyst shows promising activity and selectivity to light olefins.

### Tue-P-28
### The Effect of Varying Loadings of $CeO_2$ to a Highly Magnetic Mixture of $Fe_3O_4$–$Co_3O_4$ for $CO_2$ Hydrogenation

Allison Chan, Winny Chan, Akash Gandotra and Cheng Zhang, *Long Island University (Post), USA.*

**Short Summary:**
In this current work, we investigate the effect of cerium oxide ($CeO_2$) as a support to a mixture of $Fe_3O_4$–$Co_3O_4$ for $CO_2$ hydrogenation. We discovered that $CO_2$ conversion and $CH_4$ and CO yield increased with each loading.

### Tue-P-29

### Catalytic Regeneration of Potassium Sarcosinate Solvent to Improve Energy Efficiency of Direct Air Capture of $CO_2$

Dhruba Deka, Gyoung Jang, Radu Custelcean and Costas Tsouris, *Oak Ridge National Laboratory, USA*.

**Short Summary:**
Solvent-based absorptive $CO_2$ capture is technologically well matured, but its commercialization is challenging due to the prohibitively high solvent regeneration energy. This work demonstrates that acidic catalytic materials such as Fe-ZSM-5 can be utilized to decrease regeneration energy, thereby improving the overall energy efficiency of $CO_2$ capture process.

### Tue-P-30

### Metallic Species and Amines on Anionic Exchange Resins As Dual-Site Catalysts for the $CO_2$ - Propylene Oxide Reaction to Produce Propylene Carbonate

Gustavo A. Fuentes[1], Abraham Carrillo Campos[1], Alfonso Talavera Lopez[2] and Alfredo García Frausto[2], *(1)Universidad A. Metropolitana-Iztapalapa Mexico City, Mexico, (2)Universidad Autonoma de Zacatecas, Mexico*.

**Short Summary:**
Propylene carbonate was produced in a high-pressure batch reactor at 80°C through the reaction of $CO_2$ and propylene oxide using dual-site catalysts with a tertiary amine resin (Amberlite IRA96) coupled with metal chlorides [$Cl_2MeCl_2$], Me = Ag, Cu, Sn, Zn and Fe. The maximum yield was 80%, catalyzed by A-IRA96/$FeCl_2$.

### Tue-P-31

### Sintering and Poisoning Resistance of BEA Zeolite Supported Nickel Catalysts in $CO_2$ Methanation Reaction

Wojciech Gac[1], Witold Zawadzki[1], Grzegorz Slowik[1], Marcin Kusmierz[1], Yannick Millot[2], Laetitia Valentin[3] and Stanislaw Dzwigaj[3], *(1)Maria Curie-Sklodowska University, Poland, (2)Sorbonne Université, France, (3)Sorbonne-Universite, France*.

**Short Summary:**
It has been shown that the use of a two-step modification method of BEA zeolites improve the activity, selectivity and resistance of the catalysts to deactivation, including sintering and poisoning

# Wednesday Poster Sessions

## Exhibit Hall CD

### Conversion of Oxygenated Feedstocks Poster Session 2

**Wed-P-18**

**High Purity Hydrogen Production Via Aqueous Phase Reforming of Xylose in a Continuous Reactor over Small Platinum Nano-Catalysts**

Yoondo Kim[1,2], Hyangsoo Jeong[1,3], Yongmin Kim[1,2], Young Suk Jo[1] and Hyuntae Sohn[1,3], *(1)Korea Institute of Science and Technology (KIST), Korea, Republic of (South), (2)Korea University, Korea, Republic of (South), (3)KIST School, Korea, Republic of (South).*

**Short Summary:**

A continuous production of high purity hydrogen (99.999%) was obtained using a continuous fixed-bed hybrid reactor which includes a Pt-based catalyst containing small Pt nanoparticles with an average particle size of 1.3 nm placed on a gamma-alumina support and a home-made Pt/Ta composite membrane for hydrogen purification.

### Fundamentals of Catalytic Reaction Engineering Poster Session

**Wed-P-69**

**Consequences of Shape Selectivity for Alkene Oligomerization Catalysis**

Nibras Hijazi[1] and Jorge Gascon[2], *(1)King Abdullah University of Science and Technology, Saudi Arabia, (2)King Abdullah University of Science and Technology (KAUST), Saudi Arabia.*

**Short Summary:**

This work provides insights into the intrinsic selectivity of microporous solid acids in alkene chain growth and demonstrates how mass transfer limitations can disguise interpretations of alkene oligomerization selectivity.

### New Methods in Modeling, Simulation and Machine Learning Poster Session

**Wed-P-93**

***Ab Initio* Coverage-Dependent Microkinetic Modeling for Selective Hydrogenation of Acetylene to Ethylene on Ni-Based Catalysts**

Zahra Almisbaa[1], Khalid Almajnouni[2], Hassan Aljama[3], Luigi Cavallo[4] and Philippe Sautet[1], *(1)University of California, Los Angeles, USA, (2)Aramco Research Center at KAUST, Saudi Arabia, (3)Research & Development Center, Saudi Arabia, (4)King Abdullah University of Science and Technology (KAUST), Saudi Arabia.*

**Short Summary:**

We developed a coverage-dependent microkinetic model to describe the surface chemistry of Ni-based catalysts during the hydrogenation reactions of acetylene. Accounting for the coverage effect in DFT-based modeling provides accurate predictions for the activity and the selectivity of the catalysts.

### Conversion of Methane, Methanol and Syngas Poster Session 2

**Wed-P-1**

**Aging Studies of Dual Functional Materials for Direct Air Capture with in Situ Methanation Under Simulated Ambient Conditions: Ru Thrifting for Cost Reduction**

Yuanchunyu Lin[1] and Robert J. Farrauto[2], *(1)Columbia university, USA, (2)Columbia University, USA.*

**Short Summary:**

This work has shown that the low Ru DFM monolith (0.25%Ru, 6.1%Na2O/g-Al2O3//monolith) is stable under various ambient temperature/humidity conditions for Direct Air Capture followed by Methanation (280 °C). This would open up more alternatives to apply the technology to a realistic large-scale application with a relatively low manufacturing cost.

## Electrocatalysis and Photocatalysis Poster Session

**Wed-P-41**

**Unraveling the in-Situ Structural Transformations on Single Crystalline $IrO_2$ (110) Surface during Oxygen Evolution Reaction**

Ankita Morankar, Tristan Maxson, Zhenhua Zeng and Jeffrey Greeley, *Purdue University, USA*.

**Short Summary:**

The in-situ structural evolution of IrO2 (110) surface in acidic media is probed during oxygen evolution reaction computationally using ab-initio thermodynamic phase diagrams, while explicitly incorporating coverage, and solvation effects. Theoretical predictions for phase transitions capture the right trend observed in experimentally observed peaks in cyclic voltammograms.

## Fundamentals of Catalytic Reaction Engineering Poster Session

**Wed-P-70**

**Quantifying Active Catalytic Sites in Lewis Acidic Zeolite Sn-Beta**

Leah Ford, Alexander Spanos and Nick Brunelli, *The Ohio State University, USA*.

**Short Summary:**

Site quantification poisoning experiments are used to elucidate synthesis-structure-activity relationships for Sn-Beta, specifically investigating the effect of crystallization time on the catalysis of epoxide ring-opening. It is demonstrated that the poison and solvent selected for these experiments impact the resulting catalytic site distribution, so these factors must be considered carefully.

## New Methods in Modeling, Simulation and Machine Learning Poster Session

**Wed-P-94**

**ML Forcefields from High Throughput Catalysis Simulations**

Suman Bhasker Ranganath and Johannes Voss, *SLAC National Accelerator Laboratory, USA*.

**Short Summary:**

A protocol for the generation of optimal dataset using DFT and further training of machine learning potentials is proposed, as a potential predictive tool to accelerate screening of catalysts and reactivity trends in systems with multiple chemical species.

## Conversion of Methane, Methanol and Syngas Poster Session 2

**Wed-P-2**

**Performance of Supported Copper Catalysts for Sour Water-Gas Shift Reaction**

Ludmila Silva, Marina Freitas, Fabio B. Passos, Luis Terra and Ana Coutinho, *Universidade Federal Fluminense, Brazil*.

**Short Summary:**

Syngas obtained from gasification of residues may contain sulfur, leading to poisoning of usual WGS catalysts. $Cu/Nb_2O_5$ showed higher catalytic activity being exposed to 200 ppm of $H_2S$. This suggests a formation of new sites that could be active species for water-gas shift reaction

## Electrocatalysis and Photocatalysis Poster Session

**Wed-P-42**

**Towards Improving the Catalytic Activity of Molybdenum Phosphide Electrocatalyst for the Hydrogen Evolution Reaction**

Siyabonga Nkabinde and Patricia J. Kooyman, *University of Cape Town, South Africa*.

**Short Summary:**

This work provides a facile route to synthesize carbon supported transition metal phosphides as a strategy to increase their catalytic activity towards the hydrogen evolution reaction. Our results further demonstrate that multimetallic systems are the key to developing efficient non-noble metal electrocatalysts.

## Conversion of Oxygenated Feedstocks Poster Session 2

**Wed-P-19**

**Hydrolysis of Macauba Oil Using Heterogeneous Acid Catalysts**

Victor Santos, Ivan Xavier and Ricardo R. Soares, *Federal University of Uberlandia, Brazil*.

**Short Summary:**

γ-$Al_2O_3$ and $SiO_2$-$Al_2O_3$ show full strength of acid sites moderate, while MCM-41 shows weak strength. γ-$Al_2O_3$ has a higher density of acidic sites compared to the other catalysts. It is concluded that the OMM has potential for the development of biofuels and may contribute to the reduction of environmental impacts.

## Electrocatalysis and Photocatalysis Poster Session

**Wed-P-43**

**Mitigation of Phosphoric Acid By Ionic Liquid on PtCo/C Catalyst for High Temperature Polymer Electrolyte Fuel Cell**

Dong Hee Kim, Jong Gyeong Kim, Hyeon-Seung Jung and Chanho Pak, *Gwangju Institute of Science and Technology, Korea, Republic of (South)*.

**Short Summary:**

The IL layer loaded on the PtCo/C mitigates phosphoric acid to adsorb on the surface of catalysts, as enters oxygen molecules. Therefore, It shows excellent ORR activity even in excess phosphoric acid electrolytes by mitigating the poisoning of phosphoric acid, which is significant for high-temperature polymer electrolyte membrane fuel cell.

## Conversion of Oxygenated Feedstocks Poster Session 2

**Wed-P-20**

**Effect of Support Mixed Oxides $Al_2O_3$-& and &-$ZrO_2$ over CoMoS Phase on Hydrodeoxygenation Reactions**

Itzayana Pinzón Ramos, Cindy Garcia, Carlos Omar Castillo Araiza and Jose Antonio de los Reyes, *Universidad Autónoma Metropolitana-Iztapalapa, Mexico*.

**Short Summary:**

This work presents the evaluation of $Al_2O_3$-& and &-$ZrO_2$ mixed oxide supports in HDO reactions with CoMoS-based catalysts, where high selectivity and activity for the &-$ZrO_2$ support was obtained. In addition, different operating conditions were evaluated, which were optimized with a response surface method and these were 360°C and 5.5MPa.

## Fundamentals of Catalytic Reaction Engineering Poster Session

**Wed-P-71**

**Coupling Experimental and Ab-Initio Thermochemistry of Adsorbates in a Generalized Thermochemical Hierarchy**

Bjarne Kreitz, Kento Abeywardane and Franklin Goldsmith, *Brown University, USA*.

**Short Summary:**

A novel approach to derive more accurate heats of formation of adsorbates from DFT calculations using a structural-based error cancellation technique is presented. This study also combines for the first time available experimental heats of adsorption with the DFT results in a single thermochemical network for adsorbates on Pt(111).

## New Methods in Modeling, Simulation and Machine Learning Poster Session

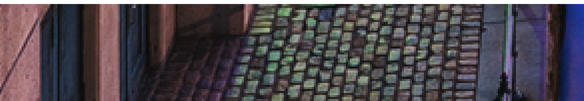
**Wed-P-95**

**Properties and Surface-Segregation of Pd/Pt Alloy Particles As a Function of Support and Gas Phase Composition**

Chen Jiachen[1], Dimitry I. Sharapa[2] and Philipp N. Plessow[2], *(1)Karlsruhe Institute of Technology, Germany, (2)Karlsruhe Institute of Technology (KIT), Germany*.

**Short Summary:**

In order to understand the shape and properties of PdPt alloy particles supported by alumina, a systematic investigation is conducted, which resulted in the discovery of a new surface termination of a-$Al_2O_3$(0001). Adsorption properties of CO were computed for comparison with experimental studies.



## Conversion of Methane, Methanol and Syngas Poster Session 2

**Wed-P-3**

### Atomic Layer Deposited Nickel Nanoparticle Catalysts for Dry Reforming of Methane

Xinhua Liang[1], Baitang Jin[2] and Shiguang Li[3], *(1)Washington University in St. Louis, USA, (2)Missouri University of Science and Technology, USA, (3)Gas Technology Institute, USA.*

**Short Summary:**

ALD prepared Ni/$Al_2O_3$ catalyst has high activity and stability due to small Ni particle size and the formation of $NiAl_2O_4$ during ALD, respectively. $CeO_2$ promotor improved the reducibility of $NiAl_2O_4$ and released Ni via formation of $CeAlO_3$, and thus increased the activity and stability of ALD prepared Ni/$Al_2O_3$ catalyst.

## Fundamentals of Catalytic Reaction Engineering Poster Session

**Wed-P-72**

### Kinetic Modeling of Anisole Hydrodeoxygenation for High Aromatic Selectivity over Ru/& Catalysts

Victor Martinez Jimenez and José Antonio De Los Reyes Heredia, *Metropolitan Autonomous University, Mexico.*

**Short Summary:**

Reaction kinetics information is crucial to determine the size of the commercial catalytic reactor and to improve the catalyst. The objective of this study is to obtain kinetic parameters that allow us to provide a quantitative framework to interpret data and to elucidate HDO reaction mechanisms for high aromatic selectivity.

## New Methods in Modeling, Simulation and Machine Learning Poster Session

**Wed-P-96**

### Modeling the Atomic Distribution of Supported Sub-Nanometer Cluster Catalysts

Salman A. Khan, Stavros Caratzoulas and Dionysios Vlachos, *University of Delaware, USA.*

**Short Summary:**

We develop actively trained machine learning potentials to model supported metal cluster catalysts. We use basin-hopping with trained machine learning potentials to discover low-energy clusters. We develop a reduced model to identify the most important features of low-energy clusters.

## Conversion of Methane, Methanol and Syngas Poster Session 2

**Wed-P-4**

### An Optimized Strategy of Simultaneous Production of Hydrogen and Carbon by Catalytic Pyrolysis in Molten Alloy Catalysts

Changgeun Oh, Hyunseok Oh, Jina Kim and Yukwon Kim, *Ajou University, Korea, Republic of (South).*

**Short Summary:**

We employed Ni-Bi and Ni-Sn mixtures of molten liquid-state alloys for a continuous production of hydrogen and carbon. In the course of optimizing the process to maximize the conversion of methane, we employed various methods of injecting methane bubbles into the molten media to control the size of bubbles.

## Electrocatalysis and Photocatalysis Poster Session

**Wed-P-44**

### Electrocatalytic Hydrogen Evolution By Bimetallic Catalysts in Presence of $Fe^{3+}$ ions As a Model Anthropogenic Contaminant

Sahanaz Parvin and Jonas Baltrusaitis, *Lehigh University, USA.*

**Short Summary:**

We have synthesized two different bimetallic catalysts, NiMo and CuCo, and investigated the effects of $Fe^{3+}$ ions in the electrolyte during HER. XRD, XAS, XPS, STEM, *in situ* Raman as well as the extensive electrochemical characterization during HER will be presented.

## Conversion of Oxygenated Feedstocks  Poster Session 2

**Wed-P-21**

**Elucidating the Influence of Alkali Metals on Phenol Tautomerization**

Isaac Onyango[1], Naseeha Cardwell[1], Yong Wang[1,2] and Jean-Sabin McEwen[1,2], *(1)Washington State University, USA, (2)Pacific Northwest National Laboratory, USA*.

**Short Summary:**

First principles-based models are used to gain fundamental insights into the influence of alkali metals and water on the HDO of phenolics in an Fe-based catalyst. These models are correlated with experiment, which show that such catalysts promote C-O bond cleavage while inhibiting the tautomerization pathway.

## New Methods in Modeling, Simulation and Machine Learning Poster Session

**Wed-P-97**

**Anharmonic Correction to the Adsorption Free Energy By Machine Learned Force Field-Based Thermodynamic Integration**

Thanh-Nam Huynh[1], Dimitry I. Sharapa[1], Tomáš Bučko[2,3] and Felix Studt[1,4], *(1)Karlsruhe Institute of Technology, Germany, (2)Slovak Academy of Sciences, Slovakia, (3)Comenius University in Bratislava, Slovakia, (4)Karlsruhe Institute of Technology (KIT), Germany*.

**Short Summary:**

This method allows for fast and accurate calculations of adsorption and desorption free energies through combination of machine learned force fields and thermodynamic integration methods. This could pave the way for detailed and precise predictions of equilibrium and rate constants for surface reactions.

## Conversion of Methane, Methanol and Syngas Poster Session 2

**Wed-P-5**

**Methane Carboxylation Using Electrochemically Activated $CO_2$**

Yucheng Yuan, Yuhan Zhang, Haoyi Li, Muchun Fei, Hongna Zhang, John Santoro and Dunwei Wang, *Boston College, USA*.

**Short Summary:**

Direct synthesis of $CH_3COOH$ from $CH_4$ and $CO_2$ is an appealing approach for the utilization of two potent greenhouse gases that are notoriously difficult to activate. We developed an integrated route to enable this reaction through electrochemical CO2RR and OER to generate CO and $O_2$, followed by $CH_4$ carbonylation.

## Electrocatalysis and Photocatalysis Poster Session

**Wed-P-45**

**Accelerating Electrocatalysts Development for Hydrogen Economy**

Tejas Bhosale, Steven Suib, Pamir Alpay and Sanjubala Sahoo, *University of Connecticut, USA*.

**Short Summary:**

In this contribution, we will present some of our combined theoretical and experimental investigations towards developing smart electrocatalysts for hydrogen production and its utilization. The goal is to understand the catalytic performances and reaction mechanisms associated with the hydrogen evolution reaction, the water-gas shift reaction and the hydrogen oxidation reaction.

## Conversion of Oxygenated Feedstocks Poster Session 2

**Wed-P-22**

**Scaled-up of an Ethanol Fuel Processor: Techno-Economic Performance for Fuel Cell Grade Hydrogen Production**

David Rodríguez-Fontalvo and Martha Cobo, *Universidad de La Sabana, Colombia*.

**Short Summary:**

Colombia's bioethanol industry has the potential to produce low emissions $H_2$ by the means of ESR, which can contribute to the Hydrogen National Roadmap. Therefore, the fuel processor based on $RhPt/CeO_2$-$SiO_2$ and $AuCu/CeO_2$ catalysts proved its worth for producing $H_2$ from bioethanol at different scales and conditions.

## Fundamentals of Catalytic Reaction Engineering Poster Session

**Wed-P-73**

**Hydrocarbon Diffusion in ZSM-5 Zeolite: Modeling the Effect of Pore Geometry, Molecule Shape & Loading**

Brian Gray, John Kuhn and Babu Joseph, *University of South Florida, USA*.

**Short Summary:**

The prediction of “configurational diffusivity” for hydrocarbons in a ZSM-5 zeolite has been examined and improved using more realistic geometric representations for diffusing molecules a flexible zeolite framework and kinetic-Monte-Carlo simulations. These result in a significant improvement in diffusivity predictions closely matching experimental studies for aromatics, alkanes and isomers.

## Conversion of Oxygenated Feedstocks Poster Session 2

**Wed-P-23**

**Production of γ-Valerolactone By Vapor-Phase Hydrogenation of Levulinic Acid over Non-Noble Metal Catalyst with Isopropanol As Hydrogen Donor**

Eliana Quiroga[1], Julia Molto[2] and Martha Cobo[1], *(1)Universidad de La Sabana, Colombia, (2)Universidad de Alicante, Spain*.

**Short Summary:**

The conversion of Levulinic acid into γ-valerolactone is a promising alternative for the development of new sustainable processes. This study aims to evaluate different conditions for this reaction over 6%Cu-14%Ni/$SiO_2$ dopped with citric acid to understand the effect of the use of H-donors.

## Fundamentals of Catalytic Reaction Engineering Poster Session

**Wed-P-74**

**Classification of Hydrocarbons Based on Surface Site Stability**

Shyama Charan Mandal[1,2], Michael L. Stone[1], Jacob Smith[3], Gennaro Liccardo[2], Melissa Cendejas[2], Bang T. Nhan[1], Abinash Kumar[4], Simon Bare[2], Stacey Bent[1], Miaofang Chi[4], Matteo Cargnello[1] and Frank Abild-Pedersen[2], *(1)Stanford University, USA, (2)SLAC National Accelerator Laboratory, USA, (3)North Carolina State University, USA, (4)Oak Ridge National Laboratory, USA*.

**Short Summary:**

Accurate and efficient prediction of binding energies of intermediates on catalytic surface is highly essential. The correlation of metal binding energies show scaling relation with the adsorbate binding energy. The binding energy of $C_1$-based and $CHCH_2$ intermediates can give the clear idea about the binding energy of higher hydrocarbon-based adsorbates.

## New Methods in Modeling, Simulation and Machine Learning Poster Session

**Wed-P-98**

**Catalytic Resonance Theory: Negative Scaling Relationships for Overcoming the Sabatier Limit**

Sallye R. Gathmann, M. Alexander Ardagh and Paul Dauenhauer, *University of Minnesota, USA*.

**Short Summary:**

Dynamic catalysis is a strategy for improving catalyst performance. Herein, we use a microkinetic model to investigate a programmable catalyst that imposes negative linear scaling behavior between the adsorption energies of a toy A-to-B reaction. Significant rate enhancement is observed, and recommendations are made for optimizing catalyst design.

## Conversion of Methane, Methanol and Syngas Poster Session 2

**Wed-P-6**

**Impact of Various Supports on the Preferential Oxidation of Carbon Monoxide over $Co_3O_4$ Nanoparticles Studied *In Situ***

Thulani Nyathi[1], Mohamed Fadlalla[1], Nico Fischer[2], Andrew York[3], Ezra Olivier[4], Emma Gibson[3], Peter Wells[5] and Michael Claeys[2], *(1)University of Cape Town, South Africa, (2)Catalysis Institute and c*change (DSI-NRF Centre of Excellence in Catalysis), University of Cape Town, South Africa, (3)Johnson Matthey Technology Centre, United Kingdom, (4)Nelson Mandela University, South Africa, (5)University of Southampton, United Kingdom*.

**Short Summary:**

For the first time, we reveal the effect of $ZrO_2$, two polymorphs of & (rutile and anatase), and $Al_2O_3$ (all as catalyst supports) on the phase transformations of $Co_3O_4$ nanoparticles, which in turn affect their activity and selectivity in the preferential oxidation of CO in $H_2$-rich gas streams.

## Electrocatalysis and Photocatalysis Poster Session

**Wed-P-46**

### Magnetic Modulation of Oxygen Evolution Electrocatalysis in Coni Electrodeposited on Fe-Modified Nickel Foam

Raj Pala, *Department Of Chemical Engineering,, India*.

**Short Summary:**

Magnetic modulation of oxygen evolution reaction in alkaline water electrolyte via Fe, Co, and Ni based anode is explored. Optimal electrocatalysts at 0.72 T is evaluated and correlations between increment in electrocatalytic activity under magnetic field and bulk magnetic properties/electrochemical impedance spectroscopy/surface electronic structure/elemental composition/nature of surface oxides/hydroxides is presented.

## Fundamentals of Catalytic Reaction Engineering Poster Session

**Wed-P-75**

### Mechanistic Insights and Design Principles for Alcohol Oxidation Reactions Mediated By Ultrasound-Derived Free Radicals.

Ari Fischer, Jaideep S. Soodan and Tej Choksi, *Nanyang Technological University, Singapore*.

**Short Summary:**

DFT-based microkinetic models establish reactivity trends for sonochemical alcohol oxidation and identify experimental conditions at which ultrasound-derived radical initiators each propagate several alcohol oxidation turnovers. Such models can aid the process intensification of ultrasound reactors to minimize energy inputs by maximizing the productivity of each radical initiator.

## New Methods in Modeling, Simulation and Machine Learning Poster Session

**Wed-P-99**

### Improved Theoretical Predictions of Small Molecule Adsorption on Silanols and Silica-Supported Isolated Titanium Sites with QM/MM

Branden Leonhardt[1], Martin Head-Gordon[2] and Alexis Bell[3], *(1)University of California Berkeley, USA, (2)Lawrence Berkeley National Laboratory, USA, (3)University of California, Berkeley, USA*.

**Short Summary:**

We demonstrate an accurate approach to calculating the $\Delta H_{ads}$ of small polar molecules to isolated Si-OH on silica and silica supported Ti sites using QM/MM. Large models are needed to capture support effects; and a strained Ti site is required (causing an enhanced $\Delta H_{ads}$) to be within error of experiment.

## Conversion of Methane, Methanol and Syngas Poster Session 2

**Wed-P-7**

### Understanding the Aromatic Cycle of the MTO Process through Mechanistic Theoretical Investigations

Philipp Plessow, *Karlsruhe Institute of Technology (KIT), Germany*.

**Short Summary:**

We discuss a revised version of the paring mechanism that avoids the formation of antiaromatic intermediates and gives significantly lower barriers. Proximate acid sites for H-SSZ-13 are shown to lower the barriers for the side-chain mechanism. Together, the computed mechanisms give realistic kinetics for the formation of ethylene and propylene.

## Electrocatalysis and Photocatalysis Poster Session

**Wed-P-47**

### Coupling $CO_2$ Capture and Electrochemical Reduction Using Azolide Ionic Liquids

Jon-Marc McGregor, Joaquin Resasco and Joan Brennecke, *The University of Texas at Austin, USA*.

**Short Summary:**

A class of ionic liquids based on azolide anions enables combined $CO_2$ capture and conversion. These ionic liquids promote CO production rates over Ag electro-catalysts by co-catalyzing $CO_2$ activation. Insights gained from this work will enable novel electrolyte designs for efficient and selective $CO_2$ conversion to desired fuels and chemicals.

## Conversion of Oxygenated Feedstocks Poster Session 2

**Wed-P-24**

### Selective Dehydration of Methyl Lactate to Acrylates Using Spatially Designed Amine Additives to FAU Zeolite Catalysts

Christopher Nicholas[1], Benjamin Hoekstra[1], Yutong Pang[2,3], ChoongSze Lee[2,3] and Paul Dauenhauer[2,3], *(1)Låkril Technologies Corporation, USA, (2)University of Minnesota, Twin Cities, USA, (3)National Science Foundation Center for Chemical Innovation, USA*.

**Short Summary:**

Selective dehydration of lactic acid to acrylic acid has been a major challenge over the last 25 years. Introduction of a nonreactive titrant to the FAU zeolite base such as pyridine, alkyl substituted pyridines, or multifunctional amines can suppress methyl lactate decarbonylation and improve dehydration selectivity to greater than 95%.

## Electrocatalysis and Photocatalysis Poster Session

**Wed-P-48**

### Alkali Metal Cation Promoters for $CO_2$ Electroreduction in Acid-Fed Membrane Electrode Assemblies

Shashwati da Cunha and Joaquin Resasco, *The University of Texas at Austin, USA*.

**Short Summary:**

State-of-the-art $CO_2$ reduction devices waste carbon and energy because of carbonate crossover and competing hydrogen evolution. Cations can steer selectivity towards $CO_2R$, and acidic pH conditions mitigate crossover. We assess $CO_2R$ performance in a zero-gap membrane electrode assembly with acidic anolyte by suspending cations on the cathode surface.

## Conversion of Oxygenated Feedstocks Poster Session 2

**Wed-P-25**

### Conversion of Oleaginous Biomass to Sustainable Aviation Fuel Via Decarboxylation/Decarbonylation over Supported Ni-Cu Catalysts

Great Umenweke, Robert Pace and Eduardo Santillan-Jimenez, *University of Kentucky, USA*.

**Short Summary:**

Inexpensive supported Ni-Cu catalysts have been found to be active and stable formulations capable of converting several oleaginous biomass feedstocks to Sustainable Aviation Fuel via decarbonylation/decarboxylation. In a continuous experiment lasting 6 days, conversion remained quantitative and most products fell within the jet fuel range irrespective of time on stream.

## Fundamentals of Catalytic Reaction Engineering Poster Session

**Wed-P-76**

### Effects of Solvation Shells on Brønsted Acidity and Their Consequences in Electrophilic Addition Catalysis

Abel Tetteh Sika-Nartey and Cathy Chin, *University of Toronto, Canada*.

**Short Summary:**

Solvents and halides can help to manipulate and tune the reaction landscapes of Brønsted acid catalyzed reactions. We report that by tuning the immediate solvation shell of phenol with polar aprotic solvents and halides, phenol deuteration turnover rates increases by at least two orders of magnitude.

## New Methods in Modeling, Simulation and Machine Learning Poster Session

**Wed-P-100**

### Discovering Trends in the Work Function of Mxenes through Machine Learning

Pranav Roy and Tej Choksi, *Nanyang Technological University, Singapore*.

**Short Summary:**

We developed a neural network model to predict MXene work functions. This model predicts work functions with a mean absolute error of 0.25 eV. Feature importance analyses indicate a strong influence of surface terminations. Reduced-order models exhibit transferability on an expanded dataset while maintaining the accuracy of the original models.

## Conversion of Methane, Methanol and Syngas Poster Session 2

**Wed-P-8**

**Effect of the Vanadia Structure on the Kinetics of Methanol Oxidative Dehydrogenation**

Gabriel Galdames, Cristian Fuenzalida, Cristobal Lillo, Paola Santander, Romel Jiménez and Alejandro Karelovic, *Universidad de Concepción, Chile*.

**Short Summary:**

Kinetic models for the methanol oxidative dehydrogenation to formaldehyde, methyl formate and dimethoxymethane were developed on vanadium supported catalysts. At higher vanadium surface coverages, the activity decreases due to an increase of the methanol adsorption enthalpy product of the multilayer formation, while favoring the methyl formate formation at lower temperatures.

## Fundamentals of Catalytic Reaction Engineering Poster Session

**Wed-P-77**

**Strain and Ligand Effects in the 1D Limit: Reactivity of Steps**

Onyinyechukwu Njoku, Kara Smeltz, Paige Fronczak and Ian McCrum, *Clarkson University, USA*.

**Short Summary:**

Our models for understanding strain and ligand effects on the reactivity of alloy catalysts, developed for model flat surfaces, must be altered at defect sites such as steps. As these defect sites are typically the “active site” for many (electro)catalytic reactions, understanding the behavior of (alloy) defect sites is important.

## New Methods in Modeling, Simulation and Machine Learning Poster Session

**Wed-P-101**

**Towards Integrating Experimental and Theoretical Data for High Quality Predictions of Material Performance Towards Electrochemical Reactions**

Shyam Deo[1,2], Melissa Kreider[1,2], Gaurav Kamat[1], Michaela Burke Stevens[1], Kirsten Winther[1], Johannes Voss[1], Frank Abild-Pedersen[1] and Thomas F. Jaramillo[1], *(1)SLAC National Accelerator Laboratory, USA, (2)Stanford University, USA*.

**Short Summary:**

We highlight a combined theory and experimental approach to the discovery and application of novel electrocatalytic materials for the oxygen reduction process (ORR) and oxygen evolution process (OER) (collectively referred as OxR) . The resulting chemically intuitive models are aimed to identify optimum catalyst structure to guide experimental synthesis.

## Conversion of Methane, Methanol and Syngas Poster Session 2

**Wed-P-9**

**Insights into the Effect of Alkali Dopants on $Li_4SiO_4$ Absorbent for Equilibrium-Enhanced Hydrogen Production**

Snehesh Shivananda Ail[1], Marco J. Castaldi[1], Charles Coe[2] and Michael Smith[2], *(1)The City College of New York, USA, (2)Villanova University, USA*.

**Short Summary:**

The SEWGS results with lithium orthosilicate absorbents, in combination with the lower onset temperature for $CO_2$ sorption, suggests potential utility of alkali-doped LOS composite samples for SESMR. The results show a significant increase in hydrogen yield above equilibrium concentrations and a reduction in operating temperature, thereby offering potential energy savings.

## Electrocatalysis and Photocatalysis Poster Session

**Wed-P-49**

**Understanding the Activity and Stability of Bimetallic Cu Catalysts for $CO_2$r**

Joel Graves and Joaquin Resasco, *The University of Texas at Austin, USA*.

**Short Summary:**

Alloying is a promising approach for improving catalytic performance in $CO_2$R. In this study, surface segregation in bimetallic copper catalysts under $CO_2$R conditions is shown to limit these improvements. Understanding the mechanism of this phenomenon over a range of alloy compositions will offer new electrocatalyst design principles for myriad chemistries.

## Conversion of Oxygenated Feedstocks Poster Session 2

**Wed-P-26**

**Potential Application of Furfural and Levulinic Acid As Combined Feed for Catalytic 2-Methyltetrahydrofuran Production**

Youngbin Kim, Reibelle Raguindin and Jeong Gil Seo, *Hanyang University, Korea, Republic of (South).*

**Short Summary:**

In this study, Furfural and Levulinic Acid, which are two of the most promising biomass-derived platform chemicals, were used as combined feed for the continuous and batch production of 2-Methyltetrahydrofuran, a fuel additive or green solvent.

## Conversion of Methane, Methanol and Syngas Poster Session 2

**Wed-P-10**

**Catalytic Methane Pyrolysis over Fe/$Al_2O_3$ for the Production of Carbon-Neutral Hydrogen**

Enrico Sartoretti[1], Piercosimo Vedele[1], Fabio Salomone[1], Chiara Novara[1], Fabrizio Giorgis[1], Massimiliano Antonini[2] and Samir Bensaid[1], *(1)Politecnico di Torino, Italy, (2)Hysytech srl, Italy*.

**Short Summary:**

Different Fe/$Al_2O_3$ materials were investigated as catalysts for methane pyrolysis for the production of carbon-free hydrogen. Solution combustion co-synthesis allows a better dispersion of small Fe crystallites in the $Al_2O_3$ framework and this is associated with a higher catalytic activity. The kinetics of the catalyzed reaction was also elucidated.

## Electrocatalysis and Photocatalysis Poster Session

**Wed-P-50**

**Electrocatalytic Reduction of Peroxydisulfate for Efficient and Selective Oxidation of Alcohols**

Mayank Tanwar[1], Seyyedamirhossein Hosseini[2], Jordyn Janusz[2], Andrew Pendergast[2], Henry White[2] and Matthew Neurock[1], *(1)University of Minnesota, Twin Cities, USA, (2)University of Utah, USA*.

**Short Summary:**

Alcohol oxidation is initiated by the redox-mediated electrocatalytic reduction of peroxydisulfate to generate the highly oxidizing sulfate radical anion, providing a selective synthetic route for the oxidation of alcohols carried out under mild conditions.

## Conversion of Oxygenated Feedstocks Poster Session 2

**Wed-P-27**

**Catalytic Depolymerization and Hydrolysis of Cellulose over ZSM-5 and Molten Salts Reaction Media**

Mateus Paiva[1], Robert Wojcieszak[1], Fábio Noronha[1] and Guillaume Vanhove[2], *(1)Université de Lille, CNRS, Centrale Lille, France, (2) Université de Lille, CNRS, France*.

**Short Summary:**

This study reports the use of ZSM-5 zeolite as heterogeneous catalyst for cellulose one-pot solubilization, depolymerization, and hydrolysis when associated with different molten salts hydrates as a reaction media. It was found that glucose and high-added value products can be obtained using milder reaction conditions.

## Fundamentals of Catalytic Reaction Engineering Poster Session

**Wed-P-78**

**Dynamics of $TiO_2$-Supported Single-Atom Catalysts (SACs) and Their Consequences in Hydrogenation Catalysis**

Linxiao Chen[1], Libor Kovarik[1], Adam Hoffman[2], Jiyun Hong[2], Sarah Allec[1], Debora Meira[3], Manh-Thuong Nguyen[1], Roger Rousseau[1,4], Simon Bare[2] and Janos Szanyi[1], *(1)Pacific Northwest National Laboratory, USA, (2)SLAC National Accelerator Laboratory, USA, (3)Argonne National Laboratory, USA, (4)Oak Ridge National Laboratory, USA*.

**Short Summary:**

This poster presents the dynamic evolution of Pd, Pt and Rh single atoms supported on anatase & under conditions related to hydrogenation catalysis, and how the dynamic behaviors affect the reaction chemistry.

## Conversion of Oxygenated Feedstocks  Poster Session 2

**Wed-P-28**
**Iron-Catalyzed Conversion of Bio-Oil into Lithium-Ion Battery Anode**
Shaikat Chandra Dey[1], Trevor Vook[1], William J. Sagues[1], Sang-Don Han[2], Mark R. Nimlos[2], Stephen S. Kelley[1] and Sunkyu Park[1], *(1)North Carolina State University, USA, (2)National Renewable Energy Laboratory, USA*.

**Short Summary:**
This study reports for the first time the synthesis of battery-grade graphite electrode from bio-oil, a renewable feedstock, via iron-catalyzed graphitization at 1500 °C in a tube furnace under nitrogen flow. The synthesis temperature is comparatively lower and the synthesis time is potentially shorter than the current graphite production technology.

## Fundamentals of Catalytic Reaction Engineering Poster Session

**Wed-P-79**
**Probing the Influence of Adsorbate-Adsorbate Interactions on H* and O* Coverage over Model Pt Nanoparticles**
Ayodeji Omoniyi and Alyssa Hensley, *Stevens Institute of Technology, USA*.

**Short Summary:**
Catalyst design for biomass upgrading is hindered by insufficient insight into the interplay between adsorbate coverage and reaction environment, with current models focusing on individual facets and low coverages. Here, we use multi-scale models to establish reaction environment-adsorbate coverage connections for representative biomass-derived species over multi-faceted Pt nanoparticles.

## Conversion of Methane, Methanol and Syngas Poster Session 2

**Wed-P-11**
**Tuning Metal-Support Interactions in Nickel-Embedded Zeolite Catalysts for Dry Reforming of Methane**
Junyan Zhang, Aditya Savara, Zili Wu and Felipe Polo-Garzon, *Oak Ridge National Laboratory, USA*.

**Short Summary:**
This work studies the dry reforming of methane (DRM) over nickel-embedded zeolites catalysts. Different nickel species were encapsulated into a series of zeolite catalysts by tuning the synthesis condition. Their distinct metal-support interactions result in distinguishable differences in catalysts' reactivity, durability, and site evolution in DRM reaction.

## Electrocatalysis and Photocatalysis Poster Session

**Wed-P-51**
**Accessing Chemically Diffuse Carbon Feedstock through Potentiodynamic Oxidation: Change Is Good**
Faviola Villariny-Rosado[1] and Omar Abdelrahman[2], *(1)University of Massachusetts Amherst, USA, (2)University of Minnesota, USA*.

**Short Summary:**
Formic acid is a promising energy storage chemical derived from biomass carbohydrates, which can exist at low concentrations in carbon feedstocks. Dynamic catalysis provides a possible solution by accessing the maximum catalytic turnover by oscillating the applied potential at surface resonance frequencies.

## Fundamentals of Catalytic Reaction Engineering Poster Session

**Wed-P-80**
**CO Oxidation over Atomically Dispersed Pt$_1$/&: Molecular Dynamics-Informed Reaction Pathways**
Selin Bac, Nicholas Humphrey and Shaama Mallikarjun Sharada, *University of Southern California, USA*.

**Short Summary:**
There has been growing evidence of the dynamic character of atomically dispersed catalysts under reaction conditions. Such character is yet to be explicitly and systematically incorporated in mechanistic studies. Our work aims to enlighten the effects of adsorption sites of single atoms and their dynamic nature on CO oxidation mechanisms/rates.

## Conversion of Methane, Methanol and Syngas Poster Session 2

**Wed-P-12**

**Study of the Promoter Effect of Manganese in a Catalyst Supported in Niobia in the Fischer-Tropsch Synthesis**

Hídila Souza Teixeira da Silva, Gabriel Garcia Silva, Ana Gabriela Martins Silva, Diogo Pimentel de Sá da Silva and Ricardo R. Soares, *Universidade Federal de Uberlândia, Brazil*.

**Short Summary:**

The results demonstrate that the presence of manganese reduces the formation of $CH_4$ and $CO_2$. In addition, the activity, selectivity towards heavy hydrocarbons ($C_{5+}$), and olefin/paraffin ratio increase. Characterization results indicate that Mn and $Nb_2O_5$ facilitate the dissociative adsorption of CO, which leads to a greater probability of chain growth.

## Electrocatalysis and Photocatalysis Poster Session

**Wed-P-52**

**NiO/ZnO Heterojunction Nanorod Catalyst for Electrochemical Methane Conversion**

Heewon Min and Jun Hyuk Moon, *Sogang University, Korea, Republic of (South).*

**Short Summary:**

We present a NiO/ZnO shell/core nanorod catalyst used to enhance electrochemical methane conversion. The built-in potential and the 1D morphology speed charge transfer. We analyze ethanol productivity as a function of nanorod length. We identify the conversion pathway to ethanol by isotopic labeling and DFT calculations.

## Conversion of Oxygenated Feedstocks  Poster Session 2

**Wed-P-29**

**Tailoring Olefin Distribution Via Tuning Lanthanide Metals in Beta-Zeolite Catalysts for Ethanol Upgrading**

Meijun Li, Stephen Purdy, Michael Cordon, Junyan Zhang, Zhenglong Li, Brian Davison and Andrew Sutton, *Oak Ridge National Laboratory, USA*.

**Short Summary:**

*We* have developed a feasible and promising way to tailor the olefin product distributions via adapting lanthanides in bimetallic catalysts, providing flexibility in constructing desirable feedstocks for renewable jet and diesel fuel production. Mechanistic investigations on the nature and confining environment of lanthanides have revealed their impact on olefin distribution.

## Electrocatalysis and Photocatalysis Poster Session

**Wed-P-53**

**Unraveling the Iron-Water Interface for Electrochemical Steel Production**

Lance Kavalsky and Venkatasubramanian Viswanathan, *Carnegie Mellon University, USA*.

**Short Summary:**

A promising green alternative to the current steelmaking process is through iron electrowinning. Here we apply DFT to probe the iron surface chemistry in water and develop a mechanistic understanding of this process. The findings will be contextualized with future experimental directions discussed.

## Conversion of Oxygenated Feedstocks  Poster Session 2

**Wed-P-30**

**Conversion of Bio-Ethanol into Olefins and Synthesis-Gas**

Tolkyn S. Baizhumanova[1], Svetlana Tungatarova[2], Gulnar N. Kaumenova[2], Galina Xanthopoulou[3], Dmitry Murzin[4] and George Vekinis[3], *(1)al-Faraby Kazakh National University, Kazakhstan, (2)D.V. Sokolsky Institute of Fuel, Catalysis and Electrochemistry, Kazakhstan, (3)Institute of Nanoscience and Nanotechnology, NCSR Demokritos, Greece, (4)Åbo Akademi University, Finland*.

**Short Summary:**

It was developed the new Ni-, Cu-, Cr-, Ce-, La/$Al_2O_3$-ZSM-5 catalysts for conversion of bioethanol into olefins and synthesis-gas. Integrated technology for the catalytic conversion of bioalcohols is a solution to the growing global energy needs and ensures the creation of environmentally friendly technologies.

## Fundamentals of Catalytic Reaction Engineering Poster Session

**Wed-P-81**

### Effects of Alkyl Chain Length on Vapor-Phase Alkene Epoxidations with $H_2O_2$ over Ti-BEA

Ohsung Kwon, Zeynep Ayla and David Flaherty, *University of Illinois Urbana-Champaign, USA*.

**Short Summary:**

Steady-state rates and activation barriers for vapor-phase alkene epoxidation with gaseous $H_2O_2$ strongly depend on alkyl chain lengths ($C_3$-$C_{10}$). Changes in rates and activation barriers reflect noncovalent interactions induced by the solvation of reactive species and the reorganization of spontaneously condensed solvents in microporous structures, even without a bulk liquid-phase.

## Conversion of Methane, Methanol and Syngas Poster Session 2

**Wed-P-13**

### DFT and TD-DFT Studies on the Mechanism of Methane Oxidative Coupling on Au-& Catalyst

Vidya Kaipanchery, Renata Tokarz-Sobieraj and Dorota Rutkowska-Zbik, *Jerzy Haber Institute of Catalysis and Surface Chemistry PAS, Poland*.

**Short Summary:**

Methane transformations into useful chemicals usually require harsh experimental conditions. Recently, the Au-& catalyst operating under mild photocatalytic conditions was proposed. In here we propose the mechanism of methane activation over this catalyst and elucidate the role of its components in the reaction.

## Fundamentals of Catalytic Reaction Engineering Poster Session

**Wed-P-82**

### Rhodium Structural Changes during CO Oxidation: The Effect on the Kinetics

Silvia Marino[1], Lai Wei[2], Marina Cortes-Reyes[3], Yisun Cheng[4], Paul Laing[4], Giovanni Cavataio[4] and William Epling[1], *(1)University of Virginia, USA, (2)Cummins Inc., USA, (3)University of Malaga, Spain, (4)Ford Motor Company, USA*.

**Short Summary:**

Rhodium structural changes during CO oxidation was observed on several catalysts characterized by different particle size. The temperature at which these structural changes occur depend on the particle size. Combining kinetic and spectroscopy data allowed us to quantify the extent of the structural changes and calculate the correct turnover frequency.

## Conversion of Methane, Methanol and Syngas Poster Session 2

**Wed-P-14**

### $H_2$-Reduced Phosphomolybdate Promotes Room-Temperature Aerobic Oxidation of Methane to Methanol

Ning Yan, *National University of Singapore, Singapore*.

**Short Summary:**

We report a Pd-containing phosphomolybdate catalyst, which, after H2 activation converts methane and $O_2$ almost exclusively to methanol at room temperature. Pd enables rapid $H_2$ activation and H spillover to phosphomolybdate for Mo reduction, while facile $O_2$/methane activation occurs on the reduced phosphomolybdate sites.

## Electrocatalysis and Photocatalysis Poster Session

**Wed-P-54**

### Electrocatalytically-Assisted Hydrocarbon Activation in Solid Oxide Electrochemical Cell-Type Reactors: Improving Olefin Selectivity

Seval Gunduz, Jaesung Kim, Matthew Ferree, Anne Co and Umit Ozkan, *The Ohio State University, USA*.

**Short Summary:**

Light olefins are key building blocks in a wide variety of industries for the production of goods that the modern world relies on. The electrocatalytically-assisted hydrocarbon activation process offers an alternative/small-scale/on-board production of light olefins from an abundant/cheap source, shale-gas, with minimum carbon-footprint when coupled with a renewable energy source.

## Conversion of Oxygenated Feedstocks  Poster Session 2

**Wed-P-31**

### Hierarchical Zeolites As Potential Catalysts for Cyclohexanone Oxidation Using Hydrogen Peroxide

Mykhailo Kurmach[1], Alyona Samotoy[1], Svitlana Sontik[1,2,3], Pavlo Yaremov[1], Oleksiy Shvets[1] and Nataliya Shcherban[1], *(1)L.V. Pisarzhevskii Institute of Physical Chemistry of the National Academy of Sciences of Ukraine, Ukraine, (2)Enamine Ltd, Ukraine, (3)Taras Shevchenko National University of Kyiv, Ukraine*.

**Short Summary:**

Obtained in this work Sn- and Zr-containing zeolites can be used in industry as efficient catalysts for Bayer-Villiger oxidation of cyclohexanone using $H_2O_2$ as a “green” oxidant, and other processes requiring Lewis acid sites.

## Conversion of Methane, Methanol and Syngas Poster Session 2

**Wed-P-15**

### Nature of the Reactive Oxygen Species in the Selective Methanol Partial Oxidation to Formaldehyde on Silver Catalysts

Emrah Ozensoy, *Bilkent University, Turkey*.

**Short Summary:**

This work highlights three critical aspects governing catalytic activity and selectivity in methanol partial oxidation to formaldehyde: electronic nature of the oxygen species, morphology of the silver catalyst surface, and stability of the intermediates and products formed. The results provide insights towards the rationally design of prospective efficient catalysts.

## Electrocatalysis and Photocatalysis Poster Session

**Wed-P-55**

### Phase-Dependent Catalytic Activity of Molybdenum Carbide Surfaces for Formic Acid Electro-Oxidation

Ankit Kumar Gautam and Alexander V. Mironenko, *University of Illinois Urbana-Champaign, USA*.

**Short Summary:**

We investigated and compared the catalytic activity of α-MoC and β-$Mo_2C$ as an inexpensive substitute of Pt for formic acid electro-oxidation. We developed surface Pourbaix diagrams for $Mo_XC_Y$ surfaces and reveal a substantial degree of surface oxidation which enables oxidation in an electrochemical environment.

## Conversion of Oxygenated Feedstocks  Poster Session 2

**Wed-P-32**

### Conversion of Aqueous Dihydroxyacetone to Lactic Acid over Metal Phosphate Catalysts in a Continuous Flow Reactor

Pawel Chmielniak[1], Carsten Sievers[1], Giada Innocenti[2], Michael Stellato[2], Qandeel Almas[2], Andrew Medford[1], Giuseppe Fornasari[2] and Fabrizio Cavani[2], *(1)Georgia Institute of Technology, USA, (2)Università di Bologna, Italy*.

**Short Summary:**

The conversion of dihydroxyacetone (DHA) to lactic acid (LA) is a good model for the up conversion of biomass to value-added chemicals. We propose a bi-molecular reaction mechanism for this reaction and support this claim with kinetics measurements.

## Fundamentals of Catalytic Reaction Engineering Poster Session

**Wed-P-83**

### Impact of Catalyst Microstructure and Soot Deposits on CO and Hydrocarbon Profiles in Catalytic Filter Measured By Spaci-MS

Miroslav Blazek[1], Petr Koci[1], Aldo Lanza[2] and Andrew York[2], *(1)University of Chemistry and Technology, Czech Republic, (2)Johnson Matthey Technology Centre, United Kingdom*.

**Short Summary:**

Filters with different microstructure and locations of Pt/γ-$Al_2O_3$ catalyst were prepared. Octane and CO oxidation was tested on fresh, soot-loaded and regenerated filters. Concentration profiles were monitored by SpaciMS. The results suggest that the pollutant slip at increased flow rates results from mass transfer limitations at the level of microstructure.

## Conversion of Oxygenated Feedstocks Poster Session 2

**Wed-P-33**

**Carboxylic Acid Decarbonylation on Nickel: The Critical Role of the Acid Binding Geometry**

Keerthan Rao, Robert Pace, Hannah Suarez, Eduardo Santillan-Jimenez and Chad Risko, *University of Kentucky, USA*.

**Short Summary:**

The decarboxylation of a model carboxylic acid over a nickel catalyst was examined by in-situ DRIFTS and DFT analysis. Both DRIFTS and DFT suggest the primary binding mode of the carboxylic acid to nickel is bidentate and that decarboxylation proceeds through dehydroxylation followed by decarbonylation of a radical intermediate.

## Fundamentals of Catalytic Reaction Engineering Poster Session

**Wed-P-84**

**Catalytic Significance of the Metal-Oxygen Coordination Sphere in Methanol Oxidative Dehydrogenation**

William Broomhead[1], Lili Zhang[1], Wei Tian[2], Jose Herrera[2] and Cathy Chin[1], *(1)University of Toronto, Canada, (2)Western University, Canada*.

**Short Summary:**

The reducibility of various metal-lattice oxygen coordination spheres of supported metal oxides, and their variation with the loading or support identity, was elucidated by kinetic interrogation in methanol oxidative dehydrogenation. Coupled thermochemical frameworks yield H-H and C-H activation scaling relations for the design of effective metal oxide catalysts.

## Conversion of Methane, Methanol and Syngas Poster Session 2

**Wed-P-16**

**Microwave-Assisted Conversion of Natural Gas into Aromatics**

Daniel Haynes, Swarom Kanitkar, Xinwei Bai, Pranjali D. Muley and Victor Abdelsayed, *National Energy Technology Laboratory, USA*.

**Short Summary:**

The results showed that the microwave-assisted methane conversion reaction could outperform the traditional thermal one, however, the stability is still poor under microwave conditions. Different catalyst-loading approaches were used in this study to increase the catalyst-microwave coupling and different characterization tools were used to understand the catalyst deactivation.

## Electrocatalysis and Photocatalysis Poster Session

**Wed-P-56**

**Computational Discovery of PGM-Free Catalysts for Selective Production of $H_2O_2$ Via Water Oxidation**

Vitaly Alexandrov, *University of Nebraska-Lincoln, USA*.

**Short Summary:**

We employ DFT calculations within the computational hydrogen electrode (CHE) approach using the VASP code to identify Pt-group metal free (PGM-free) catalysts based on doped graphene for active and selective electrochemical synthesis of $H_2O_2$ through 2-electron water oxidation.

## Fundamentals of Catalytic Reaction Engineering Poster Session

**Wed-P-85**

**Kinetic Description of Dynamic Catalysis**

Brandon Foley[1] and Neil Kanth Razdan[2], *(1)Lawrence Livermore National Laboratory, USA, (2)Massachusetts Institute of Technology, USA*.

**Short Summary:**

In this work, we develop a mathematically-based description of dynamic catalysis that (i) enables facile derivation of closed-form rate laws analogously to static systems and (ii) reduces the computational cost of calculating the dynamic-steady-state rate by $\gtrsim 10^8\times$ in reference to precedent approaches.

## Conversion of Methane, Methanol and Syngas Poster Session 2

**Wed-P-17**

### Defect Engineering Control on $La_xCe_{x-1}O_{2-x/2}$ Catalysts: Effects in Oxidative Coupling of Methane to $C_2$ Hydrocarbons

Fabiane Trindade, Bria Cisi and Andre Ferlauto, *Federal University of ABC, Brazil*.

**Short Summary:**

The tuning of structural defects and disorder of $La_xCe_{x-1}O_{2-x/2}$ catalysts was performed via $La^{3+}$ addition in molar ratios of 10-70 mol%. The oxygen species created by C-type nanodomains in $La_xCe_{x-1}O_{2-x/2}$ $x \geq 0.5$ significantly improved the $C_2$ selectivity.

## Electrocatalysis and Photocatalysis Poster Session

**Wed-P-57**

### Unraveling the Structure-Sensitive Nature of the Selective Electrocatalytic Hydrogenation of *Cis,Cis*-Muconic Acid

Deep M. Patel[1,2], Prathamesh T. Prabhu[1,2], Jean-Phillippe Tessonnier[1,2] and Luke Roling[1,2], *(1)Iowa State University, USA, (2)Center for Biorenewable Chemicals (CBiRC), USA*.

**Short Summary:**

This work provides fundamental understanding on how to maneuver the selectivity of electrocatalytic hydrogenation of *cis,cis*-muconic acid through catalyst composition, catalyst structure, and applied potential. These insights are crucial to design an efficient catalyst material for electrocatalytic production of bio-based adipic acid at an industrial scale.

## Conversion of Oxygenated Feedstocks Poster Session 2

**Wed-P-34**

### Effect of Water on C6 Carbohydrates Catalytic Conversion on Beta Zeolites

Isabel Hortal-Sánchez[1], Faysal Ibrahim[2], Edgard Lebron Rodriguez[2], Ive Hermans[2] and Nelson Cardona-Martínez[1], *(1)University of Puerto Rico at Mayagüez, USA, (2)University of Wisconsin-Madison, USA.*

**Short Summary:**

The water content in polar aprotic solvents has a strong effect over the catalytic performance for C6 carbohydrates conversion on Sn-Beta zeolites. Selection of appropriate water content in gamma-valerolactone allows the production of either alpha-hydroxy acids or difructose anhydride with high conversion and selectivity. Both products have important industrial applications.

## Electrocatalysis and Photocatalysis Poster Session

**Wed-P-58**

### Photo-Degradation of Dimethyl-Methylphosphonate on $CeO_2$ Aerogels

Travis Novak[1], Robert Balow[2], Matthew Buck[3], Debra Rolison[2] and Paul DeSario[2], *(1)US Naval Research Laboratory (NRC Postdoc), USA, (2)U.S. Naval Research Laboratory, USA, (3)United States Naval Academy, USA*.

**Short Summary:**

$CeO_2$ has high intrinsic activity against toxic organophosphorous compounds, but residual $Cl^-$ on the surface of $CeO_2$ aerogels blocks formation of terminal hydroxyls necessary for degradation. Here, we demonstrate that a simple alkaline treatment effectively removes Cl and creates $CeO_2$ aerogels highly effective for both dark and UV-enhanced dimethyl-methylphosphonate degradation.

## Conversion of Oxygenated Feedstocks Poster Session 2

**Wed-P-35**

### Performance Evaluation of Ruthenium-Based Catalysts in a Continuous Liquid-Phase HDO Reaction

Naiara C. Telis[1], Mariana Myriam Campos Fraga[2], Ricardo R. Soares[3], Klaus Raffelt[2] and Nicolaus Dahmen[2], *(1)Federal University of Uberlândia, Brazil, (2)KIT, Germany, (3)Federal University of Uberlandia, Brazil*.

**Short Summary:**

In this work, the impact of $Nb_2O_5$ as catalytic support was compared with commercial catalyst Ru/C for Hydrodeoxygenation (HDO) of syringol in a continuous reactor operating at 300 bar of hydrogen atmosphere. The reaction was taken with WHSV of 5 $h^{-1}$. $Ru/Nb_2O_5$ catalyst promotes higher syringol hydrodeoxygenation than Ru/C.

## Fundamentals of Catalytic Reaction Engineering Poster Session

**Wed-P-86**

**Enhancing Catalytic Reactivity Using Complex Forced Thermal Waveforms**

Cameron Armstrong, Fatou Diop and Andrew Teixeira, *Worcester Polytechnic Institute, USA*.

**Short Summary:**

Thermal waveforms are applied to a catalytically reactive system to observe the effect of dynamic operation on a microreactor. We find in this work dynamic operating conditions that lead to rate enhancements 5 times higher than that of the isothermal bounds.

## Conversion of Methane, Methanol and Syngas Poster Session 2

**Wed-P-102**

**Dry and Oxy-$CO_2$ Reforming over Ni Substituted Lanthanum Zirconate Pyrochlore– Activity and Stability**

Srikar Bhattar[1], Daniel Haynes[2], Dushyant Shekhawat[2] and James J. Spivey[1], *(1)Louisiana State University, USA, (2)National Energy Technology Laboratory, USA*.

**Short Summary:**

Dry reforming and Oxy-$CO_2$ reforming of methane with varying reactant concentrations is investigated using LNZ3 catalyst to optimize the activity, stability. Syngas produced from these reactions can be further converted to desired products depending on the $H_2$/CO ratio. There seems to be almost negligible coke formation for Oxy-$CO_2$ reforming reaction.

## Fundamentals of Catalytic Reaction Engineering Poster Session

**Wed-P-87**

**Effects of Acid Site Proximity in CHA Zeolites on Kinetics of Protolytic Propane Cracking and Dehydrogenation**

Bereket Bekele and Raj Gounder, *Purdue University, USA*.

**Short Summary:**

First-order protolytic propane cracking and dehydrogenation rate constants (per $H^+$) in chabazite zeolites are higher at six-membered ring (6-MR) paired $H^+$ sites than isolated sites, reflecting more entropically-stable transition states as a consequence of multi-ion-pair interactions between the carbocationic transition state, the anionic lattice charge, and the spectating $H^+$ site.

## Electrocatalysis and Photocatalysis Poster Session

**Wed-P-59**

**Data Driven Design of $Cu_xFe_yRu_{(1-x-y)}$ Catalysts for Light-Driven Production of Hydrogen**

Maya Bhat and John R. Kitchin, *Carnegie Mellon University, USA*.

**Short Summary:**

Light driven hydrogen production is promising for clean H2 production from water. This study uses a photodriven high-throughput system to form colloidal metal catalytsts *in-situ* for efficient H2 production. By leveraging parallel computational and high throughput screening approaches, we successfully pinpointed H2 active multi-metallic combinations of Cu, Ru, and Fe.

## Conversion of Oxygenated Feedstocks Poster Session 2

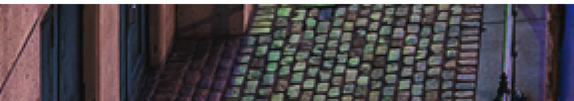
**Wed-P-36**

**Ethanol to Distillate-Range Oxygenates**

Michael Lanci, *ExxonMobil Technology and Engineering Company, USA*.

**Short Summary:**

This presentation will discuss ethanol oligomerization over a series of calcined MgAl mixed metal oxide catalysts with low amounts of Cu.



## Electrocatalysis and Photocatalysis Poster Session

### Wed-P-60

### Photocatalytic Degradation of Orange II Dye Via High Pore Volume Polymorph Zirconium-Doped Titania Under Visible Light Irradiation

Samson Owalude[1], Isaac Olowookere[2], Inosh Perera[2], Harshul Khanna[2], Elsa Njeri[2], Xueni Huang[2], Andrew Meguerdichian[2], Hamad-Tijani Ayilara[1] and Steven Suib[2], *(1)University of Ilorin, Nigeria, (2)University of Connecticut, USA*.

**Short Summary:**

This study reports a facile method of preparing rutile-anatase mixed-phase & at relatively low temperature. The Zr-doped & effectively degrades orange II dye solution up to 7 cycles through asymmetric cleavage of the azo bond as against symmetric cleavage reported by previous literatures.

## Conversion of Oxygenated Feedstocks  Poster Session 2

### Wed-P-37

### Polystyrene-Based Catalysts with Brønsted and Lewis Acidity for the One-Pot Synthesis of Hydroxymethylfurfural from Potato Starch

Ibeh S. Omodolor[1], Nkem O. Ofole[1], Sarah A. Walz[1], Maria R. Coleman[1], Ravikumar Gogar[1], Sridhar Viamajala[1], Francielle C. F. Marcos[2] and Ana C. Alba-Rubio[1,2], *(1)University of Toledo, USA, (2)Clemson University, USA*.

**Short Summary:**

Soluble and reusable polystyrene-based catalysts with Brønsted and Lewis acid sites can be effectively used for the one-pot valorization of mono- (e.g., fructose and glucose) and polysaccharides (e.g., starch) into HMF.

## Fundamentals of Catalytic Reaction Engineering Poster Session

### Wed-P-88

### Highly Dilute Transition Metal Atoms Dispersed in Supported Liquid Metal Droplets for Hydrocarbon Conversions

Kathryn MacIntosh and Rob Rioux, *Pennsylvania State University, USA*.

**Short Summary:**

Supported catalysts based on liquid droplets containing a low concentration of catalytically-active metals are a unique class of materials believed to consist of single metal atom active sites. The ability of Ga to absorb hydrogen at high temperatures suggests unique opportunities in hydrocarbon dehydrogenation reactions.

### Wed-P-89

### Reaction Network and Kinetic Modeling of By-Product Formation in Ethylene Oxychlorination for $CuCl_2/\gamma\text{-}Al_2O_3$-Based Catalysts

De Chen[1] and Dennis Neu[2], *(1)Norwegian University of Science and Technology, Norway, (2)SINTEF AS, Norway*.

**Short Summary:**

This work represents a conversion related kinetic model for by-products of ethylene oxychlorination with a detailed reaction network considering the dynamically changed active sites of a K-doped $CuCl_2/\gamma\text{-}Al_2O_3$ catalyst. The model parameters are estimated by multi-response nonlinear regression based on Mars-van Krevelen and Langmuir-Hinshelwood mechanisms.

## Electrocatalysis and Photocatalysis Poster Session

### Wed-P-61

### Enhancing Catalytic and Photocatalytic Activities of Semiconductors with Low-Atomicity Clusters

David Buceta[1], Iria Arias[1] and Manuel Arturo López Quintela[2], *(1)Nanogap, Spain, (2)University of Santiago de Compostela, Spain*.

**Short Summary:**

Depositing low-atomicity clusters on semiconductors results in large changes in electronic structure with the creation of mid gaps and surface polarons enhancing both catalytic and photocatalytic activity. Examples will be presented including CO2 hydrogenation to methane, visible-light photocatalytic hydrogen production and visible-light photocatalytic degradation of aromatics.

## Conversion of Oxygenated Feedstocks  Poster Session 2

**Wed-P-38**

### Co-Mg-Al Hydrotalcites-like Structures As Catalysts Precursors for the Hydrodeoxygenation of Stearic Acid

Ariel Aguirre-Escalante, Aida Gutiérrez-Alejandre and Rogelio Cuevas-García, *National Autonomous University of Mexico, Mexico*.

**Short Summary:**

$Co_2MgAl$ layered double hydroxides were synthesized with high metallic loading, then were calcined, and reduced at different temperatures. The catalysts were tested in the HDO of stearic acid showing good catalytic performance and high dispersion.

## Fundamentals of Catalytic Reaction Engineering Poster Session

**Wed-P-90**

### Kinetic Study and Structural Formation of a Bimetallic Cufe Catalyst

Barbara Jazmin Lino Galarza[1], Javier Rivera De la Rosa[1], Carlos Lucio Ortiz[1], Diana Bustos Martinez[1], Carlos Enrique Escarcega Gonzalez[1], Jose Andres Martinez Hernandez[1], Eduardo Maximino Sanchez Cervantes[1], Gloria Dimas Rivera[1] and Ladislao Sandoval-Rangel[2], *(1)Universidad Autónoma de Nuevo León, Mexico, (2)Tecnológico de Monterrey, Mexico*.

**Short Summary:**

The present work presents the kinetic model fitting of CuFe bimetallic catalyst, which gave a multi-reaction system that was determined by XRD, also TPR was used to analyze the reductions present and finally using TG data and Matlab(R) was fitted to solve the proposed system.

## Electrocatalysis and Photocatalysis Poster Session

**Wed-P-62**

### Surface Investigation of $MoS_x/CuInS_2$ Photocathode By in Operando Characterization for Photoelectrochemical Hydrogen Evolution

Sang Youn Chae[1], Noyoung Yoon[2], Oh Shim Joo[2] and Eun Duck Park[1], *(1)Ajou University, Korea, Republic of (South), (2)Korea Institute of Science and Technology, Korea, Republic of (South)*.

**Short Summary:**

in operando characterization is a powerful tool to reveal the surface of reaction-undergoing semiconductor photoelectrode. In this study, the $MoS_x/CuInS_2$ photocathode was prepared for photoelectrochemical hydrogen evolution. We successfully observed intermediate steps of the transformation of the $MoS_x$ layer during the reaction by in operando Raman spectroscopy under operating conditions.

## Conversion of Oxygenated Feedstocks  Poster Session 2

**Wed-P-39**

### Complete Utilization of Waste Lignin: Conversion of Lignin-Derived Guaiacol to Nylon Precursors Using Lignin-Derived Carbon Supports

Kwangjin An, *Ulsan National Institute of Science and Technology (UNIST), Korea, Republic of (South)*.

**Short Summary:**

The valorization of waste lignin for the production of high value-added chemicals is energetically and environmentally important. In this study, a new catalytic process was developed to produce raw materials for nylon production utilizing 100% of the waste lignin emitted from industrial processes.

## Electrocatalysis and Photocatalysis Poster Session

**Wed-P-63**

**Efficient and Selective Photocatalytic Conversion of Methanol Using Porous Au-$WO_3$ and Visible Light**

Robert Tracy and Christopher Landry, *University of Vermont, USA*.

**Short Summary:**

Photocatalytic conversion of $C_1$ molecules into fuels and other valuable chemicals is an important industrial research focus**.** The system described here shows the conversion of MeOH into multiple products with intermediate oxidation levels, using porous Au-$WO_3$ under mild conditions.

## Conversion of Oxygenated Feedstocks Poster Session 2

**Wed-P-40**

**Catalytic Dehydration of Glycerol over Ordered Mesoporous γ-Alumina**

Rajesh Kumar Parsapur[1], Krishnan Suthagar[1] and Parasuraman Selvam[1,2], *(1)Indian Institute of Technology-Madras, India, (2)Kumamoto University, Japan*.

**Short Summary:**

The synthesis of two distinct 3D-cubic-ordered mesoporous phases of γ-alumina by self-assembly of F108 polymer is reported. In addition, we also synthesized hierarchical nanoporous γ-alumina. All these materials have shown excellent catalytic activity in the glycerol dehydration to acrolein.

## Fundamentals of Catalytic Reaction Engineering Poster Session

**Wed-P-91**

**Selective Alkene Epoxidation on Ag-Cu Near Surface Alloys**

Yogita Soni, Qianli Xing, Laura Cramer, E. Charles H. Sykes and Prashant Deshlahra, *Tufts University, USA*.

**Short Summary:**

Ag-Cu near surface alloy (NSA) nanoparticles with Ag shell – Cu core structures are prepared via galvanic replacement. Epoxidation rates and selectivity on these structures, together with DFT calculations and surface science measurements in single-crystal NSAs are used to understand relations between dynamic structure and reactivity of NSAs.

**Wed-P-92**

**Design of Pd 2D Thin Film Catalysts with Si, $SiO_2$, ZnO, $SiN_x$, C Suports for Selective Acetylene Hydrogenation**

Zehua Li[1], Eylül Öztuna[1,2], Christian Rohner[1], Alexander Steigert[2], Martin Muske[2], Manuela Arztmann[2], Sabine Wrabetz[1], Jutta Kröhnert[1], Maria Dimitrakopoulou[1], Matus Stredansky[1], Lukas Thum[1], Wiebke Frandsen[1], Adnan Hammud[1], Frank Girgsdies[1], Daniel Delgado Munoz[1], Johannes Frisch[2], Tathiana M. Kokumai[2], Marcus Bär[2], Simone Raoux[2,3], Thomas Schmidt[1], Mauricio Prieto[1], Arno Bergmann[1], Helmut Kuhlenbeck[1], Olga Vinogradova[1], Vanessa J. Bukas[1], Thomas Lunkenbein[1], Annette Trunschke[1], Axel Knop-Gericke[1], Rutger Schlatmann[2], Karsten Reuter[1], Beatriz Roldán Cuenya[1], Robert Schlögl[1], Daniel Amkreutz[2] and Katarzyna Skorupska[1], *(1)Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany, (2)Helmholtz-Zentrum Berlin für Materialien und Energie, Germany, (3)Humboldt-Universität zu Berlin, Germany*.

**Short Summary:**

This work proves the applicability of novel 2D systems in catalysis and provides a new direction for future catalyst development and optimization with functional interface.

## Electrocatalysis and Photocatalysis Poster Session

### Wed-P-64

### Shifting the Band Gap from UV to Visible Region in Au/$CeO_2$ Nanocomposites.

Miriam Sánchez-Ordaz, Elizabeth Rojas-García, John H. Sierra-Uribe, Mara Cordero-Garcia and Sergio Gomez Torres, *Universidad Autónoma Metropolitana-Iztapalapa, Mexico*.

**Short Summary:**

The addition of gold improves the photocatalytic activity of $CeO_2$ because it decreases the recombination of the electron-hole pair and increases the capacity of the material to absorb radiation in the visible spectrum. Measurements were made in order to clarify this property for photocatalytic applications of the synthesized samples.

### Wed-P-65

### Co-Designing Photocatalytic Charge Separation and Multi-Potential Catalysis for Activation of Water and Biomass

Shu Hu, Rito Yanagi, Bin Liu and Atsu Kludze, *Yale University, USA*.

**Short Summary:**

Semiconductor photocatalysts coevolve reductive and oxidative reactions at nanoscale. We show the rational design of photocatalysts by fundamental studies of multiple concurring catalytic or redox processes and show scalable $H_2$ production with activating water and biomass. The study paves the way for utilizing biomass with carbon capture and storage.

### Wed-P-66

### Size-Dependent Electrochemical Nitrogen Reduction Catalyzed By Monodisperse Au Nanoparticles

Junrui Li[1] and Junsheng Li[2], *(1)Washington State University, USA, (2)Wuhan University of Technology, China*.

**Short Summary:**

We report size-dependent electrochemical $N_2$ reduction activities of Au nanoparticles. 8 nm Au was found to be the best among all sizes with an $NH_3$ production rate and Faradic efficiency of 17.49 $\mu$gh/mg$_{Au}$ and 5.8 %. DFT studies indicated that an optimal proportion of the surface step sites is important.

### Wed-P-67

### Differentiating between Metallic and Oxidized Tin for Electrochemical $CO_2$ Reduction Using Grand-Canonical DFT, *in-Situ* Infrared Spectroscopy and Kinetic Modeling

Todd Whittaker[1,2], Yuval Fishler[1,2], Paige Brimley[1,2], Adam Holewinski[1,2], Charles Musgrave[1,2], Wilson Smith[1,2,3] and Derek Vigil-Fowler[3], *(1)Renewable and Sustainable Energy Insitute, USA, (2)University of Colorado Boulder, USA, (3)National Renewable Energy Laboratory, USA*.

**Short Summary:**

A computational and experimental approach was used to study $CO_2$ reduction on Sn catalysts. Grand-canonical DFT and *in-situ* ATR-SEIRAS on tin and tin oxide revealed a preference for $CO_2$ to bind oxygen atoms down, explaining the formate selectivity. Microkinetic modeling also reveals the differences between tin and tin oxide.

### Wed-P-68

### Structure-Property-Performance Relationships of Cuprous Oxide Nanostructures for Dielectric Mie Resonance-Enhanced Photocatalysis

Ravi Teja Addanki Tirumala, Sundaram Bhardwaj Ramakrishnan and Marimuthu Andiappan, *Oklahoma State University, USA*.

**Short Summary:**

A novel approach in photocatalysis, that $Cu_2O$ nanoparticles(NPs) exhibiting dielectric Mie-resonances can exhibit up to an order of magnitude higher photocatalytic rate as compared with $Cu_2O$ nanostructures not exhibiting Mie-resonances. FDTD-simulations and experimental results predict a volcano-type relationship between the photocatalytic rate and the size of $Cu_2O$ nanospheres and nanocubes.

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