



**27th North American  
Catalysis Society Meeting  
May 22-27, 2022**





Greetings!

As Co-Chairmen, we look forward to welcoming you at the 27th biennial North American Meeting of the North American Catalysis Society, to be held at the Hilton Midtown, Manhattan, NY, USA on May 22-27, 2022. 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 27th North American Meeting is available on the North American Catalysis Society Meeting's website: <http://www.nam27.org/>.

Sincerely,

Handwritten signature of Marco Castaldi in black ink.

Marco Castaldi  
Co-Chair

Handwritten signature of Lucas Dorazio in black ink.

Lucas Dorazio  
Co-Chair

Handwritten signature of Israel E. Wachs in black ink.

Israel E. Wachs  
Co-Chair



# NAM27 Co-Chairs



**Marco J. Castaldi**

*Professor of Chemical Engineering  
Director, Earth System Science & Environmental Engineering  
Director, Combustion and Catalysis Laboratory  
The City College of New York (CUNY)*

Marco J Castaldi is a professor of chemical engineering at The City College of New York. He is the director of the Earth Engineering Center at City College and the Head of the U.S. Waste-to-energy research technology (WTERT) council. His research areas are combustion and catalysis with a focus on thermal conversion of solid feedstocks, such as MSW, and developing and understanding catalytic processes focused on hydrocarbon chemistry. He has received the Fulbright Global Scholar Award and is a technical Fellow of the American Institute of Chemical Engineers (AIChE) and the American Society of Mechanical Engineers (ASME). He is the past chair of the Catalysis Society of Metropolitan New York and currently serves as the NACS Representative.



**Lucas Dorazio**

*BASF Corporation, Refinery Catalyst Research & Development  
Adjunct Professor, New Jersey Institute of Technology*

Lucas Dorazio has been a practicing chemical engineer in industry for over 20 years working in a variety different engineering and research positions. He received his doctorate from Columbia University in New York City where his research was in the field of heterogeneous catalysis. He started working for BASF in year 2000, where most of that time has been spent at BASF's catalyst research center in Iselin NJ. Currently, he leads a team developing fluid catalytic cracking catalysts to support the refining industry. In addition to his work in industrial research, he is also an adjunct professor at NJIT where he teaches two courses in the field of catalysis. He has authored several journal articles and been granted several patents in the field of catalysis, and recently co-authored a textbook on the topic of industrial catalysis. He is an active member of the local catalysis community where he serves as a Director for the New York Metropolitan Catalysis Society.



**Israel E. Wachs**

*G. Whitney Snyder Professor, Chemical and Biomolecular Engineering Director, Operando Molecular Spectroscopy and Catalysis Research Lab*

In a career spanning three decades, Wachs has earned international renown for research into heterogeneous catalysis. His research focuses on the catalysis science of mixed metal oxides for numerous catalytic applications. The U.S. Environmental Protection Agency has honored Wachs with a Clean Air Excellence award for a catalytic process he invented that converts paper-mill pollutants into formaldehyde. The American Chemical Society (ACS) has given Wachs the George A. Olah Award for achievements in hydrocarbon and petroleum chemistry and the American Institute of Chemical Engineering (AIChE) has honored Wachs with the Catalysis and Reaction Engineering Division Practice Award . He is the recipient of multiple awards from local catalysis societies (Michigan, New York, Chicago and Philadelphia). In 2011, he was named a Fellow of the American Chemical Society (ACS), the highest honor bestowed by the society. In 2012, he was recognized by the German Alexander von Humboldt Foundation with a Humboldt Research Award and the International Vanadium Chemistry Organization with its Vanadis award.

# In Memory of John W. Byrne



John earned a BS in Chemistry from Penn State University, graduating Phi Beta Kappa and was a proud alum. His graduate work was at Harvard University where he earned his Ph.D. under the guidance of Prof. John A. Osborn. John then began his career in 1976 as a Research Scientist at the Engelhard Corporation laboratory in Iselin N.J. where he initially worked on novel catalysts for the cracking of gasoil into gasoline. There he invented the first catalyst to cut sulfur oxide emissions from a commercial catalytic cracking unit by over 80%. Later, he invented the first commercially viable pollution control catalyst for the reduction of nitrogen oxide emissions. He concluded his career in 2015 at BASF Corp. as a Senior Research Associate leading all R&D to develop novel biocides based on a proprietary BASF chemistry. During his career he has been an inventor on 10 US Patents.

John also cherished his professional associations outside of the laboratory. He served as Treasurer of the Catalysis Society of Metropolitan New York and more recently as a director for over 40 years. He was active in many other roles in the Catalysis Society, most recently serving on the committee organizing the 27th North American Catalysis Society Meeting in New York City. Despite his illness, he organized the local events for and was able to attend NAM27. He enjoyed every minute of his time with the more than 1400 researchers gathered from around the world.

John was a kind and good man, often described by friends and colleagues as one of the nicest and most positive people they knew. He made the world a better place. He will be dearly missed.

# NAM27 Organizing Committee

Secretary	Michele Sarazen	Princeton University
Treasurer	John Brody	ExxonMobil
Scientific Program	Fuat Celik	Rutgers, The State University of New Jersey
Scientific Program	Wolfgang Ruettinger	BASF
Poster Program	Taejin Kim	Stony Brook University
Poster Program	Xianqin Wang	NJ Institute of Technology
Poster Program	Lindsey Welch	Cedar Crest College
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Website Chair	McKenzie Kohn	Johnson Matthey
Kokes Awards	Elizabeth Biddinger	City College of New York
Kokes Awards	George Tsilomelekis	Rutgers, The State University of New Jersey
Exhibits	Al Metauro	Novita Technology

# NAM27 Acknowledgements

## ACKNOWLEDGEMENTS

The 27th NAM Organizing Committee would like to thank the following:

- The **North American Catalysis Society** for their support of NAM27.
- The **National Science Foundation, US Department of Energy and the North American Catalysis Society** for their support of the Richard J. Kokes Student Travel Awards program.
- The NAM26 organizing committee for their support, help and guidance.
- Jingguang Chen of NACS for his counsel and assistance with finances.
- The many reviewers who helped us with the record number of submissions for NAM27.
- 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 record number of abstracts and presentations.
- The fantastic staff of the Hilton New York.

## SPONSORS OF MAJOR NACS 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
- **Johnson Matthey** for sponsoring The Robert Burwell Lectureship in Catalysis Award, administered by The North American Catalysis Society
- **W.R. Grace and Company** and the **North American Catalysis Society** as the sponsors for the F.G. Ciapetta Lectureship in Catalysis Award
- **W.R. Grace and Company** for sponsoring the Paul H. Emmett Award in Fundamental Catalysis
- **Clariant** for sponsoring the Eugene J. Houdry Award in Applied Catalysis
- **ExxonMobil Research and Engineering** and **Clariant** for sponsoring the NACS Award for Distinguished Service in the Advancement of Catalysis

# THANK YOU TO OUR SPONSORS



## PLATINUM



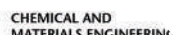
## GOLD



## SILVER



## BRONZE



# 27th 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!***

	<b>First Name</b>	<b>Last Name</b>	<b>Institution</b>	<b>Country</b>
1	Ravi Teja	Addanki Tirumala	Oklahoma State University	USA
2	Naveen	Agrawal	The Pennsylvania State University	USA
3	Divakar Reddy	Aireddy	Louisiana State University	USA
4	Rawan	Almallahi	University of Michigan-Ann Arbor	USA
5	Faisal	Alshafei	California Institute of Technology	USA
6	Safa	Alzaim	New Jersey Institute of Technology	USA
7	Allison	Arinaga	Northwestern University	USA
8	Cameron	Armstrong	Worcester Polytechnic Institute	USA
9	A.K.M. Kazi	Aurnob	Louisiana State University	USA
10	Scott	Bamonte	University of Connecticut	USA
11	Hamed	Bateni	Iowa State University	USA
12	Maya	Bhat	Carnegie Mellon University	USA
13	Akash	Biswas	Columbia University	USA
14	Katrín	Blöndal	Brown University	USA
15	Muntaseer	Bunian	The University of Alabama in Huntsville	USA
16	Jian	Chang	University of Pennsylvania	USA
17	Pak Wing	Chen	University of Houston	USA
18	Ewa	Chukwu	Clemson University	USA
19	Mara	Cordero-Garcia	Universidad Autónoma Metropolitana-Iztapalapa	Mexico
20	James	Crawford	Colorado School of Mines	USA
21	Kaixi	Deng	Stony Brook University	USA
22	Griffin	Drake	Massachusetts Institute of Technology	USA
23	Haider	Ejaz	Rutgers, The State University of New Jersey	USA
24	Jacques	Esterhuizen	University of Michigan-Ann Arbor	USA
25	Sopuruchukwu	Ezenwa	Purdue University	USA
26	Lotanna	Ezeonu	Stevens Institute of Technology	USA
27	Noah	Felvey	University of California, Davis	USA
28	Jordan	Finzel	University of California, Santa Barbara	USA
29	José Gabriel	Flores Aguilar	Universidad Autonoma Metropolitana-Azcapotzalco	Mexico
30	Sallye R.	Gathmann	University of Minnesota, Twin Cities	USA
31	Timothy	Goetjen	Northwestern University	USA
32	Anshuman	Goswami	University of Notre Dame	USA



33	Benjamin	Greydanus	University of Colorado Boulder	USA
34	Jacklyn N.	Hall	University of Houston	Mexico
35	Bryan	Hare	Georgia Institute of Technology	USA
36	Carlos	Hernández-Fontes	Universidad Nacional Autónoma de México (UNAM)	USA
37	Alexander	Hoffman	University of Florida	USA
38	Isabel	Hortal-Sánchez	University of Puerto Rico - Mayagüez	USA
39	Wenda	Hu	Washington State University	USA
40	Erwei	Huang	Stony Brook University	USA
41	Anagha	Hunoor	The Ohio State University	USA
42	Jared	Jorolemon	St. John Fisher College	USA
43	Mitchell	Juneau	University of Rochester	USA
44	Lance	Kavalsky	Carnegie Mellon University	USA
45	Doyoung	Kim	University of Delaware	USA
46	Kareesa	Kron	University of Southern California	USA
47	Kaitlyn	Lawrence	City College of New York, CUNY	USA
48	Kyung-Min	Lee	Stony Brook University	USA
49	Seungyeon (Lina)	Lee	University of Delaware	USA
50	Juliana	Levi	Arizona State University	USA
51	Jialu	Li	The University of Akron	USA
52	Junchen	Liu	New York University	USA
53	Song	Luo	University of Massachusetts Amherst	USA
54	Keka	Mandal	University of Virginia	USA
55	Silvia	Marino	University of Virginia	USA
56	Andrew S.	May	City College of New York, CUNY	USA
57	Lizbeth	Moreno Bravo	McGill University	Canada
58	Jessica A.	Muhlenkamp	University of Notre Dame	USA
59	Musa	Najimu	University of California, Irvine	USA
60	Thu	Nguyen	Rutgers, The State University of New Jersey	USA
61	Tu	Nguyen	University of California, Riverside	USA
62	Michelle	Nolen	Colorado School of Mines	USA
63	Alaba	Ojo	University of South Carolina	USA
64	Sean	Overa	University of Delaware	USA
65	Juili	Parab	University of Massachusetts Amherst	USA
66	Deependra	Parmar	University of Houston	USA
67	Laura	Paz Herrera	University of Colorado Boulder	USA
68	Ian	Peczak	Northwestern University	USA
69	Daniel E.	Pérez	Universidad Nacional Autónoma de México (UNAM)	Mexico
70	Tram	Pham	University of Oklahoma	USA
71	Hemanth Somarajan	Pillai	Virginia Polytechnic Institute and State University	USA
72	Zahra	Rajabi	University of Texas at San Antonio	USA
73	Michael	Rebarchik	University of Wisconsin-Madison	USA
74	Tomas	Ricciardulli	University of Illinois Urbana-Champaign	USA
75	Reyna	Rios	Universidad Autónoma Metropolitana-Iztapalapa	Mexico
76	Cameron	Roman	Louisiana State University	USA
77	Christopher	Rzepa	Lehigh University	USA
78	Samji	Samira	Wayne State University	USA

79	Hafeera	Shabbir	Clemson University	USA
80	Hao	Shen	Johns Hopkins University	USA
81	Michael	Smith	Princeton University	USA
82	Surya Pratap	Solanki	University of Houston	USA
83	Taylor	Spivey	University of Colorado Boulder	USA
84	Berlin	Sudduth	Washington State University	USA
85	Vaidish	Sumaria	University of California, Los Angeles	USA
86	Jiakai	Sun	University of California, Santa Barbara	USA
87	Scott	Svadlenak	Oregon State University	USA
88	Mackenzie R.	Todd	University of Maine	USA
89	Jessica	Torres	University of California, Los Angeles	Mexico
90	Adam	Twombly	Tufts University	USA
91	Anoop	Uchagawkar	The University of Kansas	USA
92	Brandon	Vance	University of Delaware	USA
93	Vyshnavi	Vennelakanti	Massachusetts Institute of Technology	USA
94	Manasi	Vyas	Colorado School of Mines	USA
95	Mingyu	Wan	University of Massachusetts Lowell	USA
96	Bo	Wang	Rice University	USA
97	Bernard	Whajah	Louisiana State University	USA
98	Colby A.	Whitcomb	University of Virginia	USA
99	Andrew	Wolek	Northwestern University	USA
100	Yinan	Xu	Purdue University	USA
101	Vamakshi	Yadav	Purdue University	USA
102	Zihao	Yan	Virginia Polytechnic Institute and State University	USA
103	Rito	Yanagi	Yale University	USA
104	Rachel	Yang	Princeton University	USA
105	Benjamin	Yeh	University of Minnesota, Twin Cities	USA
106	Adam	Yonge	Georgia Institute of Technology	USA
107	Md Raian	Yousuf	Virginia Polytechnic Institute and State University	USA
108	Citlalli	Zenteno	Instituto Mexicano del Petróleo	Mexico
109	Yuan	Zhang	University of Maryland - College Park	USA
110	Rui	Zhang	Washington State University	USA
111	Chengshuang	Zhou	Stanford University	USA

**The 27th NAM Organizing Committee would like to thank The National Science Foundation, US Department of Energy, and the North American Catalysis Society for their support of the RichardJ. Kokes Student Travel Awards program**



# NAM 27 Program Details

- 4 plenary events
- 13 technical areas across 8 parallel sessions
- 112 technical sessions
- 654 oral presentations, of which 22 keynotes
- Over 373 posters presented
- 175 individuals serving as session chairs
- 566 reviewers reviewing abstracts

NAM27 Topical Areas	Technical Program Committee	
Technical Program CoChair	Fuat Celik	Rutgers University
Technical Program CoChair	Wolfgang Ruettinger	BASF
Conversion of Biomass Resources and Polymers	Alan Allgeier	Kansas University
Conversion of Biomass Resources and Polymers	George Huber	University of Wisconsin-Madison
Conversion of Fossil Resources	Eric Stangland	Dow
Conversion of Fossil Resources	Brian Weiss	Merck
Catalysis for C1 and SynGas Chemistry	Friederike Jentoft	University of Massachusetts-Amherst
Catalysis for C1 and SynGas Chemistry	Madelyn Stalzer	ExxonMobil
Catalysis for Environmental Applications	Yuejin Li	BASF
Catalysis for Environmental Applications	Fudong Liu	University of Central Florida
Catalysis for Chemical Synthesis and Functionalization	Anne Gaffney	Idaho National Lab
Electrocatalysis and Photocatalysis	Charles Dismukes	Rutgers University
Electrocatalysis and Photocatalysis	Jennifer Strunk	Leibniz Institute for Catalysis
Homogeneous and Molecular Catalysis	David Kaphan	Argonne National Lab
Homogeneous and Molecular Catalysis	Matthew Winston	Merck
Fundamentals of Catalysis	Jingyue Liu	Arizona State University
Fundamentals of Catalysis	Michele Sarazen	Princeton University
Modelling, Simulation, and Machine Learning in Catalysis	A.J. Medford	Georgia Tech
Modelling, Simulation, and Machine Learning in Catalysis	Srinivas Rangarajan	Lehigh University
Reaction Engineering	Eric Sacia	AbbVie
Reaction Engineering	Sourav Sengupta	DuPont
Catalyst Characterization	Robert Rioux	Pennsylvania State University
Catalyst Characterization	Sanjaya Senanayake	Brookhaven National Lab
Catalyst Design and Synthesis	Travis Conant	Sabic
Catalyst Design and Synthesis	Ayman Karim	Virginia Tech
Catalyst Manufacturing	Bill Borghard	Rutgers University



# NAM27 Oral Program





# Monday May 23, 2022

## MONDAY MORNING

### Houdry Award Lecture: Deng-Yang Jan

**Session Chairs:** Lucas Dorazio, *BASF Corporation, USA* and Jeffery Bricker, *Honeywell UOP, USA*

8:00 AM Eugene J. Houdry Award Address: UOP Zeolitic Materials (UZM) in Aromatics, Derivatives and LAB Production.

**Deng (DY) Jan**, *Honeywell UOP, USA*.

## Grand Ballroom East

### Methane to Cn

**Session Chairs:** Elaine Gomez, *ExxonMobil*, and Eleni A. Kyriakidou, *University at Buffalo (SUNY), USA*.

9:30 AM **Mon-GBRE-0930** Understanding the Impact of Water on Surface Oxygen Selectivity across the Pressure Gap in Oxidative Coupling of Methane.

**Yixiao Wang**, Sagar Sourav, Ross Kunz and Rebecca Fushimi, *Idaho National Laboratory, USA*.

#### Short Summary:

A transient isotopic pulse response study has enabled precise measurement of different populations of short-lived surface oxygen species and their role in selectivity under steady-state conditions for OCM catalysts. Water has positive impact on the formation of dioxo species and also increase their surface residence time, thereby, enhancing  $C_{2+3}$  yield

9:50 AM **Mon-GBRE-0950** Optimizing Dual Membrane-Catalyst Reactor Design Via Additive Manufacturing: Application to the Oxidative Coupling of Methane.

**James Wortman**<sup>1</sup>, Valentina Igenegbai<sup>1</sup>, Rawan Almallahi<sup>1</sup>, Ali Hussain Motagamwala<sup>1</sup> and Suljo Linic<sup>2</sup>, (1)*University of Michigan-Ann Arbor, USA*, (2)*University of Michigan, USA*.

#### Short Summary:

An additive manufacturing approach was developed for synthesizing dual membrane/catalyst asymmetric reactor systems based on  $BaCe_{0.8}Gd_{0.2}O_{3-6}$  for the oxidative coupling of methane (OCM). The approach helps to address issues of low  $O_2$  flux, insufficient  $C_{2+}$  hydrocarbon yield and high fabrication cost, which are hurdles to OCM membrane reactor applications.

10:10 AM **Mon-GBRE-1010** Fe<sub>2</sub>O<sub>3</sub>@SiO<sub>2</sub> Oxygen Carriers for Selective Chemical Looping Combustion of Hydrogen in Methane Dehydroaromatization.

**Sunkyu Kim** and Raul F. Lobo, *University of Delaware, USA*.

#### Short Summary:

Fe<sub>2</sub>O<sub>3</sub>@SiO<sub>2</sub> core-shell structures as oxygen carriers are developed for the chemical looping of hydrogen combustion in methane dehydroaromatization. A SiO<sub>2</sub> coating can prevent aromatic diffusion to the Fe<sub>2</sub>O<sub>3</sub> oxygen carrier surface, achieving high methane conversion and aromatic yield by overcoming thermodynamic limitations.

10:30 AM **Mon-GBRE-1030** Dynamic Study of the Evolution of Metal Species in ZSM-5 during Activation and Reaction in Direct Methane Dehydroaromatization.

Sheima Khatib<sup>1</sup>, **Emanuel Noel Joy**<sup>1</sup>, Mustafizur Rahman<sup>1</sup>, Apoorva Sridhar<sup>1</sup>, Simon Bare<sup>2</sup>, Adam Hoffman<sup>2</sup> and Adriano Braga<sup>1</sup>, (1)*Texas Tech University, USA*, (2)*SLAC National Accelerator Laboratory, USA*.

#### Short Summary:

In this work we present our results related to the effect of activation conditions and the addition of a second transition metal (Fe, Co or Ni) to ZSM-5 in the methane dehydroaromatization reaction.

10:50 AM **Mon-GBRE-1050** How the Products in Methane Dehydroaromatization Process Impact Its Stability?.

**Antoine Beuque**<sup>1</sup>, Ludovic Pinard<sup>1</sup>, Jean-François Paul<sup>2</sup>, Elise Berrier<sup>2</sup>, Alexander Sachse<sup>1</sup> and Hao Hu<sup>2</sup>, (1)*Université de Poitiers, France*, (2)*Univ. Lille, CNRS, Centrale Lille, Univ. Artois, UMR 8181-UCCS-Unité de Catalyse et Chimie du Solide, F-59000 Lille, France, France*.

#### Short Summary:

Share of mystery remains on the deactivation in methane dehydroaromatization over Mo/ZSM-5. This work includes a comprehensive study of the products influence on the catalyst lifetime. It was evidenced for the first time, the catalyst deactivates through an inhibition effect of aromatics, which strongly chemisorb onto the molybdenum moieties.

11:10 AM **Mon-GBRE-1110** Direct Conversion of Syngas to Methyl Acetate Via Dimethyl Ether Intermediate in a Dual-Bed Fluidized-Bed Reactor.

**Woochang Sung**, Hyun Seung Jung, Jun Young Kim, Jong Wook Bae and Dong Hyun Lee, *Sungkyunkwan University, Korea, Republic of (South)*.

#### Short Summary:

It was confirmed that two series reactions could occurred in one fluidized bed reactor, and it had a lower deactivation rate value compared to the fixed bed reactor. The effect of process variables in the fluidized bed was analyzed in this study.



11:30 AM **Mon-GBRE-1130** Combined Experimental and Simulation Investigation of Oxidative Coupling of Methane over Pt/Al<sub>2</sub>O<sub>3</sub> at High Temperature.

Jaspreet Chawla, Sven Schardt, Sofia Angeli, **Patrick Lott**, Lubow Maier, Steffen Tischer and Olaf Deutschmann, *Karlsruhe Institute of Technology (KIT), Germany*.

**Short Summary:**

The study has been conducted to understand the interplay between the catalytic kinetic model and homogenous model into C<sub>2</sub> product formation under high temperature and short contact times, during oxidative coupling of methane over platinum catalyst. Both experiments and modeling studies have been conducted to validate the established results.

## MONDAY AFTERNOON

### Natural Gas to Syngas I

**Session Chairs:** Carrie Farberow, *National Renewable Energy Laboratory, USA* and Beata Kilos-Reaume, *The Dow Chemical Company, USA*.

1:10 PM **Mon-GBRE-1310** Mixed Oxides As Flexible Carbon/Oxygen Carriers for Tunable Syngas Generation and CO<sub>2</sub> Utilization Under a Cyclic Scheme.

**Sherafghan Iftikhar**<sup>1</sup>, William Martin<sup>1</sup>, Junchen Liu<sup>1</sup>, Yunfei Gao<sup>1</sup>, Iwei Wang<sup>2</sup> and Fanxing Li<sup>1</sup>, (1)*North Carolina State University, USA*, (2)*Tsinghua University, China*.

**Short Summary:**

The results of our study indicated that LaFe<sub>1-x</sub>Ni<sub>x</sub>O<sub>3</sub> perovskite is a flexible oxygen and/or carbon carrier, resulting in tunable production of syngas. Lower Fe content leads to higher H<sub>2</sub>/CO. The flexibility of LaFe<sub>1-x</sub>Ni<sub>x</sub>O<sub>3</sub> eliminates the need to use cryogenic separations and makeup gas to meet the downstream syngas composition requirements.

1:30 PM **Mon-GBRE-1330** Periodic Reactivity Trend of Earth Abundant Bimetallic Clusters for Methane Dry Reforming Reactions.

**Weifeng Tu**<sup>1</sup>, Yinan Xu<sup>2</sup>, Jeffrey Greeley<sup>2</sup> and Ya-Huei (Cathy) Chin<sup>1</sup>, (1)*University of Toronto, Canada*, (2)*Davidson School of Chemical Engineering, Purdue University, USA*.

**Short Summary:**

We systematically designed a series of Ni nanoparticles decorated with a secondary element (Cu, Co, or Fe), investigated their catalytic functions for carbon dioxide reforming of methane, and established the mechanistic details of methane dry reforming and periodic reactivity trend of bimetallic catalytic clusters on the methane C-H bond activation.

1:50 PM **Mon-GBRE-1350** Ni Nanoparticles on SrTiO<sub>3</sub> with High Coke-Resistance in Dry Reforming of Methane.

**Eunkyung Cho** and Chang Hyun Ko, *Chonnam National University, Korea, Republic of (South)*.

**Short Summary:**

Depending on the preparation method, metallic nickel supported on perovskite SrTiO<sub>3</sub> showed different catalytic activity and coke resistance. Metallic nickel supported on SrTiO<sub>3</sub> by impregnation method lost its catalytic activity by severe coke deposition. However, metallic nickel supported on SrTiO<sub>3</sub> during catalyst preparation step displayed reasonable activity and coke-resistance.

2:10 PM **Mon-GBRE-1410** Excess-Methane Dry Reforming over Yttrium Promoted Ni/KIT-6 Catalysts for Synthesis Gas Production.

Katarzyna Świrk<sup>1</sup>, Patrick Da Costa<sup>2</sup> and **Magnus Rønning**<sup>1</sup>, (1)*Norwegian University of Science and Technology (NTNU), Norway*, (2)*Sorbonne Université, France*.

**Short Summary:**

The yttrium promoted Ni/KIT-6 catalysts were analyzed under excess-methane dry reforming. The measured H<sub>2</sub>/CO molar ratio was in the range of 0.83-0.77 which is suitable for the FT synthesis when using Fe-based catalyst. This could be a future alternative for the use of these materials in upgrading biogas to syngas.

2:30 PM **Mon-GBRE-1430** Numerical Investigation of the Kinetics of Methane Dry Reforming at Low Temperature.

**Han Wang**<sup>1</sup>, Sunky Kim<sup>2</sup> and Erdem Sasmaz<sup>1</sup>, (1)*University of California, Irvine, USA*, (2)*University of Delaware, USA*.

**Short Summary:**

The detailed elementary reaction mechanisms of DRM over the Pt<sup>x</sup>-NiCe@SiO<sub>2</sub> and Pt<sup>0.25</sup>-NiCe/SiO<sub>2</sub><sup>WI</sup> impregnated catalysts were studied. The effects of catalyst morphology and Pt-Ni interaction on the DRM activity were examined by multiple reaction models. The modeling in this work explains the promotion effect of SAA on the yolk-shell catalysts.

2:50 PM **Mon-GBRE-1450** Nickel Embedded Silica Catalyst for Highly Durable Performance of Dry Reforming of Methane (DRM).

**Haehyun Min** and Sung Bong Kang, *Gwangju Institute of Science and Technology, Korea, Republic of (South)*.

**Short Summary:**

We report the highly durable Ni-embedded silica catalyst (NiES) for the superior catalytic dry reforming of methane (DRM) activity. We also proved no clue of deactivation behavior over the NiES catalyst up to 500 hours of operation and extremely high catalytic capacity up to 450 L<sub>g<sub>cat</sub></sub><sup>-1</sup>h<sup>-1</sup>.

## Natural Gas to Syngas II

**Session Chairs:** Coleman Kronawitter, *University of California, Davis, USA* and Carsten Sievers, *Georgia Institute of Technology, USA*.

3:30 PM **Mon-GBRE-1530** Mechanisms and Kinetics of Exsolved Ni-Fe Catalysts – Influence on Catalyst Performance for Dry Reforming of Methane. Soham Shah<sup>1</sup>, Luz Cruz<sup>1</sup>, Mingjie Xu<sup>2</sup>, Jiyun Hong<sup>3</sup>, Xiaoqing Pan<sup>2</sup>, Simon Bare<sup>3</sup> and **Kandis Leslie Abdul-Aziz**<sup>1</sup>, (1)*University of California, Riverside, USA*, (2)*University of California, Irvine, USA*, (3)*SLAC National Accelerator Laboratory, USA*.

**Short Summary:**

This work studied the exsolution kinetics of Ni-Fe from  $\text{LaFe}_{1-x}\text{Ni}_{3-x}\text{O}_{3-x}$  precursors by coupling gas-phase reaction studies with *operando* X-ray absorption spectroscopy and *in situ* scanning electron transmission microscopy. Insights are gained on the influence of the reductive thermal treatment on the structure evolution of Ni-Fe catalysts and the DRM performance.

3:50 PM **Mon-GBRE-1550** Spatio-Temporal Features of Coupled Oxidation and Reforming of Methane on Pt+Pd/Al<sub>2</sub>O<sub>3</sub> Monolith Catalyst.

Jonathan Ratcliff and **Michael P. Harold**, *University of Houston, USA*.

**Short Summary:**

This study is focused on determining the spatial interplay between total/partial methane oxidation with reforming reactions in the rich methane regime, utilizing in-situ spatial temperature and concentration techniques. These methods reveal both mass coupling through the availability of O<sub>2</sub> and thermal coupling between the exothermic oxidation and endothermic reforming chemistries.

4:10 PM **Mon-GBRE-1610** Role of h-BN Support in Determining Active Rhodium Oxide Phase and Its Application to Syngas Production from Methane Partial Oxidation.

**Younhwa Kim**<sup>1,2</sup>, Sungsu Kang<sup>1,2</sup>, Chyan Kyung Song<sup>3</sup>, Jongbaek Sung<sup>2</sup> and Jungwon Park<sup>2</sup>, (1)*Seoul National University, Korea, Republic of (South)*, (2)*Institute for Basic Science (IBS), Korea, Republic of (South)*, (3)*School of Chemical and Biological Engineering, Korea, Republic of (South)*.

**Short Summary:**

We investigate the new role of h-BN support in preferentially growth of rhodium oxide nanoparticles owing to the distinctive metal oxide-support interaction. Moreover, we achieve highly controlled methane partial oxidation to syngas with keeping the H<sub>2</sub>/CO ratio of 2.

4:30 PM **Mon-GBRE-1630** Coking-Resistant Ni/MgAl<sub>2</sub>O<sub>4</sub> Catalyst for Partial Oxidation of Methane: The Impact of the Physicochemical Properties of the Support.

**Abbas Khaleel** and Abdurashed Pillantakath, *United Arab Emirates University, United Arab Emirates*.

**Short Summary:**

The study aimed at correlating between the coking resistance of Ni/MgAl<sub>2</sub>O<sub>4</sub> in partial oxidation of methane and the preparation method of its support. The catalysts over sol-gel-prepared and g-AlOOH-based MgAl<sub>2</sub>O<sub>4</sub>, showed significantly higher coking resistance with only negligible amounts of soft carbon observed on the spent catalysts.

5:10 PM **Mon-GBRE-1710** Zeolite-Supported Ultra-Small Nickel As Catalyst for Oxidative Conversion of Methane to Syngas.

**Shuhei Yasuda**, Takeshi Matsumoto and Toshiyuki Yokoi, *Tokyo Institute of Technology, Japan*.

**Short Summary:**

We found facile catalyst such a zeolite-supported nickel catalyst as an efficient catalyst for the partial oxidation of methane to syngas production.

## Grand Ballroom West

### MONDAY MORNING

#### Fundamentals of Catalysis: Fundamental Mechanisms I

**Session Chairs:** Gina Noh, *The Pennsylvania State University, USA* and William F. Schneider, *University of Notre Dame, USA*.

9:30 AM **Mon-GBRW-0930** Predicting a Key Catalyst-Performance Descriptor for Oxide-Supported Metal Nanoparticles: Metal Chemical Potential.

**Charles T. Campbell**, Zhongtian Mao and John Rumpitz, *University of Washington, USA*.

**Short Summary:**

The chemical potential of transition metal atoms in oxide-supported nanoparticles correlates with surface reactivity and sinter resistance. Based on microcalorimetric measurements, the chemical potential is shown to be predictable versus particle size and the adhesion energy of the particle to the support, and this adhesion energy correlates with metal oxophilicity.

9:50 AM **Mon-GBRW-0950** Catalytic Requirements for Alkanol C-H and C-O Bond Scission on Transition Metal Oxide Surfaces.

**William Broomhead**<sup>1</sup>, Wei Tian<sup>2</sup>, Jose Herrera<sup>2</sup> and Ya-Huei (Cathy) Chin<sup>1</sup>, (1)*University of Toronto, Canada*, (2)*Western University, Canada*.

**Short Summary:**

The mechanistic roles of redox and acid sites on transition metal oxide surfaces in the C-H and C-O bond scission of alkanols were elucidated by kinetic interrogation of methanol partial oxidation and 2-butanol dehydration reactions. Structure-activity relations were developed as a basis for the design of selective metal oxide catalysts.

10:10 AM **Mon-GBRW-1010** Active Centers of Inverse Catalysts.

**Yurong Wu**<sup>1</sup>, Weiqing Zheng<sup>1</sup>, Alfred Worrada<sup>1</sup>, Tianjun Xie<sup>1</sup>, Sagar Sourav<sup>1</sup>, Stavros Caratzoulas<sup>1</sup>, George Tsilomelekis<sup>2</sup> and Dionisios G. Vlachos<sup>1</sup>, (1) *University of Delaware, USA*, (2) *Rutgers, The State University of New Jersey, USA*.

**Short Summary:**

Pt-WO<sub>x</sub> inverse catalyst is one widely used bifunctional catalyst in biomass upgrade. The identification and control of the Brønsted acid sites (BAS) remain elusive, requiring extensive *in-situ* spectroscopic characterizations. We systematically study the dynamics of BAS of Pt-WO<sub>x</sub>/SiO<sub>2</sub> catalysts, which is a prerequisite for developing M-MO catalysts with desired properties.

10:30 AM **Mon-GBRW-1030** Controlling Near-Surface Hydrogen Bonding Interactions and Catalyst Selectivity Using Organic Monolayers.

Alexander Jenkins<sup>1</sup>, Patrick D. Coan<sup>1</sup>, Carrie Farberow<sup>2</sup>, Michael B. Griffin<sup>2</sup>, Charles Musgrave<sup>1</sup> and **J. Will Medlin**<sup>3</sup>, (1) *University of Colorado Boulder, USA*, (2) *National Renewable Energy Laboratory, USA*, (3) *University of Colorado at Boulder, USA*.

**Short Summary:**

A combination of computational and experimental methods was used to study hydrogen bonding interactions between organic modifiers and reactive intermediates on metal surfaces. Hydrogen bonding interactions were found to preferentially stabilize hydroxylated reaction intermediates, leading to shift in adsorbate scaling relations and observed catalyst selectivity.

10:50 AM **Mon-GBRW-1050** H<sub>2</sub>-D<sub>2</sub> and H<sub>2</sub>O-D<sub>2</sub> Isotopic Exchange Pathways on Pt Nanoparticles.

**Samuel Leung**<sup>1</sup>, Sai Chen<sup>1</sup>, David Hibbitts<sup>2</sup> and Enrique Iglesia<sup>1</sup>, (1) *University of California, Berkeley, USA*, (2) *University of Florida, USA*.

**Short Summary:**

H<sub>2</sub>-D<sub>2</sub> isotopic exchange reactions are mediated by noncompetitive adsorption routes that circumvent recombinative desorption pathways and thus cannot be used to unequivocally show reversibility of H<sub>2</sub> chemisorption on Pt surfaces during surface catalysis. H<sub>2</sub>O inhibits H<sub>2</sub> adsorption via partial titration of Pt surfaces rather than by destabilization of H-Pt interactions.

11:10 AM **Mon-GBRW-1110** Effects of Bromide Adsorption on the Direct Synthesis of Hydrogen Peroxide on Pd Nanoparticles.

**Pranjali Priyadarshini**<sup>1,2</sup>, Tomas Ricciardulli<sup>2</sup>, Jason Adams<sup>2</sup>, Yangsik Yun<sup>2</sup> and David Flaherty<sup>2,3</sup>, (1) *Georgia Institute of Technology, USA*, (2) *University of Illinois Urbana-Champaign, USA*, (3) *University of California, Berkeley, USA*.

**Short Summary:**

H<sub>2</sub>O<sub>2</sub> is a green alternative to harmful chlorinated oxidizers if it can be produced selectively by direct synthesis (H<sub>2</sub> + O<sub>2</sub> → H<sub>2</sub>O<sub>2</sub>). The irreversible adsorption of Br on Pd nanoparticles increase the steady-state H<sub>2</sub>O<sub>2</sub> selectivities in pure water by direct synthesis, requiring no further addition of liquid-phase bromide.

11:30 AM **Mon-GBRW-1130** Role of Support Acidity in Activation and Deactivation of Heterogeneous Re-Based Catalysts for Olefin Metathesis.

**Lijun Gao** and Susannah L. Scott, *University of California, Santa Barbara, USA*.

**Short Summary:**

Olefin metathesis play an important role in chemical processed. The high price of Re combined with low catalysts stability have limited commercial application. This study will provide new insight into the role of acidity in supported Re-based catalyst which will be helpful for development of more robust catalysts.

## MONDAY AFTERNOON

### Fundamentals of Microporous Catalysis I

**Session Chairs:** Michele Sarazen, *Princeton University, USA* and Eric Duskocil, *BP, USA*.

1:10 PM **Mon-GBRW-1310** Kinetic Effects of Framework Al Density on Cu Ion Mobility during NO<sub>x</sub> Selective Catalytic Reduction with NH<sub>3</sub> in Chabazite Zeolites.

**Siddarth Krishna**<sup>1</sup>, Casey Jones<sup>1</sup>, Anshuman Goswami<sup>2</sup>, David Dean<sup>1</sup>, Jeffrey T. Miller<sup>1</sup>, William F. Schneider<sup>2</sup> and Rajamani Gounder<sup>1</sup>, (1) *Purdue University, USA*, (2) *University of Notre Dame, USA*.

**Short Summary:**

Experimental kinetic measurements and *operando* X-ray absorption spectra of Cu-chabazite zeolites of varying Cu and Al densities reveal that the framework Al anionic charges regulate the mobility of NH<sub>3</sub>-solvated extraframework Cu cationic active sites that dynamically interact during NO<sub>x</sub> reduction catalysis, a manifestation of non-mean-field reactivity behavior.

1:30 PM **Mon-GBRW-1330** Modeling the Active Site Structure of a Heterogeneous Nickel (II) Cation Complex Catalyst Under Different Environmental Conditions.

**Stephen Vicchio**<sup>1</sup>, Zhihengyu Chen<sup>2</sup>, Karena Chapman<sup>2</sup> and Rachel Getman<sup>1</sup>, (1) *Clemson University, USA*, (2) *Stony Brook University, USA*.

**Short Summary:**

Heterogeneous catalysts exhibit dynamic changes in structure as a function of environmental conditions. For metal complexes supported on solid supports, the structural response to different conditions is difficult to elucidate. Herein, we model a supported Ni(II) metal complex under different reducing conditions to demonstrate the structural response of the catalyst.

1:50 PM **Mon-GBRW-1350** Distribution of Al Species and Their Impacts on Alkane Cracking in MFI Zeolites.

**Tram Pham**, Vy T. Nguyen, Bin Wang and Steven P. Crossley, *University of Oklahoma, USA*.

**Short Summary:**

By utilizing cation titration and pulsed water treatments, we revealed the important role of extra framework Al species and Al distribution including acid sites in pairs and their location in the generation of highly active sites for alkane cracking in MFI zeolites.

2:10 PM **Mon-GBRW-1410** Catalytic Consequences of Intracrystalline Diffusional Constraints for Propene Oligomerization over Brønsted Acid Zeolites.

Elizabeth Bickel and Rajamani Gounder, *Purdue University, USA*.

**Short Summary:**

Rates, selectivities, and deactivation of zeolite catalysts for propene oligomerization reflect the combined influences of kinetics and intrapore diffusional constraints imposed by occluded hydrocarbon products, which change in composition with pressure and temperature; these insights are revealed by interrogating zeolites synthesized with independently varied Al arrangement, density, and crystallite size.

2:30 PM **Mon-GBRW-1430** Metal Nanoparticle Location Effects in Pd/Zeotype Bifunctional Catalysts for Hydroconversion of N-Alkanes.

Luc C.J. Smulders<sup>1</sup>, Jochem H. van de Minkelis<sup>1</sup>, Min Tang<sup>1</sup>, Tegan Roberts<sup>2</sup>, Glenn Sunley<sup>2</sup>, Petra E. de Jongh<sup>1</sup> and Krijn P. de Jong<sup>1</sup>, (1)*Utrecht University, Netherlands*, (2)*BP plc, United Kingdom*.

**Short Summary:**

Heat treatment of Pd ion exchanged zeotypes affects Pd particle location: catalysts were prepared with majority of particles *in* the pore network or *on* the zeotype crystals. Furthermore, catalysts were prepared with Pd located on alumina binder material. Pd location impacts the activity and selectivity during hydroconversion of *n*-alkanes.

2:50 PM **Mon-GBRW-1450** Probing Surface-Adsorbate Interactions and Energetics through Active Particle Dynamics.

Benjamin Greydanus<sup>1</sup>, J. Will Medlin<sup>2</sup> and Daniel K. Schwartz<sup>3</sup>, (1)*University of Colorado Boulder, USA*, (2)*University of Colorado at Boulder, USA*, (3)*University of Colorado, USA*.

**Short Summary:**

Here, we show the utility of active particles for in-situ quantification of the affinity and saturation coverage of adsorbates onto metal catalytic surfaces under steady-state reaction conditions. The energetics of this process were directly probed by measuring the isotherms at elevated temperatures.

## Fundamentals of Microporous Catalysis II

**Session Chairs:** Sarika Goel, *Honeywell UOP, USA* and Brett Loveless, *ExxonMobil Research and Engineering, USA*.

3:30 PM **KEYNOTE Mon-GBRW-1530** Mechanisms of Communication between Active Sites in Zeolites and Consequences for Acid and Redox Catalysis. Rajamani Gounder, *Purdue University, USA*.

**Short Summary:**

Active sites in zeolites communicate with one another through bound co-adsorbates or upon their solvation by reactants to form complexes with localized mobility, leading to marked consequences for the kinetics and mechanisms of acid and redox catalysis and to strong dependences of reactivity on the spatial arrangement of active sites.

4:10 PM **Mon-GBRW-1610** Effects of Al Position, Confinement, and Clustering on Methanol Dehydration Rates and Kinetics in MFI.

Alexander Hoffman<sup>1</sup>, Songhyun Lee<sup>2</sup>, Ryoh-Suke Sekiya<sup>1,3</sup>, Claire Nimlos<sup>2,4</sup>, Rajamani Gounder<sup>2</sup> and David Hibbitts<sup>1</sup>, (1)*University of Florida, USA*, (2)*Purdue University, USA*, (3)*Georgia Institute of Technology, USA*, (4)*National Renewable Energy Laboratory, USA*.

**Short Summary:**

The effects of Al location on turnover rates remain unclear despite many years of study. We use DFT to evaluate methanol dehydration barriers at all 12 T-sites to quantify confinement effects in MFI. We include methanol clusters in our study, which alter kinetic behavior but were excluded from previous analyses.

4:30 PM **Mon-GBRW-1630** Role of Brønsted and Lewis Acid Sites in Zeolites for Hydride Transfer.

Eric Hernandez and Friederike C. Jentoft, *University of Massachusetts Amherst, USA*.

**Short Summary:**

Hydride transfer during the transformation of 1-butanol on HZSM-5 zeolites with various Si/Al ratios is evident by formation of cyclopentenyl cations on the surface (as detected by in situ IR and UV-vis spectroscopy) and the evolution of alkanes. The cation concentration correlates with Brønsted (and not Lewis) acid concentration.

4:50 PM **Mon-GBRW-1650** Reaction Pathways and Kinetic Descriptors of Iron- and Chromium-Based Metal-Organic Frameworks for Aryl Alkene Oxidation.

Rachel Yang and Michele Sarazen, *Princeton University, USA*.

**Short Summary:**

Detailed reaction pathways and kinetic mechanisms are formulated for iron and chromium carboxylate metal-organic frameworks during aryl oxidation utilizing H<sub>2</sub>O<sub>2</sub>. Metal properties impact reactive intermediate and metalocycle transition state stabilizations that result in different reactivities and oxygenate product distributions. Framework functionalization yields insight into electronic structures that improve observed selectivities.

5:10 PM **Mon-GBRW-1710** Chemistry of Sites on Fe<sub>3o</sub> Nodes of the Metal-Organic Framework MIL-100: Catalyst for Methanol Dehydration.

Yue Xiao<sup>1</sup>, Minxin Zhang<sup>1</sup>, Bruce Gates<sup>2</sup> and Dong Yang<sup>1</sup>, (1)*Nanjing Tech University, China*, (2)*University of California, Davis, USA*.

**Short Summary:**

We investigated the bonding of formate, methoxy, and hydroxy ligands to MIL-100(Fe) node sites, providing evidence showing the presence of defects and demonstrating the collaborative roles of node defect and vacancy sites in methanol dehydration catalysis and determining a new MOF catalyst deactivation mechanism, whereby Fe<sup>3+</sup> is reduced to Fe<sup>2+</sup>.

## MONDAY MORNING

## Atomically-Dispersed Metal Catalysts I

**Session Chairs:** Sara Jacob, *ExxonMobil Research and Engineering, USA* and Lucun Wang, *Idaho National Laboratory, USA*.

9:30 AM **Mon-GRAM-0930** Bifunctional Heterogeneous Pair-Site Catalysts.

Ji Qi<sup>1</sup>, Insoo Ro<sup>1</sup>, Seungyeon Lee<sup>2</sup>, Mingjie Xu<sup>3</sup>, Xingxu Yan<sup>3</sup>, Xiaoqing Pan<sup>3</sup>, Dionisios G. Vlachos<sup>2</sup>, Stavros Caratzoulas<sup>2</sup> and **Phillip Christopher**<sup>1</sup>, (1)*University of California, Santa Barbara, USA*, (2)*University of Delaware, USA*, (3)*University of California, Irvine, USA*.

**Short Summary:**

Our results demonstrate that heterogeneous atomically dispersed pairs can act as bifunctional active sites with emergent reactivity for reactions performed in industry using homogeneous catalysts, and allow detailed analyses of their reaction mechanisms. For ethylene hydroformylation and methanol carbonylation, >95% product selectivity was demonstrated at industrially viable product formation rates.

9:50 AM **Mon-GRAM-0950** Design of Pt<sub>1</sub>Zn<sub>1</sub> Nano-Alloy Catalysts for Propane Dehydrogenation through Interface Tailoring Via Atomic Layer Deposition.

Piyush Ingale<sup>1</sup>, **Robert Baumgarten**<sup>1</sup>, Kristian Knemeyer<sup>1</sup>, Phil Preikschas<sup>1</sup>, Elias Frei<sup>2</sup>, Stefan Kotrel<sup>2</sup>, Michael Geske<sup>1</sup>, Raoul Naumann d'Alnoncourt<sup>1</sup>, Arne Thomas<sup>3</sup> and Frank Rosowski<sup>2,3</sup>, (1)*BasCat – UniCat BASF JointLab: Technische Universität Berlin, Germany*, (2)*BASF SE, Germany*, (3)*Technische Universität Berlin, Germany*.

**Short Summary:**

This work highlights the significance of ALD as synthetic tool to introduce new interfaces in the catalysts. An ultra-thin functional layer of ZnO is deposited via ALD on SiO<sub>2</sub> followed by IWI of Pt nanoparticles. The supported Pt<sub>1</sub>Zn<sub>1</sub> nanoparticles formed after activation are benchmarked against industrial Oleflex like PDH catalyst

10:10 AM **Mon-GRAM-1010** Accelerating Hydrogenation While Suppressing Hydrogen Evolution: Proof of Single-Atom Alloy Strategy for Hcs Production in Electrocatalytic CO<sub>2</sub> Reduction.

**Manjeet Chhetri**<sup>1</sup>, Zehua Jin<sup>1</sup>, John Yeager<sup>1</sup>, Case Sandor<sup>1</sup>, Sungsik Lee<sup>2</sup>, Cameron Bodenschatz<sup>3</sup> and Ming Yang<sup>1</sup>, (1)*Clemson University, USA*, (2)*Argonne National Laboratory, USA*, (3)*NASA Glenn Research Center, USA*.

**Short Summary:**

The present work demonstrates the proof of concept single atom alloy strategy using platinum group metals on Copper catalysts' surface which would otherwise seem to be effective in hydrogen evolution reaction, can be adopted to CO<sub>2</sub> reduction to achieve enhanced hydrocarbon formation.

10:30 AM **Mon-GRAM-1030** Atomically Dispersed Pd in Flame Synthesized Pd/CeO<sub>2</sub> Catalyst for Methane Oxidation Reactions.

**Musa Najimu** and Erdem Sasmaz, *University of California, Irvine, USA*.

**Short Summary:**

This work showed the synthesis of different Pd structures on CeO<sub>2</sub> using flame spray pyrolysis. The high temperature synthesis can stabilize atomically dispersed Pd species which are active for low temperature methane oxidation.

10:50 AM **Mon-GRAM-1050** Ethylene-to-Propene (ETP) Conversion over Ni(II) Single Sites on Tailored Silica-Alumina Supports.

**Zixuan Chen** and Christoph Müller, *ETH Zürich, Switzerland*.

**Short Summary:**

Application of the ALD of TMA onto dehydroxylated silica allows the precise control of the abundance of strong BAS on the support. The abundance of strong BAS is found to correlate directly with the ETP activity of Ni(II) single sites supported on such ALD-prepared silica-aluminates.

11:10 AM **Mon-GRAM-1110** Boosting Support Reducibility and Metal Dispersion By Exposed Surface Atom Control for Highly Active Supported Metal Catalysts.

**Myeong Gon Jang**<sup>1</sup>, Sinmyung Yoon<sup>2</sup>, Dongjae Shin<sup>1</sup>, Hyung Jun Kim<sup>1</sup>, Rui Huang<sup>1</sup>, Euseob Yang<sup>2</sup>, Jihun Kim<sup>2</sup>, Kug-Seung Lee<sup>1</sup>, Kwangjin An<sup>2</sup> and Jeong Woo Han<sup>1</sup>, (1)*Pohang University of Science and Technology (POSTECH), Korea, Republic of (South)*, (2)*Ulsan National Institute of Science and Technology (UNIST), Korea, Republic of (South)*.

**Short Summary:**

The synthetic strategy of facet control combined with metal doping in a well-defined structure is introduced for the first time to control the catalytic activity. This research will contribute to improving the catalytic activity through understanding of the relationship between the shape of oxide and the doped and loaded metals.

11:30 AM **Mon-GRAM-1130** Atomically Precise Design of Heterogeneous Catalysts for Enhanced Parahydrogen-Induced Polarization Nuclear Magnetic Resonance.

**Helena Hagelin-Weaver**<sup>1</sup>, Bochuan Song<sup>1</sup>, Hanqin Zhao<sup>1</sup>, Diana Choi<sup>1</sup>, Yan Xin<sup>2</sup> and Clifford R. Bowers<sup>1</sup>, (1)*University of Florida, USA*, (2)*Florida State University, USA*.

**Short Summary:**

Heterogeneous catalysts were designed to improve parahydrogen-induced polarization nuclear magnetic resonance signals. To reduce hydrogen diffusion and allow pairwise addition of dihydrogen, single atom platinum supported on ceria shapes were used, and strong metal support interactions were induced on titania-supported rhodium catalysts. Both methods were shown to improve NMR signals.



## MONDAY AFTERNOON

### Atomically-Dispersed Metal Catalysts II

**Session Chairs:** Feng Gao, *Pacific Northwest National Laboratory, USA* and Elaine Gomez, *ExxonMobil, .*

1:10 PM **Mon-GRAM-1310** Atomically Dispersed Platinum *on* and *in* a MgO Support: Catalysts for CO Oxidation.

Yizhen Chen<sup>1</sup>, **Rachita Rana**<sup>1</sup>, Zhennan Huang<sup>2</sup>, Jorge Perez-Aguilar<sup>1</sup>, Xiao Zhao<sup>3</sup>, Thomas Blum<sup>4</sup>, Adam Hoffman<sup>5</sup>, Miquel Salmeron<sup>3</sup>, Miaofang Chi<sup>2</sup>, Coleman Kronawitter<sup>1</sup>, Fernando Vila<sup>6</sup>, Ambarish Kulkarni<sup>1</sup>, Simon Bare<sup>5</sup> and Bruce Gates<sup>1</sup>, (1)*University of California, Davis, USA*, (2)*Oak Ridge National Laboratory, USA*, (3)*Lawrence Berkeley National Laboratory, USA*, (4)*University of California, Irvine, USA*, (5)*SLAC National Accelerator Laboratory, USA*, (6)*University of Washington, USA*.

**Short Summary:**

We report a comparison of MgO-supported surface and subsurface platinum catalysts that are atomically dispersed, with evidence of their structures under working conditions and evidence of how metal–support coordination determines the catalytic properties for CO oxidation.

1:30 PM **Mon-GRAM-1330** Combined Experimental, Density Functional Theory, and Microkinetic Modeling for Mechanism Determination on Single Atom Catalysts.

Shyam Deo, Linxi Wang, Kayla Eudy, Zayne Weber, **Griffin Canning**, Robert Rioux and Michael Janik, *The Pennsylvania State University, USA*.

**Short Summary:**

Single transition metal atoms supported on oxides provide tunable and emergent catalytic properties. We prepared single atom catalysts with late transition metals supported on ceria nanocubes. Characterization, kinetic measurements, DFT calculations, and microkinetic modeling (MKM) using Bayesian inference are combined to determine the elementary catalytic mechanism of catalytic CO oxidation.

1:50 PM **Mon-GRAM-1350** Site-Density-Sensitive Pt1/Moxc Catalysts for the Low-Temperature Reverse Water Gas Shift Reaction..

**Ewa Chukwu**<sup>1</sup>, Lindsay Molina<sup>1</sup>, Conner Rapp<sup>1</sup>, Luis Morales<sup>1</sup>, Stavros Karakalos<sup>2</sup> and Ming Yang<sup>1</sup>, (1)*Clemson University, USA*, (2)*University of South Carolina, USA*.

**Short Summary:**

Increasing active sites density as a facile strategy for promoting the Intrinsic activity of single atoms catalysts might not hold in all cases, especially when both the supported metal and supports directly participate in the reaction pathways.

2:10 PM **Mon-GRAM-1410** Electronic Modulation of Pt Atomically Dispersed on Oxides Aiming Catalytic Applications.

Leonardo S. Sousa, Renan B. Guerra, Caio C. Oliveira and **Daniela Zanchet**, *University of Campinas, Brazil*.

**Short Summary:**

Through the design and heterogenization of coordination compounds, it was possible to modulate the catalytic activity of Pt atomically dispersed on TiO<sub>2</sub>. For the Reverse Water Gas Shift reaction, our catalyst showed an increase of two times in activity, higher stability and selectivity when compared to a conventional Pt/TiO<sub>2</sub> catalyst.

2:30 PM **KEYNOTE Mon-GRAM-1430 Synthesis of Supported Single Atom Catalysts Via Chelate Fixation.** Abolfazl Shakouri, Horie Adabi Firouzjaie, Stavros Karakalos, **Christopher T. Williams** and John R. Regalbuto, *University of South Carolina, USA*.

**Short Summary:**

Heterogeneous single atom catalysts have tremendous potential but a facile synthesis at high metal loadings remains a challenge. Herein, we present a simple, scalable method for doing so, applicable to a wide variety of metals and carbon and oxide supports.

### Bimetallic and Mixed Oxide Catalysts

**Session Chairs:** Marc Porosoff, *University of Rochester, USA* and Zhehao Wei, *Air Liquide, .*

3:30 PM **Mon-GRAM-1530** Effects of Metal Doping and Particle Shape in Nanocrystal-Based Catalysts for the Direct Synthesis of Hydrogen Peroxide.

**Silke Behrens**, *Karlsruhe Institute of Technology (KIT), Germany*; *Karlsruhe Institute of Technology (KIT), Germany*.

**Short Summary:**

Model catalysts were synthesized from shape-selective Pd<sub>3</sub>Pb nanocrystals and employed to study the effects of Pb doping and nanocrystal shape on the catalytic performance in direct H<sub>2</sub>O<sub>2</sub> synthesis. Especially Pd<sub>3</sub>Pb nanocrystals of cubic shape reveal a high H<sub>2</sub>O<sub>2</sub> productivity because of their ordered structure, well-defined morphology, and alloy effect.

3:50 PM **Mon-GRAM-1550** Enhancing Reactivity in Olefin Metathesis of Ethylene and 2-Butene to Propylene over Mo-Based Bimetallic Single-Site Catalysts.

**Anoop Uchagawkar**<sup>1</sup>, Denis Johnson<sup>1,2</sup>, Anand Ramanathan<sup>1,3</sup> and Bala Subramaniam<sup>1</sup>, (1)*The University of Kansas, USA*, (2)*University of Pittsburgh at Johnstown, USA*, (3)*Currently at Chevron Phillips Chemical Company, 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.

4:10 PM **Mon-GRAM-1610** From Formation Phase Studies to Catalyst Design Strategies for Rh-Based Alcohol Synthesis Catalysts.

**Phil Preikschas**<sup>1</sup>, Martin Konrad<sup>1</sup>, Katharina Trapp<sup>1</sup>, Milivoj Plodinec<sup>2</sup>, Julia Bauer<sup>1</sup>, Ralph Kraehnert<sup>1</sup>, Raoul Naumann d'Alnoncourt<sup>1</sup> and Frank Rosowski<sup>3,4</sup>, (1)BasCat – UniCat BASF JointLab: Technische Universität Berlin, Germany, (2)Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany, (3)BASF SE, Germany, (4)Technische Universität Berlin, Germany.

**Short Summary:**

A lack of long-term catalytic studies and spent sample characterization limits our fundamental understanding of specific promoter effects, hampering an improvement of Rh-based catalysts. Therefore, formation phase studies have been conducted to clarify the role of Mn and Fe as promoters yielding new catalyst design strategies.

4:30 PM **Mon-GRAM-1630** Facilitate Hydrogen Dissociation over Dilute Nanoporous Ti-Cu Catalysts.

**Jennifer Lee**<sup>1</sup>, Zhen Qi<sup>2</sup>, Alexandre Foucher<sup>3</sup>, Hio Tong Ngan<sup>4</sup>, Kevin Dennis<sup>5</sup>, Jun Cui<sup>5</sup>, Philippe Sautet<sup>4</sup>, Eric Stach<sup>3</sup>, Robert Madix<sup>1</sup>, Juergen Biener<sup>2</sup> and Cynthia Friend<sup>1</sup>, (1)Harvard University, USA, (2)Lawrence Livermore National Laboratory, USA, (3)University of Pennsylvania, USA, (4)University of California, Los Angeles, USA, (5)Ames Laboratory, USA.

**Short Summary:**

We successfully demonstrated the use of early transition metal Ti to promote H<sub>2</sub> dissociation over nanoporous Cu materials via steady-state HD exchange reaction experiments. Based on various characterization techniques together with DFT calculations, isolated, metallic Ti in Cu is proposed to be the active site for the promotional effect observed.

4:50 PM **Mon-GRAM-1650** Tuning of Composition, Mesostructure and Activity of Cobalt-Based Mixed Spinel Oxides for Oxygen Evolution Reaction.

**Anna Rabe**<sup>1,2</sup>, Felix Hiege<sup>3</sup>, Maximilian Jaugstetter<sup>3</sup>, Felix Haase<sup>4</sup>, Arno Bergmann<sup>4</sup>, Julia Bükér<sup>3</sup>, Adarsh Koul<sup>3</sup>, Wolfgang Schuhmann<sup>3</sup>, Martin Muhler<sup>3</sup>, Beatriz Roldan Cuenya<sup>4</sup>, Kristina Tschulik<sup>3</sup> and Malte Behrens<sup>1,5</sup>, (1)University of Duisburg-Essen, Germany, (2)University of Kiel, Germany, (3)Ruhr University Bochum, Germany, (4)Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany, (5)Christian-Albrechts-Universität zu Kiel, Germany.

**Short Summary:**

This work investigates real structure-reactivity relationships of systematically substituted cobalt-based spinels in several oxygen evolution reactions. Conventional controlled co-precipitation is applied, and a new microemulsion-assisted approach is established, which leads to highly active Co<sub>2</sub>FeO<sub>4</sub> catalysts. The enhanced activity of the newly prepared materials is investigated with *operando* and *in-situ* experiments.

5:10 PM **Mon-GRAM-1710** Breaking the Scaling Relations in Oxygen Reduction Reaction on MoO<sub>y</sub>/Pt(CuNi)<sub>x</sub> Catalyst Toward Enhanced Activity.

Dezhen Wu, Xiaochen Shen, Yanbo Pan, Libo Yao and **Zhenmeng Peng**, The University of Akron, USA.

**Short Summary:**

The scaling relations of reaction intermediates in oxygen reduction reaction was broken by depositing MoO<sub>y</sub> on Pt(CuNi)<sub>x</sub> nanoparticles. The specific-area activity was increased with a group of Pt(CuNi)<sub>x</sub> nanoparticle catalysts, thanks to the dual-site cascade reaction mechanisms at the MoO<sub>y</sub>/Pt(CuNi)<sub>x</sub> interfaces.

## Mercury Ballroom

### MONDAY MORNING

#### Challenges for Future Industrial Processes

**Session Chairs:** Kandis Leslie Abdul-Aziz, University of California, Riverside, USA and Jun Wang, SABIC, USA.

9:30 AM **Mon-MEBR-0930** Production of Hydrogen Peroxide in Two-Phase System Using MOF-Based Photocatalysts.

**Hiroshi Yamashita**, Osaka University, Japan.

**Short Summary:**

Application of metal organic frameworks (MOFs) as photocatalysts for H<sub>2</sub>O<sub>2</sub> production is very novel. A MOF composed of Ti<sub>8</sub>O<sub>8</sub>(OH)<sub>4</sub> clusters interconnected by 2-aminoterephthalic acid linkers (MIL-125-NH<sub>2</sub>) can produce a photoexcited state composed of Ti<sub>8</sub>O<sub>8</sub>(OH)<sub>4</sub><sup>+-</sup> and a hole at an adjacent organic linker under visible light irradiation for photocatalytic H<sub>2</sub>O<sub>2</sub> production.

9:50 AM **Mon-MEBR-0950** Rational Design of Electrocatalysts for High-Temperature Solid Oxide Electrochemical Cells: Oxygen and Carbon Dioxide Electrocatalysis.

**Juliana Carneiro**, Elif Tezel, Xiangkui Gu and Eranda Nikolla, Wayne State University, USA.

**Short Summary:**

In this work we developed a theory-guided design principle that provides significant insights into high-temperature O<sub>2</sub> and CO<sub>2</sub> electrocatalysis in SOECs. Our results revealed that the strength of surface oxygen binding, described by the oxophilicity of the electrocatalyst, can be used as an activity and stability descriptor.

10:10 AM **Mon-MEBR-1010** Balancing Mass Transport and Kinetics in Adiponitrile Electrosynthesis: From Electrolyte Design to Dynamic Potential Control.

**Miguel Modestino**, New York University, USA.

**Short Summary:**

This presentation will discuss how careful formulation of electrolytes can lead to adiponitrile (ADN) electrosynthesis with selectivity of >83%. Furthermore, dynamic potential control can be used to balance mass transport and kinetics in organic electrosynthesis, leading to a 30% enhancement in ADN production rates with respect to direct current operation.

10:30 AM **Mon-MEBR-1030** On the Role of Support Oxygen-Groups in the Electrochemical Oxidation of Glucose over Pt/Carbon Nanofiber Catalysts.

Matthijs van der Ham<sup>1</sup>, Tomas Haasterecht, van<sup>1</sup>, Marc Koper<sup>2</sup> and **J.H. (Harry) Bitter<sup>1</sup>**, (1)Wageningen University & Research, Netherlands, (2) Leiden University, Netherlands.

**Short Summary:**

The the performance of Pt supported on carbon nanofibers for the electrocatalytic oxidation of glucose to (di)carboxylic acids is determined by the number of oxygen groups on the surface of the carbon.

10:50 AM **Mon-MEBR-1050** Enhancing Acetate Selectivity By Coupling Anodic Oxidation in Carbon Monoxide Electroreduction.

**Sean Overa** and Feng Jiao, *University of Delaware, USA*.

**Short Summary:**

By tailoring membrane properties and anode partial oxidation selectivity, a highly durable and selective carbon monoxide electrolyzer was produced capable of generating 3.2 M acetate at a purity of 97.8 %. This system achieved 100 hours stability and >500 mA cm<sup>-2</sup> towards CO reduction at <2.4 V.

11:10 AM **Mon-MEBR-1110** Unifying Concepts in Electro- and Thermocatalysis Towards Hydrogen Peroxide Production.

**Jason Adams**, Matthew Kromer, Joaquin Rodriguez-Lopez and David Flaherty, *University of Illinois Urbana-Champaign, USA*.

**Short Summary:**

The direct synthesis of H<sub>2</sub>O<sub>2</sub> from H<sub>2</sub> and O<sub>2</sub> couples the electrocatalytic oxygen reduction (ORR) and hydrogen oxygen reactions (HOR) over metal nanoparticles. These systems show similar rates and selectivities at equivalent electrochemical potentials. Consequently, thermocatalytic rates depend on rates of HOR and the stability of O-O bonds during ORR.

11:30 AM **Mon-MEBR-1130** Highly Active Nitrogen – Doped Carbon Nanostructures As Bromine Evolution Reaction Electrocatalysts.

**Dishari Basu**, Deeksha Jain, Jonathan Hightower, Vance Gustin, Aravind Asthagiri, Anne Co and Umit S. Ozkan, *The Ohio State University, USA*.

**Short Summary:**

This work demonstrates the application of a noble metal free carbon-based catalyst i.e. nitrogen doped carbon nanostructures (CNx) as a promising alternative for a novel electrocatalytic bromine production process via electrochemical bromide oxidation at room temperature, eliminating the traditional requirement for toxic chlorine gas as the oxidant.

## MONDAY AFTERNOON

### Synthesis of Fuels

**Session Chairs:** Gianvito Vile, *Politecnico di Milano, Italy* and Eranda Nikolla, *Wayne State University, USA*.

1:10 PM **Mon-MEBR-1310** Electrocatalytic Methane Oxidation to Ethanol on Iron-Nickel Hydroxide Nanosheets.

**Jialu Li**, Libo Yao, Dezhen Wu and Zhenmeng Peng, *The University of Akron, USA*.

**Short Summary:**

Effective decomposition of methane is of high desirability but remains challenging. Herein, we report an electrochemical methane oxidation process with Fe-Ni-OH as the catalyst in the aqueous alkaline electrolyte under ambient conditions. The maximum product formation rate of ethanol has reached 9.09 mmol/g<sub>catalyst</sub>·h on Fe<sub>3</sub>-Ni<sub>7</sub>-OH under 1.46 V vs. RHE.

1:30 PM **KEYNOTE Mon-MEBR-1330** Regulating Surface Oxide Activity for Decarbonizing Chemicals and Fuels. **Yang Shao-Horn**, *Massachusetts Institute of Technology, USA*.

**Short Summary:**

In this talk we will discuss how to tune oxide electronic structure and design oxide surfaces to control the kinetics of key reactions central to making of chemicals and fuels using electrons from renewables.

2:10 PM **Mon-MEBR-1410** An Intensified Photocatalytic Process of CO<sub>2</sub> Conversion to Fuels Via Direct Utilization of Bicarbonates.

**Rito Yanagi<sup>1</sup>**, Tianshuo Zhao<sup>2</sup> and Shu Hu<sup>1</sup>, (1)Yale University, USA, (2)University of Pennsylvania, USA.

**Short Summary:**

Photocatalysts promise solar fuels production at scale. I first introduce our oxide coatings for efficient and durable photocatalysis. We then present how the charge transfer kinetics sensitively determine the charge separation. Finally, we employ our coatings to achieve H<sub>2</sub> evolution at record efficiency and CO<sub>2</sub> conversion from bicarbonate directly.

2:30 PM **Mon-MEBR-1430** Sunlight-Powered Reverse Water Gas Shift Reaction (rWGS) Using a Plasmonic Au/TiO<sub>2</sub> Nanocatalyst.

Pau Martinez Molina<sup>1</sup>, Nicole Meulendijks<sup>1</sup>, Man Xu<sup>1</sup>, Marcel Verheijen<sup>2,3</sup>, Tim Den Hartog<sup>4</sup>, Pascal Buskens<sup>1,5</sup> and **Francesc Sastre<sup>1</sup>**, (1)The Netherlands Organisation for Applied Scientific Research, Netherlands, (2)Eindhoven University of Technology, Netherlands, (3)Eurofins Materials Science, Netherlands, (4)Zuyd University of Applied Sciences, Netherlands, (5)Hasselt University, Netherlands.

**Short Summary:**

The Au/TiO<sub>2</sub> catalyst can promote efficiently the reverse Water Gas Shift reaction (rWGS) under solar light irradiation at ambient temperatures. An apparent quantum efficiency of 4.78% was reached with a CO selectivity of 98% and a production rate of 429 mmol<sub>Au</sub><sup>-1</sup> h<sup>-1</sup> without external heating.

2:50 PM **Mon-MEBR-1450** Observation and Models of Plasma-Catalytic Nitrogen Oxidation.

Hanyu Ma<sup>1</sup>, Rakesh Sharma<sup>2</sup>, Stefan Welzel<sup>2</sup>, Richard van de Sanden<sup>2</sup>, Mihalis Tsampas<sup>2</sup> and **William F. Schneider**<sup>1</sup>, (1)University of Notre Dame, USA, (2)Dutch Institute for Fundamental Energy Research, Netherlands.

**Short Summary:**

Plasma-catalytic nitrogen oxidation to NO is demonstrated at conditions of no background plasma or catalytic production. Microkinetic models quantitatively capture behavior and guide optimization.

## Nitrogen Activation

**Session Chairs:** Bryan Goldsmith, *University of Michigan-Ann Arbor, USA* and Nirala Singh, *University of Michigan-Ann Arbor, USA*.

3:30 PM **Mon-MEBR-1530** High-Temperature Electrocatalytic NH<sub>3</sub> Production on Strontium Iron Molybdate-Type Double Perovskite Oxynitride Cathodes.

**Seval Gunduz**, Matthew Ferree, Jaesung Kim, Anne Co and Umit S. Ozkan, *The Ohio State University, USA*.

**Short Summary:**

An alternative electrochemical process can be engineered for small-scale applications that has the potential to enable on-site/sustainable/scalable/energy-efficient ammonia production. In this study, double-perovskite oxides/oxynitrides which possess the benefits of both perovskite-oxide and nitride materials were synthesized, characterized ex-situ/in-situ/operando and tested in an SOEC for NH<sub>3</sub> production from N<sub>2</sub> and H<sub>2</sub>O.

3:50 PM **Mon-MEBR-1550** Electrochemical Reduction of Gaseous Nitrogen Oxides on Transition Metals at Ambient Conditions.

**Feng Jiao**, *University of Delaware, USA*.

**Short Summary:**

We investigate a series of transition metal catalysts for electrocatalytic reduction of gaseous nitric oxide (NO) and nitrous oxide (N<sub>2</sub>O) at ambient condition in a gas-fed electrolyzer configuration.

4:10 PM **Mon-MEBR-1610** Waste to an Asset, Synthesis of Ammonia from Nitrate Reduction.

**Samira Siahrostami**, *University of Calgary, Canada*.

**Short Summary:**

We use computational analysis to investigate the electrochemical production of ammonia from nitrate reduction.

4:30 PM **Mon-MEBR-1630** Species and Pathways Involved in Synthesis of Ammonia By Plasma Catalysis.

**Brian Bayer**, Peter Bruggeman and Aditya Bhan, *University of Minnesota, Twin Cities, USA*.

**Short Summary:**

This study utilizes molecular beam mass spectrometry to quantitatively correlate formation of ammonia with consumption of vibrationally excited and radical species derived from nitrogen and hydrogen in atmospheric pressure nonthermal plasma to determine which species and pathways are involved in the synthesis of ammonia over different transition metal surfaces.

## Rendezvous Trianon

### MONDAY MORNING

#### Alkane Oxydehydrogenation I

**Session Chairs:** Jeff Kloosterman, *Air Products, USA* and Partha Nandi, *Corporate Research, ExxonMobil Research and Engineering, USA*.

9:30 AM **Mon-RZVS-0930** Rate Analysis and Product Inhibition in Bulk Oxide Catalysis: The Case of Ethane Oxidation over Nickel Oxide.

**Xiaohui Zhao**, Jeffrey D. Rimer and Praveen Bollini, *University of Houston, USA*.

**Short Summary:**

Inhibition of H<sub>2</sub>O and CO<sub>2</sub> as common oxidation products makes rigorous rate measurement very challenging. We have developed a mathematic model to interpret the kinetic data of ethane oxidation over bulk nickel oxide measured with and without product co-feeds to illustrate the necessity of inspecting both regimes for kinetic study.

9:50 AM **Mon-RZVS-0950** Selective Oxidation of Propane with Perovskites.

**Jinhu Dong**<sup>1</sup>, Gregor Koch<sup>1</sup>, Pierre Kube<sup>1</sup>, Spencer J. Carey<sup>1</sup>, Kristian Knemeyer<sup>2</sup>, Frank Rosowski<sup>2,3</sup>, Robert Schlögl<sup>1,4</sup> and Annette Trunschke<sup>1</sup>, (1) Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany, (2)Technische Universität Berlin, Germany, (3)BASF SE, Germany, (4)Max Planck Institute for Chemical Energy Conversion, Germany.

**Short Summary:**

Selective oxidation of propane have been systematically investigated with perovskite catalysts by varying A-site (La, Pr, Nd, and Sm) and B-site (Cr, Mn, Fe, and Co), providing a general overview and understanding. We also provide some insights into modulation of the propylene selectivity by surface deposition on Mn-containing perovskites.

10:10 AM **Mon-RZVS-1010** Molten Salt Promoted Perovskite Oxide Redox Catalysts for Anaerobic Oxidative Dehydrogenation of Light Alkanes.  
**Leo Brody** and Fanxing Li, *North Carolina State University, USA*.

**Short Summary:**

We present acceptor-doped, redox-active perovskite oxides promoted with molten alkali metal salts for highly selective oxidative dehydrogenation of alkanes to olefins. With high olefin selectivity and yield, as well as favorable heat of reactions, the core-shell redox catalyst has excellent potential to be effective for intensified light alkane conversion.

10:30 AM **Mon-RZVS-1030** Chemical Looping Oxidative Dehydrogenation of Ethane: Elucidating the Role of Alkali Metal Salt Promoters to Suppress Overoxidation.

**Giancarlo Luongo**, Felix Donat and Christoph Müller, *ETH Zürich, Switzerland*.

**Short Summary:**

The molecular O<sub>2</sub> feed in the oxidative dehydrogenation (ODH) of ethane is replaced by oxygen storage materials that release in situ gaseous O<sub>2</sub> in a chemical looping scheme, without compromising the selectivity towards the desired product when suitable alkali metal salt coatings are applied.

10:50 AM **Mon-RZVS-1050** Pd-PdO Phase Transformation Under H<sub>2</sub>O<sub>2</sub> Environments and Its Consequences on the Selective Oxidation of Alkanes to Alkanols.

**Manasi Vyas**, Diego Gomez-Gualdron and Stephanie Kwon, *Colorado School of Mines, USA*.

**Short Summary:**

By combining experimental and theoretical methods, this work provides a mechanistic understanding of C-H activation routes by electrophilic oxygen species on Pd-PdO catalysts and demonstrates a potential route to directly oxidize propane with H<sub>2</sub>O<sub>2</sub> to form alkanol products using Pd at mild temperatures ( $\leq 433$  K).

11:10 AM **Mon-RZVS-1110** Chemical Looping Propane Oxidative Dehydrogenation Studies As an Alternative Route for Propylene Production.

**Caitlin Moffat**<sup>1</sup>, S. David Jackson<sup>1</sup>, Emma Gibson<sup>1</sup> and David Morgan<sup>2</sup>, (1)*University of Glasgow, United Kingdom*, (2)*Cardiff University, United Kingdom*.

**Short Summary:**

Vanadia catalysts were tested in chemical looping PODH studies. O<sub>2</sub>, N<sub>2</sub>O and CO<sub>2</sub> oxidants were utilised for the regeneration step to establish the effectiveness of softer oxidants. Our studies have displayed the potential for enhanced propylene yields by obtaining specific V<sup>5+</sup>/V<sup>4+</sup> ratios which may be crucial in overcoming selectivity limitations.

## MONDAY AFTERNOON

### Alkane Oxydehydrogenation II

**Session Chairs:** Krishna Janmanchi, *The Dow Chemical Company, USA* and Brian Weiss, *ExxonMobil Process Technology Company, USA*.

1:10 PM **Mon-RZVS-1310** Highly Selective Iron Oxide-Based Catalysts for on-Purpose Ethylene Production Via CO<sub>2</sub>-Assisted Ethane Dehydrogenation.

**Stavros-Alexandros Theofanidis**<sup>1</sup>, G. T. Kasun Kalhara Gunasooriya<sup>2</sup>, Ioanna Itskou<sup>1</sup>, Maria Tasioula<sup>1</sup> and Angeliki Lemonidou<sup>1</sup>, (1)*Aristotle University of Thessaloniki, Greece*, (2)*Technical University of Denmark, Denmark*.

**Short Summary:**

In this work, the on-purpose ethylene production via CO<sub>2</sub>-assisted oxidative dehydrogenation of ethane over iron oxide-based catalysts, supported on mixed oxides (NiO-MgO-ZrO<sub>2</sub>), was investigated. Experimental and theoretical methods were coupled to elucidate the nature of active sites affecting the selective and unselective reaction pathways.

1:30 PM **Mon-RZVS-1330** CexZr1-XO2 Supported CrOx Catalysts for CO<sub>2</sub>-Assisted Oxidative Dehydrogenation of Propane with Enhanced Selectivity and Stability.

**Jian Dou**, Joey Funderburg, Arnab Bose and Fanxing Li, *North Carolina State University, USA*.

**Short Summary:**

Ce doped, 5wt.%/Ce<sub>x</sub>Zr<sub>1-x</sub>O<sub>2</sub> catalysts demonstrated enhanced selectivity and stability for propylene production via CO<sub>2</sub>-ODH process. Comprehensive characterization coupled with designed catalytic experiments identified the active state of the Cr cation and elucidated coke formation as the cause for catalyst deactivation, providing insight for developing efficient CO<sub>2</sub>-ODH catalyst for olefin production.

1:50 PM **Mon-RZVS-1350** First Principles Analysis of Oxidative Dehydrogenation of Ethane on Iron Sulfide Catalysts Using Sulfur As a Soft Oxidant.

**Anik Biswas**<sup>1</sup>, Yinan Xu<sup>1</sup>, Xinrui Zhang<sup>2</sup>, Allison Arinaga<sup>2</sup>, Tobin J. Marks<sup>2</sup> and Jeffrey Greeley<sup>1</sup>, (1)*Davidson School of Chemical Engineering, Purdue University, USA*, (2)*Northwestern University, USA*.

**Short Summary:**

Iron sulfide catalysts can provide a high ethylene yield of 76% in sulfur-oxidative dehydrogenation of ethane (SODHE). C-H bond activation of ethane is the rate-determining step of SODHE reaction on the 001-S surface of FeS<sub>2</sub>, which is the energetically most favorable FeS<sub>2</sub> surface at high reaction temperatures (>800°C).

2:10 PM **Mon-RZVS-1410** Experimental and Theoretical Investigation of Siliceous Vanadium-Containing BEA Zeolites and Their Application in Odh of Light Alkanes.

Małgorzata Smoliło-Utrata<sup>1</sup>, Katarzyna Samson<sup>1</sup>, Małgorzata Ruggiero-Mikołajczyk<sup>1</sup>, Agnieszka Drzewiecka-Matuszek<sup>1</sup>, Jacek Gurgul<sup>1</sup>, **Dorota Rutkowska-Zbik**<sup>1</sup>, Laetitia Valentin<sup>2</sup>, Frederic Averseng<sup>2</sup>, Yannick Millot<sup>2</sup> and Stanislaw Dzwigaj<sup>2</sup>, (1)*Jerzy Haber Institute of Catalysis and Surface Chemistry PAS, Poland*, (2)*Sorbonne Université, France*.



### Short Summary:

Oxidative dehydrogenation (ODH) of light alkanes with V-based catalysts is a promising alternative to fill the gap between olefin demand and production. We show that pseudo-tetrahedral V species, formed in vanadium-containing siliceous BEA zeolites prepared by two-step post-synthesis method, are active centers of ODH of light alkanes into light alkenes.

2:30 PM **Mon-RZVS-1430** Mixed Metal Oxide Catalysts for Oxidative Dehydrogenation of Ethane to Ethylene.

Mozhdeh Parizad<sup>1</sup>, **John Meynard Tengco**<sup>1</sup>, Gregory Tate<sup>2</sup>, Weijian Diao<sup>3</sup> and John R. Monnier<sup>1</sup>, (1)University of South Carolina, USA, (2)University of California, Berkeley, USA, (3)Villanova University, USA.

### Short Summary:

MoVNbTeSbOx catalysts with high content of crystalline M1 phase were prepared having high activity and selectivity for ethane ODH, making ODH an economically viable route for ethylene production. Studying the formation of M1 phase in such metal oxides can help in further understanding catalyst structure-function relationship in the ODH process.

2:50 PM **Mon-RZVS-1450** Kinetic Studies of Selective Partial Oxidation of Ethane with Cu/CHA.

**Randall Meyer**<sup>1</sup>, Pedro Serna<sup>2</sup> and Takayuki Iida<sup>2</sup>, (1)Corporate Strategic Research, USA, (2)ExxonMobil Research and Engineering, USA.

### Short Summary:

Cu/CHA catalysts have been employed in the selective partial oxidation of ethane to ethylene via a cooperative effect of the Cu oxidation site and the acid site of the zeolite for dehydration of the presumed alcohol intermediate for ethylene production.

## Characterization of Complex Catalytic Materials and Systems

**Session Chairs:** Luis Bollman, Dow, and Long Qi, Ames Laboratory and Iowa State University, USA.

3:30 PM **Mon-RZVS-1530** X-Ray Diffraction Tomography and Deep Learning for Real-Time Characterisation of Catalytic Reactors and Electrochemical Energy Devices.

Hongyang Dong<sup>1</sup>, Keith Butler<sup>2</sup>, Dorota Matras<sup>3,4</sup>, Stephen Price<sup>5</sup>, Yaroslav Odarchenko<sup>5</sup>, Rahul Khatry<sup>6</sup>, Andrew Thompson<sup>6</sup>, Vesna Middelkoop<sup>7</sup>, Simon D. M. Jacques<sup>5</sup>, Andrew M. Beale<sup>1,8</sup> and **Antonios Vamvakeros**<sup>5</sup>, (1)University College London, United Kingdom, (2)Science and Technology Facilities Council, United Kingdom, (3)Diamond Light Source, United Kingdom, (4)The Faraday Institution, United Kingdom, (5)Finden Ltd, United Kingdom, (6)National Physical Laboratory, United Kingdom, (7)Vito NV, Boeretang 200, BE-2400 MOL, Belgium, Belgium, (8)UK Catalysis Hub, United Kingdom.

### Short Summary:

In this work, the development and application of cutting-edge applied deep learning approaches for chemical imaging and tomography methods are presented. An example is the PQ-Net neural network which analysed in 10s of seconds experimental X-ray diffraction computed tomography data (20,000 diffraction patterns) with accuracy equivalent to the Rietveld method.

3:50 PM **Mon-RZVS-1550** Fixed-Bed Reactor for Operando Structure-Activity Profiling.

Birte Wollak<sup>1</sup>, Raimund Horn<sup>1,2</sup>, Ann-Christin Dippel<sup>3</sup>, Marina Sturm<sup>3</sup>, Diego Espinoza<sup>1</sup>, Olof Gutowski<sup>3</sup>, Thomas L. Sheppard<sup>2,4</sup>, Dmitry Doronkin<sup>4</sup>, **Oliver Korup**<sup>1,2</sup> and Michael Schmidt<sup>2</sup>, (1)Hamburg University of Technology, Germany, (2)Reacnostics GmbH, Germany, (3)Deutsches Elektronen-Synchrotron DESY, Germany, (4)Karlsruhe Institute of Technology (KIT), Germany.

### Short Summary:

Appropriate operando measurements in heterogeneous catalysis are essential to reveal complex structure-activity relationships of catalysts at work. Here a combined methodological approach for simultaneous spatially-resolved gas composition, temperature and synchrotron x-ray absorption or diffraction measurements is shown using a catalytic profile reactor under industrially-relevant and kinetically well-defined reaction conditions.

4:10 PM **Mon-RZVS-1610** The Role of Melting in SiO<sub>2</sub>-Supported AVox-Catalysts (A: Li, Na, K, Rb, and Cs) for Propane Oxidation.

**Ezgi Erdem**<sup>1,2</sup>, Pierre Kube<sup>1</sup>, Andrey Tarasov<sup>1</sup>, Yuanqing Wang<sup>1</sup>, Spencer J. Carey<sup>1</sup>, Michael Hävecker<sup>1,3</sup>, Frank Rosowski<sup>2,4</sup>, Robert Schlögl<sup>1,3</sup> and Annette Trunschke<sup>1</sup>, (1)Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany, (2)Technische Universität Berlin, Germany, (3)Max Planck Institute for Chemical Energy Conversion, Germany, (4)BASF SE, Germany.

### Short Summary:

The doping of silica supported vanadium oxide with alkali causes partial or complete melting of the surface layer. The impact of melting on the performance in propane oxidation is studied and the surface dynamics are analyzed by a combination of operando techniques.

4:30 PM **Mon-RZVS-1630** Probing the Electronic, Atomic and Nanoscale Structure of Ni-Ga/SiO<sub>2</sub> Catalysts for CO<sub>2</sub> Hydrogenation to Methanol Via Operando X-Ray Absorption Spectroscopy and X-Ray Total Scattering.

**Nora Zimmerli**, Paula Macarena Abdala and Christoph Müller, ETH Zürich, Switzerland.

### Short Summary:

Here, we present a detailed structure-performance analysis of Ni-Ga/SiO<sub>2</sub> catalysts under CO<sub>2</sub> hydrogenation conditions using operando X-ray absorption spectroscopy and X-ray total scattering. The use of these complementary techniques is key to characterize the structure of the active phases in the Ni-Ga system across the electronic, atomic and nanoscale.

4:50 PM **Mon-RZVS-1650** Zeolite Encapsulated Molybdenum Sulfide Clusters Mimicking the Nitrogenase Enzyme's Active Site.

**Roland Weindl**<sup>1</sup>, Rachit Khare<sup>1</sup>, Hui Shi<sup>1,2</sup> and Johannes A. Lercher<sup>1,3</sup>, (1)Technical University of Munich, Germany, (2)Yangzhou University, China, (3)Pacific Northwest National Laboratory, USA.

### Short Summary:

Transition metal sulfides (TMS) are workhorse catalysts in the refining of crude oil and are gaining major importance as replacement for noble metals in electrocatalysis. We have synthesized TMS clusters resembling the nitrogenase enzyme's active site in structure and reactivity. Our

findings provide an intriguing path towards bio-inspired hydrogenation catalysis.

5:10 PM **Mon-RZVS-1710** Synergistic Interfaces in Metal-Metal Oxide Inverted Systems for Catalytic Upgrading.

**Laura Paz Herrera**<sup>1</sup>, Lucas Freitas De Lima E Freitas<sup>2</sup>, Eranda Nikolla<sup>2</sup> and J. Will Medlin<sup>3</sup>, (1)University of Colorado Boulder, USA, (2)Wayne State University, USA, (3)University of Colorado at Boulder, USA.

**Short Summary:**

This investigation is aimed at characterizing and understanding metal-metal oxide bifunctional interfaces in inverted Pd@MO<sub>2</sub> (M = Ti, Ce, Zr) catalytic structures. Systematic variations of synthesis and reactivity parameters for CO oxidation were probed. Inverted catalytic systems displayed higher activity than supported structures, with Pd@ZrO<sub>2</sub> as the best performing catalyst.

## Sutton North

### MONDAY MORNING

#### Catalytic Conversion of Plastics I

**Session Chairs:** James Dorman, Louisiana State University, USA and Ana R. C. Morais, University of Kansas, USA.

9:30 AM **Mon-SUNO-0930** Selective Conversion of Polyolefin Waste to Liquid Hydrocarbons Via Hydrocracking over Bifunctional Ru/Acid Catalysts.

**Julie Rorrer**<sup>1</sup>, Amani Ebrahim<sup>2</sup>, Ydna Questell-Santiago<sup>1</sup>, Clara Troyano-Valls<sup>1</sup>, Arun Asundi<sup>2</sup>, Gregg T. Beckham<sup>3</sup>, Simon Bare<sup>2</sup> and Yuriy Roman<sup>1</sup>, (1)Massachusetts Institute of Technology, USA, (2)SLAC National Accelerator Laboratory, USA, (3)National Renewable Energy Laboratory, USA.

**Short Summary:**

The depolymerization of polyolefins via hydrogenolysis over Ru-based catalysts has emerged as a promising method of upcycling waste plastics to produce liquid alkanes. In this study, we utilized bifunctional Ru/acid catalysts to improve selectivity and activity for polyethylene and polypropylene depolymerization by promoting a hydrocracking mechanism, suppressing methane formation.

9:50 AM **Mon-SUNO-0950** Operando Micro-Spectroscopy Reveals the Important Role of a Hydrocarbon Pool for Polyolefin Conversion.

**Ina Vollmer**, Michael Jenks, Florian Meirer and Bert M. Weckhuysen, Utrecht University, Netherlands.

**Short Summary:**

Obtaining aromatics via catalytic conversion of polyolefins could boost recycling rates. A discarded refinery catalyst forms less deactivating species than the fresh catalyst, while yielding 20 wt.% aromatics. Here, we study the underlying reaction mechanism with *operando* micro-spectroscopy to reveal the importance of a pool of active intermediates.

10:10 AM **KEYNOTE Mon-SUNO-1010 Catalytic Plastics Upcycling Technologies for a Circular Economy.** Dionisios G. Vlachos, University of Delaware, USA; University of Delaware, USA.

**Short Summary:**

We will discuss the role of catalysis in circular economy and specifically on plastics recycling and upcycling.

10:50 AM **Mon-SUNO-1050** Catalytic Conversion of Model Plastic Pyrolysis Oil to Olefins and Aromatics over ZSM-5.

**Houqian Li**<sup>1</sup>, Son Dong<sup>1</sup>, Ivo Hermans<sup>2</sup> and George Huber<sup>1</sup>, (1)University of Wisconsin-Madison, USA, (2)University of Wisconsin-Madison, USA.

**Short Summary:**

We reported a study elucidating the fundamental chemistry in the catalytic upgrading of plastic pyrolysis oil. Model compound for plastic pyrolysis oil was evaluated by zeolites and the reaction mechanism was proposed based on the kinetic measurements.

11:10 AM **Mon-SUNO-1110** Design of Sequential Catalytic Solvolysis Process for Selectively Deconstructing Waste Plastics.

**Hongfei Lin**, Washington State University, USA.

**Short Summary:**

The grand challenge of recycling waste plastics is the heterogeneity of comingled plastic wastes, containing various incompatible polymers. We will discuss the sequential catalytic solvolysis processes that convert various plastics in a plastic mixture, such as polyesters, polyamides, and polyolefins, to value-added products such as monomers or hydrocarbon fuels.

11:30 AM **Mon-SUNO-1130** Incentivizing the Upcycling of Waste PVC By Tandem Hydrothermal Dechlorination and Catalytic Hydrogenation.

**Scott Svadlenak** and Konstantinos Goulas, Oregon State University, USA.

**Short Summary:**

Simultaneous hydrothermal dechlorination and catalytic hydrogenation of PVC plastic at mild temperatures with traditional hydrogenation catalysts can produce an HDPE type resin. The treated plastic product displays melt behavior consistent with polyethylene illuminating a possible new chemical upcycling pathway for PVC waste management.

## MONDAY AFTERNOON

### Lignin I: Fundamentals

**Session Chairs:** Patrisha Bugayong, *Benedictine College, USA* and Eric Sacia, *AbbVie, USA*.

1:10 PM **Mon-SUNO-1310** Quantitative Analysis of Solvent Effects in Liquid-Phase Aryl Ether Hydrogenolysis and Phenol Hydrogenation.

Ali Chamas<sup>1</sup>, Jason A. Chalmers<sup>1</sup>, Long Qi<sup>1,2</sup> and **Susannah L. Scott<sup>1</sup>**, (1)*University of California, Santa Barbara, USA*, (2)*USDOE Ames Laboratory, USA*.

**Short Summary:**

In reductive lignin depolymerization, the rate of phenolic hydrogenation varies by two orders of magnitude and is correlated with adsorption on the catalyst. Using *operando* <sup>13</sup>C MAS-NMR spectroscopy, the rates of aryl ether hydrogenolysis and subsequent phenol hydrogenation were quantified in a wide range of protic and aprotic solvents.

1:30 PM **Mon-SUNO-1330** Lignin Chemistry and Valorization Based on Structural Insights.

**Steffan Green<sup>1</sup>**, Brandon Kinn<sup>1</sup>, Thomas Binder<sup>1</sup>, Erik Hagberg<sup>2</sup> and Bala Subramaniam<sup>1</sup>, (1)*The University of Kansas, USA*, (2)*Archer Daniels Midland Company, USA*.

**Short Summary:**

Strategies to valorize lignin often fail to progress into commercial applications. Using structural insights, we delineate the features of lignin from corn residues in the rational design of a realizable corn-based biorefinery. We report a holistic approach for the scalable extraction and valorization of lignin from corn residues.

1:50 PM **Mon-SUNO-1350** *In-Situ* Characterization of Depolymerization over Heterogeneous Catalysts.

**Marcus Foston**, *Washington University in St. Louis, USA*.

**Short Summary:**

*In-situ* small angle neutron scattering (SANS) was used on lignin samples to probe their polymer coil size and conformational changes that occur at reaction conditions and upon interaction with copper-doped porous metal oxide catalyst.

2:10 PM **Mon-SUNO-1410** Beware of Diffusion Limitations in Catalytic Biomass Conversion: Mesoscale Reaction-Diffusion Phenomena Governing Lignin-First Biomass Fractionation.

**Nicholas E. Thornburg<sup>1</sup>**, M. Brennan Pecha<sup>1</sup>, David G. Brandner<sup>1</sup>, Michelle L. Reed<sup>1</sup>, Josh V. Vermaas<sup>1</sup>, William E. Michener<sup>1</sup>, Rui Katahira<sup>1</sup>, Todd B. Vinzant<sup>1</sup>, Thomas D. Foust<sup>1</sup>, Bryon S. Donohoe<sup>1</sup>, Yuriy Roman<sup>2</sup>, Peter N. Ciesielski<sup>1</sup> and Gregg T. Beckham<sup>1</sup>, (1)*National Renewable Energy Laboratory, USA*, (2)*Massachusetts Institute of Technology, USA*.

**Short Summary:**

**Consequences of confinement:** Biomass conversion is central to the renewable production of important chemicals and fuels. A new, feedstock-centric mesoscale modeling framework informs condensed-phase fractionation strategies by decoupling underlying reaction kinetics from mass and heat transport, elucidating the consequences of biomass pore and particle size on observable laboratory catalyst measurements.

2:30 PM **Mon-SUNO-1430** Deoxygenation Mechanism of Phenol over Ru(0001) Surface.

**Haider Ejaz** and Fuat E. Celik, *Rutgers, The State University of New Jersey, USA*.

**Short Summary:**

Phenol hydrodeoxygenation was studied over Ru(0001) surface and the mechanism for production of a variety of products was investigated. Dispersion forces were considered and a tautomerization pathway was found to be the best one. Hydrogenation was found to increase the feasibility of deoxygenation and production of cyclic hydrocarbons.

2:50 PM **Mon-SUNO-1450** Magnetic Core-Shell Catalyst for the Microwave-Assisted Reductive Depolymerization of Lignin.

**Elisa Acciardo<sup>1</sup>**, Silvia Tabasso<sup>2</sup>, Maela Manzoli<sup>2</sup> and Samir Bensaid<sup>1</sup>, (1)*Politecnico di Torino, Italy*, (2)*University of Turin, Italy*.

**Short Summary:**

A facile method was investigated to synthesize a magnetic catalyst, consisting in a hierarchical structure based on Fe<sub>3</sub>O<sub>4</sub> coated with alumina and impregnated with palladium. Catalytic tests for the reductive depolymerization of a lignin representative compound have proven that Pd/Fe<sub>3</sub>O<sub>4</sub>@Al<sub>2</sub>O<sub>3</sub> is a promising catalyst for the valorization of renewable resources.

### Furans

**Session Chairs:** Basudeb Saha, *University of Delaware, USA*; Rikarbon, *USA* and Joshua Terrian, *Archer Daniels Midland, .*

3:30 PM **Mon-SUNO-1530** Surface Mechanisms for Furfural Electrooxidation to Value-Added Chemicals Probed By ATR-Seiras.

**Joseph Hasse<sup>1,2</sup>**, Todd Whittaker<sup>1,2</sup> and Adam Holewinski<sup>1,2</sup>, (1)*University of Colorado Boulder, USA*, (2)*Renewable and Sustainable Energy Institute, USA*.

**Short Summary:**

The furfural oxidation reaction was studied using attenuated total reflectance surface enhanced infrared absorption spectroscopy (ATR-SEIRAS), accompanied by modulation excitation spectroscopy (MES), to investigate dominant surface moieties over a wide spectral and potential range in a variety of materials. Down pathway products, identified in high conversion electrolyses, were also investigated.

3:50 PM **Mon-SUNO-1550** Mechanistic Study of Furfural Electrochemical Hydrogenation and Hydrogenolysis over Cu Catalyst in Sulfuric Acid. Steven M. Watt<sup>1,2</sup>, Andrew S. May<sup>2</sup> and **Elizabeth J. Biddinger**<sup>1,2</sup>, (1)*The Graduate Center of the City University of New York, USA*, (2)*City College of New York, CUNY, USA*.

**Short Summary:**

The mechanism of furfural electrochemical hydrogenation and hydrogenolysis in acidic electrolytes on copper was studied by measuring the initial rate of product formation during potentiostatic bulk electrolysis. A non-competitive Langmuir-Hinshelwood type mechanism was determined with the hydrogenation product and hydrogenolysis product produced in separate, parallel reactions.

4:10 PM **Mon-SUNO-1610** Aqueous Phase Furfural Hydrogenation Using Dilute Limit Alloy Bimetallic Catalysts.

**Leandro De Castro**<sup>1,2</sup>, Christopher T. Williams<sup>2</sup> and John R. Regalbuto<sup>2</sup>, (1)*University of the Philippines Los Baños, Philippines*, (2)*University of South Carolina, USA*.

**Short Summary:**

To our knowledge, this is the first report on the use of single atom alloy-based catalysts in aqueous phase hydrogenation reaction. Single atom alloys of platinum, palladium and ruthenium show improved precious metal usage efficiency as compared with nanoparticle counterparts

4:30 PM **Mon-SUNO-1630** On-Line FTIR-MS Gas Phase Analysis of 2,5-Dimethylfuran Valorization over Zeolites.

**Christopher Sauer**<sup>1</sup>, Anders Lorén<sup>2</sup>, Andreas Schaefer<sup>1</sup> and Per-Anders Carlsson<sup>1</sup>, (1)*Chalmers University of Technology, Sweden*, (2)*RISE Research Institutes of Sweden, Sweden*.

**Short Summary:**

The catalytic conversion of biomass-derived 2,5-dimethylfuran over zeolites was followed by time-resolved on-line analysis. Mostly olefins and BTX aromatics are formed in the beginning, and their formation is linked. With increasing time on stream and deactivation of certain active sites, the product distribution shifts towards isomers of 2,5-dimethylfuran.

4:50 PM **Mon-SUNO-1650** Metal Functionalized Graphene Oxide Hybrid Catalysts for the Microwave Assisted Catalytic Synthesis of HMF.

Yui Hirano<sup>1</sup>, Shinya Hayami<sup>2</sup> and **Jorge Beltramini**<sup>2</sup>, (1)*Kumamoto University, Japan*, (2)*Queensland University of Technology, Australia*.

**Short Summary:**

In this study, we focused on the use of graphene oxide (GO) as catalyst support. Here, we demonstrate the effectiveness of a GO/metal oxide nanoparticle hybrid catalyst in transforming carbohydrates to HMF starting with glucose as a model compound.

5:10 PM **Mon-SUNO-1710** Production of Biorefinery Products in the Hydrogenation of Furfural Using a Bimetallic Catalyst of Pd and Fe Synthesized By of Gobernadora (*Larrea tridentate*) Extract.

**Javier Rivera de la Rosa**<sup>1</sup>, Carlos Lucio Ortiz<sup>1</sup>, Diego Alexander González Casamachin<sup>1</sup>, Bárbara Jazmín Lino Galarza<sup>1</sup> and Ladislao Sandoval-Rangel<sup>2</sup>, (1)*Universidad Autónoma de Nuevo León, Mexico*, (2)*Tecnológico de Monterrey, Mexico*.

**Short Summary:**

In this work, hydrogenation of furfural to produce open-ring compounds, which can be considered biorefinery products, is presented using a new real bimetallic catalyst of Pd and Fe synthesized using Gobernadora (*Larrea tridentate*) extract from the northwestern region of Mexico as a reducing agent.

## Sutton South

### MONDAY MORNING

#### Electro and Photo Catalysis

**Session Chairs:** Michal Bajdich, *SLAC National Accelerator Laboratory, USA* and Fanglin Che, *University of Massachusetts Lowell, USA*.

9:30 AM **KEYNOTE Mon-SUSO-0930 Sustaining the Planet Via (Photo)(Electro)Catalysis, from First Principles.** **Emily Carter**, *Princeton University, USA*.

**Short Summary:**

Insights into (photo)(electro)catalysis by a diverse set of materials (transition metal oxyhydroxides, functionalized semiconductor and metal electrodes, metal nanoparticles, cation-substituted perovskites) will be presented to create a virtuous cycle of artificial (photo)synthesis, exploiting energy from sunlight or other renewable sources, water, air, and carbon dioxide to synthesize fuels and chemicals.

10:10 AM **Mon-SUSO-1010** First-Principles Informed Microkinetic Modeling of Electrocatalytic Reactions on Graphene-Based Single-Atom Catalysts.

**Michael Rebarchik**, Saurabh Bhandari, Thomas Kropp and Manos Mavrikakis, *University of Wisconsin-Madison, USA*.

**Short Summary:**

A potential-dependent microkinetic model was developed to evaluate the electrocatalytic performance of graphene-based single-atom catalysts towards the oxygen reduction and evolution reactions. Our findings highlight the importance of considering kinetics, coverage effects, and reaction conditions when evaluating electrochemical activity and suggest that co-adsorbed species are important determinants of catalytic performance.

10:30 AM **Mon-SUSO-1030** The Role of Roughening to Enhance Selectivity to C<sub>2</sub>+ Products during CO<sub>2</sub> Electroreduction on Copper.  
**Joakim Halldin Stenlid**<sup>1,2</sup>, Joseph Gauthier<sup>3</sup>, Alexis T. Bell<sup>3</sup>, Martin Head-Gordon<sup>4</sup> and Frank Abild-Pedersen<sup>1</sup>, (1)SLAC National Accelerator Laboratory, USA, (2)Stanford University, USA, (3)University of California, Berkeley, USA, (4)Lawrence Berkeley National Laboratory, USA.

**Short Summary:**

Elucidating atomic scale origin of enhancing effect of surface roughening on C<sub>2</sub> selectivity in electroreduction of CO<sub>2</sub>

10:50 AM **Mon-SUSO-1050** Theoretical Studies of Electrochemical Proton-Coupled Electron Transfer.

**Robert Warburton**, Phillips Hutchison, William Lake, Alexander Soudackov and Sharon Hammes-Schiffer, *Yale University, USA*.

**Short Summary:**

The impact of interfacial electric fields on electrochemical PCET is investigated using DFT calculations. PCET mechanisms are studied using vibrational Stark shift probes and graphite-conjugated molecular catalysts to understand constant-potential PCET thermodynamics.

11:10 AM **Mon-SUSO-1110** Modelling Potential-Dependent Electrochemical Activation Barriers - Revisiting the Alkaline Hydrogen Evolution Reaction.

**Frank Abild-Pedersen**<sup>1</sup>, Jiang Li<sup>1,2</sup>, Joakim Halldin Stenlid<sup>2</sup>, Thomas Ludwig<sup>1,2</sup> and Philomena Lamoureux<sup>1,2</sup>, (1)SLAC National Accelerator Laboratory, USA, (2)Stanford University, USA.

**Short Summary:**

We have simulated the kinetics of HER on Pt surfaces under alkaline condition and explicitly included treatment of statistical fluctuations of the solvent. Our results reproduce the trend in experimental data. We identify that the distribution of the electrode-water distance has a large effect on the transfer barriers.

11:30 AM **Mon-SUSO-1130** Oxides Supported Transition Metal Single Atoms for Oxygen Electrocatalysis.

**G. T. Kasun Kalhara Gunasooriya** and Jens K. Nørskov, *Technical University of Denmark, Denmark*.

**Short Summary:**

In this work, oxides supported transition metal single-atom catalysts (SACs) for oxygen electrocatalysis was investigated. The stability and activity of SACs were carefully studied and machine learning models were used to identify descriptors and to predict adsorption energies. Based on these theoretical findings, rational catalyst design principles are established.

## MONDAY AFTERNOON

### Machine Learning in Catalysis: Approaches I

**Session Chairs:** Siddharth Deshpande, *University of Delaware, USA* and Hongliang Xin, *Virginia Polytechnic Institute and State University, USA*.

1:10 PM **Mon-SUSO-1310** Graph Based Methods for Atomistic Modeling of Heterogeneous Catalysts.

**Siddharth Deshpande**, Pushkar Ghanekar and Jeffrey Greeley, *Purdue University, USA*.

**Short Summary:**

Accurately modeling heterogeneous catalytic systems requires accounting for characteristics such as defect morphologies, and adsorbate-adsorbate interactions, amongst others. This work presents a graph-theory based workflow to systematically overcome these challenges. Utilization of packages, Surfgraphs and ACE-GCN, is demonstrated to identify complex catalytic morphologies by systemic enumeration and screening procedures.

1:30 PM **Mon-SUSO-1330** Open Catalyst Project: Advancements in Building a Universal Machine Learning Potential.

**Muhammed Shuaibi** and Zachary Ulissi, *Carnegie Mellon University, USA*.

**Short Summary:**

The Open Catalyst Project aims to develop new ML methods and models to accelerate the catalyst simulation process for renewable energy technologies. In this talk we present some of the latest advancements made towards building a universal machine learning potential.

1:50 PM **Mon-SUSO-1350** Reduce, Reuse, Recycle: Data Benchmarking and Accessibility for Faster Research with the Catalyst Property Database.

**Kurt Van Allsburg**, Qiyuan Wu, Sean Tacey and Carrie Farberow, *National Renewable Energy Laboratory, USA*.

**Short Summary:**

When data—such as computed reaction energetics—is used in catalyst design, it is almost always generated by researchers themselves, even if similar data has been published previously. The [Catalyst Property Database](#) (CPD) seeks to reduce this duplication of effort by creating a centralized, searchable database of quality catalyst property data.

2:10 PM **Mon-SUSO-1410** Predicting Energetics of Entire Reaction Pathways Via Machine Learning.

Sarah Stratton, Chukwudi Nwaokorie, Gbolade Kayode and **Matthew Montemore**, *Tulane University, USA*.

**Short Summary:**

Because the descriptor-based screening approach makes assumptions that do not always hold, we developed a machine-learning model for predicting the energetics of entire reaction pathways. This allows more sophisticated screening and kinetic analysis. We applied this model to screen 11,000 alloys for methane steam reforming.

2:30 PM **Mon-SUSO-1430** A Computational Workflow for Intermetallic Catalyst Discovery.

**Angela Nguyen**<sup>1</sup>, Unnatti Sharma<sup>2</sup>, Rushi Gong<sup>1</sup>, Griffin Canning<sup>1</sup>, Shunli Shang<sup>1</sup>, Robert Rioux<sup>1</sup>, Zi-Kui Liu<sup>1</sup>, Zachary Ulissi<sup>2</sup> and Michael Janik<sup>1</sup>, (1) *The Pennsylvania State University, USA*, (2) *Carnegie Mellon University, USA*.

**Short Summary:**

Intermetallic compounds have precise local atomic composition and structure, and the arrangement of multiple metals in an active site can be systematically manipulated. We integrate a series of computational tools, together with experiment, to determine intermetallic compositions that expose precisely structured active sites to catalyze selective hydrogenation reactions.



2:50 PM **Mon-SUSO-1450** Bridging the Gap between Simple and Complex Surfaces: A Combined DFT and Transfer Learning-Driven Workflow to Determine Stability of Complex Alloy Catalysts.

**Gaurav Deshmukh**<sup>1</sup>, Pushkar Ghanekar<sup>1</sup> and Jeffrey Greeley<sup>2</sup>, (1)*Purdue University, USA*, (2)*Davidson School of Chemical Engineering, Purdue University, USA*.

**Short Summary:**

A combined DFT and transfer learning-based workflow is utilized to rigorously study segregation of Pt on the (211) stepped facet of Pt<sub>3</sub>Ni. Surface phase diagrams reveal a relationship between Pt-skin stability and the surface coordination environment. This workflow is further extended to study electrochemical stability of high-entropy alloys.

## Machine Learning in Catalysis: Approaches II

**Session Chairs:** Sean Tacey, *National Renewable Energy Laboratory, USA* and Robert Warburton, *Yale University, USA*.

3:30 PM **Mon-SUSO-1530** WhereWulff: An Automated and Democratized Framework for High-Throughput Computational Chemistry.

**Javier Heras Domingo**, Rohan Sanspeur and Zachary Ulissi, *Carnegie Mellon University, USA*.

**Short Summary:**

Despite excitement around ML for catalyst discovery, machine learning models are only as good as the data they are trained on. Through an automated workflow called "WhereWulff", this work sets the stage for high-quality oxide surface chemistry data origination that will feed future predictive efforts to screen for OER catalysts.

3:50 PM **Mon-SUSO-1550** A Generalizable Closed-Loop Framework for Accelerated Discovery of Electrochemical Nitrogen Reduction Catalysts.

**Lance Kavalsky**<sup>1</sup>, Vinay I. Hegde<sup>2</sup>, Eric Muckley<sup>2</sup>, Lydia M. Tsvierioti<sup>1</sup> and Venkatasubramanian Viswanathan<sup>1</sup>, (1)*Carnegie Mellon University, USA*, (2)*Citrine Informatics, USA*.

**Short Summary:**

We showcase a generalizable computational closed-loop framework applied towards identification of single-atom alloy candidate electrocatalysts for ammonia synthesis. The design-space is explored via a sequential learning approach, with an acquisition function that incorporates cost and stability metrics. We will highlight promising candidates found using this framework.

4:10 PM **Mon-SUSO-1610** Accelerating Geometric Optimizations By Finetuning Open Catalyst Project Models with Active Learning.

**Joseph Musielewicz** and Zachary Ulissi, *Carnegie Mellon University, USA*.

**Short Summary:**

Active learning enables the acceleration of density functional theory (DFT) geometric optimizations for catalyst screening. Graph neural networks (GNNs) pretrained on the Open Catalyst 2020 dataset provide a cheap, but sophisticated, representation of the physics underlying DFT. Geometric optimizations can be further accelerated by finetuning these GNNs using active learning.

4:30 PM **Mon-SUSO-1630** Simultaneously Accounting for Compositional and Structural Variations in High Entropy Alloy Catalysts Using Neural Network.

**Zhuole Lu**, Zhi Wen Chen and Chandra Veer Singh, *University of Toronto, Canada*.

**Short Summary:**

A robust neural network model has been developed to predict for adsorption energy on high-entropy alloy catalysts, taking into account both compositional and structural variations. The trained model is highly accurate (mean absolute error of 0.094 eV) and provided atomistic insights for site-specific catalytic properties.

4:50 PM **Mon-SUSO-1650** Addressing the Complexity of AI Distributions Using Multiscale Atomic Zeolite Simulation Environment (MAZE).

**Jiawei Guo** and Ambarish Kulkarni, *University of California, Davis, USA*.

**Short Summary:**

Multiscale Atomistic Zeolite Simulation Environment (MAZE) is a new zeolite-focused software toolkit that facilitates high-throughput calculations and machine learning model development by greatly simplifying and standardizing multistep workflows.

5:10 PM **Mon-SUSO-1710** A Local Solution for Automated Data Acquisition and Storage in Catalysis.

Abdulrhman Moshantaf, Michael Wesemann, Patrick Oppermann, Heinz Junkes, Robert Schlögl and **Annette Trunschke**, *Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany*.

**Short Summary:**

Ensuring reproducible and scalable synthesis and reliable kinetic analysis in catalysis research requires standardization of experiments. We present here a system for automated data acquisition and storage based on handbooks using EPICS for experiment control and a database (archive) for data storage and transfer.

## Trianon Ballroom

### MONDAY MORNING

#### NOx Abatement and Three Way Catalysis I

**Session Chairs:** Bryan Goldsmith, *University of Michigan-Ann Arbor, USA* and Tae Jin Kim, *Stony Brook University, USA*.

9:30 AM **Mon-TRBR-0930** *Operando* XAS Characterization of  $\text{Cu}_x\text{Co}_{3-x}\text{O}_4$  Direct NOx Decomposition Catalysts during Transient Product Formation. **Jiyun Hong**<sup>1</sup>, Torin C. Peck<sup>2</sup>, Simon Bare<sup>1</sup> and Charles A. Roberts<sup>2</sup>, (1)*SLAC National Accelerator Laboratory, USA*, (2)*Toyota Research Institute - North America, USA*.

**Short Summary:**

*Operando* X-ray absorption spectroscopy (XAS) has been performed on  $\text{Cu}_x\text{Co}_{3-x}\text{O}_4$  catalysts under NO decomposition reaction conditions with simultaneous product detection via mass spectrometry. Analyzing the XAS data of transient and steady-state portions of the reaction step will identify the structure that is related to the undesired  $\text{NO}_2$  formation.

9:50 AM **Mon-TRBR-0950** Stoichiometric Natural Gas Engine Three-Way Catalyst Robustness to Fuel Sulfur.

**Mi-Young Kim**, Jian Gong, Krishna Kamasamudram, Michael Cunningham and Aleksey Yezerets, *Cummins Inc., USA*.

**Short Summary:**

This study demonstrates the impact of sulfur on NG TWC's overall performance with the help of the 4-mode test protocol. The insights on fuel sulfur robustness of TWC can facilitate designing the sulfur tolerant TWC and attaining the optimal desulfation strategies in CH<sub>4</sub> emission control on stoichiometric natural gas engines.

10:10 AM **Mon-TRBR-1010** NO Reduction By CO over NiO<sub>x</sub>/CeO<sub>2</sub> Catalysts: Effect of Synthesis Conditions (oxidation and reduction).

**Kyung-Min Lee** and Tae Jin Kim, *Stony Brook University, USA*.

**Short Summary:**

This work is mainly focused on investigation of the impact of catalyst synthesis conditions (e.g., oxidation and reduction) on the physicochemical properties of NiO<sub>x</sub>/CeO<sub>2</sub> catalyst and the catalytic response for NO reduction by CO reaction.

10:30 AM **Mon-TRBR-1030** Impact of Atmosphere on Precious Metal Sintering and Importance of Vapor Phase Carriers.

**Andrew (Bean) Getsoian**, *Ford Motor Company, USA*.

**Short Summary:**

Precious metal sintering during catalyst aging is a major driver of cost for automotive catalysts. This work uses computational thermodynamics to assess the stabilities of potential carrier molecules such as PdCO and Pd(OH)<sub>2</sub> that may form under catalyst aging conditions, and shows how such species facilitate Ostwald ripening.

10:50 AM **KEYNOTE Mon-TRBR-1050 Thermally Stable Single Atom Catalysts.** **Yong Wang**, *Pacific Northwest National Laboratory, USA; Washington State University, USA*.

**Short Summary:**

We discuss our recent advances in the study of thermally-durable single atom catalysts prepared by atom trapping, and the fundamental principles to activate such single-atom-catalysts. We further discuss thermally stable SACs for CO oxidation, unburnt hydrocarbon (HC) oxidation, and NOx reduction.

11:30 AM **Mon-TRBR-1130** Industrial Challenges for Gasoline TWC Cold Start: Developing Pd/CeO<sub>2</sub> Systems.

**Tamsin Bell**, Kerry Simmance, Nicola Collis, Amy Kolpin and David Thompsett, *Johnson Matthey Technology Centre, United Kingdom*.

**Short Summary:**

This work addresses key industrial issues of gasoline cold start: inhibition chemistry and thermal durability. Herein, we report Pd/CeO<sub>2</sub> with fresh ambient activity and superior aged activity compared to Pd/Al<sub>2</sub>O<sub>3</sub>. Testing catalysts in relevant full gas mixtures and harsh ageing is critical to understand the limitations of these catalytic systems.

### MONDAY AFTERNOON

#### NOx Abatement and Three Way Catalysis II

**Session Chairs:** Mi-Young Kim, *Cummins Inc., USA* and Eleni A. Kyriakidou, *University at Buffalo (SUNY), USA*.

1:30 PM **Mon-TRBR-1330** Spatiotemporal Resolution of NO Profiles over a NOx Storage Catalyst By PLIF.

**Sui Wan**, Kevin Keller, Patrick Lott, Thomas Häber, Rainer Suntz and Olaf Deutschmann, *Karlsruhe Institute of Technology (KIT), Germany*.

**Short Summary:**

The 2D spatially and temporally resolved absolute NO concentration profiles over a NOx storage catalyst are obtained with quenching corrected phase-locked PLIF. With a detailed reaction mechanism, the simulations capture the NO evolution over the Pt/BaO/Al<sub>2</sub>O<sub>3</sub> catalyst and give detailed insight into reaction dynamics.

1:50 PM **Mon-TRBR-1350** Direct NO Decomposition of Rh Supported Metal Oxide Catalyst: Deactivation and Regeneration Strategy.

**Wo Bin Bae**<sup>1</sup>, Do Yeong Kim<sup>1</sup>, Minkyu Kim<sup>2</sup> and Sung Bong Kang<sup>1</sup>, (1)*Gwangju Institute of Science and Technology, Korea, Republic of (South)*, (2)*Yeungnam University, Korea, Republic of (South)*.

**Short Summary:**

Our results showed that the dissociated oxygen triggers the catalyst deactivation for the direct NO decomposition (DND) reaction. The intermittent CO dosing to the catalyst could resolve the self-poisoning of dissociated oxygen on the active sites of the Rh/PrO<sub>2</sub>. This study will provide a useful insight of the DND catalyst.

2:10 PM **Mon-TRBR-1410** Dynamics of Ceria-Zirconia Redox: Kinetics, Thermodynamics, and Transport.

**Andrew Hwang**<sup>1</sup>, Andrew (Bean) Getsoian<sup>2</sup>, Jason Wu<sup>2</sup> and Enrique Iglesia<sup>1</sup>, (1)University of California, Berkeley, USA, (2)Ford Motor Company, USA.

**Short Summary:**

We examine the kinetics, thermodynamics, and transport phenomena involved in reduction and oxidation of ceria-zirconia solid solutions (CZO) and CZO-supported Pt nanoparticles.

2:30 PM **Mon-TRBR-1430** Multifunctional Catalyst Evaluations and Comparisons for the Simultaneous Reduction of CO, NOx and Hydrocarbon Emissions.

**Todd J. Toops** and Pranaw Kunal, Oak Ridge National Laboratory, USA.

**Short Summary:**

We investigate a wide range of multi-component catalyst systems containing HCTs, PNAs, and DOCs using an emissions merit function. This identified that a 1:1:4 ratio of PNA:HCT:DOC was the most effective emissions reduction configuration and had similar reactivity as a physical mixture or as a PNA-HCT-DOC multi-bed reactor.

2:50 PM **Mon-TRBR-1450** Pd and Rh Three-Way Catalysts and Their Distinct Responses to Lean-Rich Cycling Aging.

**Yuntao Gu**<sup>1</sup>, Wei Li<sup>1</sup>, Fudong Liu<sup>2</sup>, Xiaolai Zheng<sup>3</sup>, Yuejin Li<sup>3</sup>, Nicholas Nelson<sup>4</sup>, Kenneth Rappe<sup>4</sup> and William Epling<sup>5</sup>, (1)General Motors Global R&D, USA, (2)University of Central Florida, USA, (3)BASF Corporation, USA, (4)Pacific Northwest National Laboratory, USA, (5)University of Virginia, USA.

**Short Summary:**

The objective of this work is to better understand the responses of Pd and Rh single atom species to a high temperature oscillating feed that toggles between oxidative and reductive environments. We report the distinct deactivation phenomena of Pd and Rh after due to different redox and particle sintering kinetics.

## NOx Abatement and Three Way Catalysis III

**Session Chairs:** Tamsin Bell, Johnson Matthey Technology Centre, United Kingdom and Andrew (Bean) Getsoian, Ford Motor Company, USA.

3:30 PM **Mon-TRBR-1530** Impact of Catalyst Formulation and Operating Conditions on H<sub>2</sub>-SCR for deNO<sub>x</sub> of Hydrogen-Fueled Engines.

**Michael Borchers**, Kevin Keller, Patrick Lott and Olaf Deutschmann, Karlsruhe Institute of Technology (KIT), Germany.

**Short Summary:**

Our study reveals a variety of challenges in the application of H<sub>2</sub>-SCR for NO<sub>x</sub> removal from H<sub>2</sub>-fueled internal combustion engines. A comprehensive knowledge of the impact of gas composition and catalyst formulation on the activity and selectivity, as presented herein, is crucial for advances in H<sub>2</sub>-SCR technology.

3:50 PM **Mon-TRBR-1550** Mechanism Understanding for NOx Storage, Release and Reduction on Pt Doped Ceria Based Catalysts.

**Oisin Hamill**<sup>1</sup>, Nancy Artioli<sup>1</sup>, Alexandre Goguet<sup>1</sup>, Nicola Collis<sup>2</sup>, Paul Millington<sup>2</sup>, Jillian Collier<sup>2</sup> and Loredana Mantarosie<sup>2</sup>, (1)Queen's University Belfast, United Kingdom, (2)Johnson Matthey Technology Centre, United Kingdom.

**Short Summary:**

NOx storage capacity and reducibility of Platinum-Ceria catalysts is enhanced by doping with the rare-earth metal Samarium. Morphological and catalyst activity changes, caused by doping, result in a decrease in the NOx reduction temperature. This is particularly important for the application of these catalysts to reduce NOx during cold-start operation.

4:10 PM **Mon-TRBR-1610** DeNOx and deN<sub>2</sub>O Catalysts for Industrial Application: Fe-FER or Fe-ZSM5?

**Alberto Garbujo**<sup>1</sup>, Roberto Lanza<sup>2</sup>, Emmanuel Rohart<sup>3</sup>, Arnaud Lahougue<sup>3</sup> and Pierdomenico Biasi<sup>1</sup>, (1)CASALE SA, Switzerland, (2)Verdant Chemical Technologies AB, Sweden, (3)EnerCat - ALSYS Group, France.

**Short Summary:**

Two industrial catalysts were investigated under relevant industrial conditions before and after aging treatments. Results showed that Fe-FER is the most stable catalyst and exhibits high performance. Fe-FER is extremely selective in N<sub>2</sub> even after severe aging while the Fe-ZSM5 exhibited a larger undesired N<sub>2</sub>O generation.

4:30 PM **Mon-TRBR-1630** Three-Way Catalyst Reactivity of Net-Zero Carbon Fuels for Advanced Combustion Engine Emissions Control.

**Sreshtha Sinha Majumdar** and Josh A. Pihl, Oak Ridge National Laboratory, USA.

**Short Summary:**

Fuel composition has a significant impact on emissions control of regulated pollutants such as NMOG, CO and NOx. Evaluation of the reactivity of net-zero carbon fuels on emissions control catalysts under engine-exhaust relevant conditions will inform the selection of future fuels while ensuring compliance with the stringent emissions regulations.

# Tuesday May 24, 2022

## Grand Ballroom

### TUESDAY MORNING

#### Emmett Award Lecture: Thomas Jaramillo

Session Chairs: Marco Castaldi, *City College of New York (CUNY), USA*

8:00 AM Paul H. Emmett Award Address: Designing Catalysts and Chemical Processes for Global Sustainability.

Thomas F. Jaramillo, *SLAC National Accelerator Laboratory, USA; Stanford University, USA.*

## Grand Ballroom East

### (Reverse) Water-Gas-Shift

Session Chairs: Tracy Lohr, *Shell, USA* and Sunitha Tadepalli, *International Flavors and Fragrances, .*

9:30 AM **Tue-GBRE-0930** Plasma-Assisted Catalysis for Low-Temperature Reverse Water-Gas Shift.

Patrick Barboun and Jeffrey Baldwin, *Naval Research Lab, USA.*

#### Short Summary:

In this talk, plasma-assisted catalysis is applied to driving the reverse water-gas shift reaction to achieve high yields of CO at low temperature relative to the analogous thermal process over Ni and Cu based catalysts.

9:50 AM **Tue-GBRE-0950** High Metal Loading Silica-Encapsulated Catalysts for Low-Temperature Reverse Water Gas Shift Reaction.

Sin Kim Tang, Kelvin Kwok, Wang Bo, Luwei Chen and Armando Borgna, *Institute of Chemical and Engineering Sciences, A\*STAR, Singapore.*

#### Short Summary:

High-loading transition metal (10-70 wt%) catalysts were deposited on mesoporous silica for low-temperature reverse water gas shift reaction that is suitable for CO<sub>2</sub> utilization applications. Cu and Fe catalysts were superior in CO selectivity compared to Ni and Co, while co-precipitation was more effective than incipient wetness impregnation.

10:10 AM **Tue-GBRE-1010** Kinetic Analysis of CO<sub>2</sub> Activation By Means of Reverse Water-Gas Shift Reaction on Rh and Pt Surfaces.

Luca Nardi and Matteo Maestri, *Politecnico di Milano, Italy.*

#### Short Summary:

This work proposes a mechanistic understanding of the Reverse Water-Gas shift reaction in a wide set of operating conditions on 4%Rh/Al<sub>2</sub>O<sub>3</sub> and 4%Pt/Al<sub>2</sub>O<sub>3</sub> catalysts. This provides fundamental insights on the CO<sub>2</sub> activation over metal-support catalysts, paving the way for novel catalytic design.

10:30 AM **Tue-GBRE-1030** Intermetallic Ni<sub>3</sub>Zn Catalyst for High-Pressure RWGS Toward CO<sub>2</sub>-to-Liquid Applications.

Nágila Maluf, Adriano Braga, Liane Rossi, Maitê Gothe and Pedro Miguel Vidinha Gomes, *University of São Paulo, Brazil.*

#### Short Summary:

Here we developed a Ni<sub>3</sub>Zn catalyst that suppressed the formation of methane and therefore increased the yield to CO in the CO<sub>2</sub> hydrogenation at high pressure; a step forward the production of syngas at high pressure allowing the integration of RWGS and gas-to-liquid processes (MeOH/C<sub>2+</sub>) under similar pressure conditions.

10:50 AM **Tue-GBRE-1050** Reverse Water-Gas Shift Using a Highly Active and Selective Mn-Based Catalyst.

Jerrick Mielby, Mikkel Kock Larsen and Søren Kegnæs, *Technical University of Denmark, Denmark.*

#### Short Summary:

Mn/ZrO<sub>2</sub> is a highly active and selective catalyst for the reverse water-gas shift reaction that converts CO<sub>2</sub> and H<sub>2</sub> into CO and H<sub>2</sub>O. Results from *operando* modulation excitation phase-sensitive detection diffuse reflectance infrared spectroscopy (ME-PSD-DRIFTS) using isotopic CO<sub>2</sub> labeling indicate that the reaction follows an associative reaction pathway.

11:10 AM **Tue-GBRE-1110** Tailoring Metal Active Sites and Support for Sour Water-Gas Shift Reaction.

Fabio B. Passos, Ludmila Silva, Luis Terra, Ana Coutinho and Christian Sousa, *Universidade Federal Fluminense, Brazil.*

#### Short Summary:

Sour water gas shift reaction is influenced by how active sites interact with sulfur poison and reactants. Pt/Nb<sub>2</sub>O<sub>5</sub> was suitable to be used in sour water-gas shift reaction and the use of Nb<sub>2</sub>O<sub>5</sub> was beneficial for Au and CuO-ZnO catalysts. CuO-ZnO/HAP catalyst showed higher sulfur resistance compared to CuO-ZnO/Al<sub>2</sub>O<sub>3</sub>.

11:30 AM **Tue-GBRE-1130** Investigations to Intensified Hydrogen Production Via Sorption Enhanced Water Gas Shift Reaction.

Sneesh Shivanandra<sup>1</sup>, Marco J. Castaldi<sup>1</sup>, Anthony Wallace<sup>2</sup>, Charles Coe<sup>2</sup> and Michael Smith<sup>2</sup>, (1)City College of New York, CUNY, USA, (2) Villanova University, USA.

#### Short Summary:

This work shows the use of high temperature (600 – 650°C) and rapid CO<sub>2</sub> absorbing (0.21 mg<sub>CO<sub>2</sub></sub><sup>-1</sup> g<sup>-1</sup> min<sup>-1</sup>) surfactant-mediated Li<sub>4</sub>SiO<sub>4</sub> composite with 1wt.% Pt/Al<sub>2</sub>O<sub>3</sub> catalysts for SEWGS reactions. To our best knowledge, there have been no earlier reports of SEWGS operation at 650 C.

## TUESDAY AFTERNOON

### Creative C1 Chemistry

**Session Chairs:** Eleni A. Kyriakidou, *University at Buffalo (SUNY), USA* and Tracy Lohr, *Shell, USA*.

1:10 PM **Tue-GBRE-1310** Discovery of Sulfide Catalysts for the Selective Vapor-Phase Methoxycarbonylation of Ethylene.

**David Barton**<sup>1</sup>, Beata Kilos-Reaume<sup>1</sup>, Paulami Majumdar<sup>1</sup>, Steven Corthals<sup>2</sup> and Gerolamo Budroni<sup>2</sup>, (1)*The Dow Chemical Company, USA*, (2)*Dow Benelux, Netherlands*.

**Short Summary:**

Methyl propionate, an intermediate to produce methylmethacrylate, is commercially produced from ethylene, CO, and methanol using a homogeneous Pd catalyst. A recent discovery of a heterogeneous cobalt sulfide catalyst that is highly selective in the vapor phase at moderate pressure will be highlighted and nature of the active site discussed.

1:30 PM **KEYNOTE Tue-GBRE-1330 Oxidative Propane Dehydrogenation Using CO<sub>2</sub> over Vanadium Containing Small-Pore Zeolites.** Meera Shah, Marco Rigamonti and **Michiel Dusselier**, *KU Leuven, Belgium*.

**Short Summary:**

The oxidative dehydrogenation of propane with CO<sub>2</sub> is reported using small-pore zeolites containing intraporous V species. We discovered a very active catalyst that selectively delivers high space-time yields for both propylene and CO, pointing to a direct mechanism where CO<sub>2</sub> itself reoxidizes the active V site.

2:10 PM **Tue-GBRE-1410** Oxidative Dehydrogenation of Ethane with CO<sub>2</sub> over Metal Oxide Overlayer Supported Fe<sub>x</sub>Ni<sub>y</sub>: Overlayer Support Effects. Shaine Raseale<sup>1</sup>, **Wijnand Marquart**<sup>1</sup>, Gonzalo Prieto<sup>2</sup>, Michael Claeys<sup>1</sup> and Nico Fischer<sup>1</sup>, (1)*Catalysis Institute and c\*change (DSI-NRF Centre of Excellence in Catalysis), University of Cape Town, South Africa*, (2)*Max-Planck-Institut für Kohlenforschung, Germany*.

**Short Summary:**

Weakly acidic metal oxide (MO<sub>x</sub>)-supported Fe<sub>x</sub>Ni<sub>y</sub> nanoalloys are inactive while strongly acidic MO<sub>x</sub>-supported Fe<sub>x</sub>Ni<sub>y</sub> nanoalloys are active for CO<sub>2</sub> and ethane conversion. Activity for either oxidative dehydrogenation (ODHE) or dry-reforming and pathway to ODHE depends on both the metal oxide acid sites strength and the composition of Fe<sub>x</sub>Ni<sub>y</sub> nanoalloys.

2:30 PM **Tue-GBRE-1430** Environmentally Benign Methane-Assisted Catalytic Desulfurization.

**Hao Xu** and Hua Song, *University of Calgary, Canada*.

**Short Summary:**

A desulfurization process for dibenzothiophene under methane over a creative combination of two catalysts is realized, generating a new sulfur-containing product CS<sub>2</sub>, as an important intermediate and non-polar solvent. This study pioneers a transformational desulfurization route, whose practical potential is also supported by the desulfurization practices of real-world samples.

2:50 PM **Tue-GBRE-1450** Terminal Amines, Nitriles and Olefins through Catalytic CO Hydrogenation in the Presence of Ammonia..

Norbert Kruse<sup>1</sup>, **Hafsa Karroum**<sup>2</sup>, Sergey Chenakin<sup>3</sup> and Vincent Dubois<sup>4</sup>, (1)*Pacific Northwest National Laboratory, USA*, (2)*Washington State University, USA*, (3)*G.V. Kurdyumov Institute for Metal Physics of the N.A.S. of Ukraine, Ukraine*, (4)*LABIRIS, Belgium*.

**Short Summary:**

We report on the “one step - one pot” synthesis of chain-lengthened aliphatic amines and nitriles from CO/H<sub>2</sub>/NH<sub>3</sub> gas feeds using potassium-promoted Co/MnO<sub>x</sub> catalysts. We show that the reaction can be tuned via adjustments of the H<sub>2</sub>/CO ratio so as to favor the production of either terminal amines or nitriles.

### Natural Gas Conversion

**Session Chairs:** Elaine Gomez, *ExxonMobil*, and Dongxia Liu, *University of Maryland - College Park, USA*.

3:30 PM **Tue-GBRE-1530** Highly Integrated 3D Printed Micro-Reactor for Methane Reforming.

Nadi Braidy, Jean-François Pélouquin, Dino Mehanovic, Dany Francoeur, **William Leclerc**, Luc Fréchette and Mathieu Picard, *Université de Sherbrooke, Canada*.

**Short Summary:**

We demonstrate the performance of a microreactor for dry and steam methane reforming. The microreactor comprises an evaporator, heat exchanger, and a bed made of microchannels loaded with Ni-alumina. 99% CH<sub>4</sub> conversion is demonstrated with H<sub>2</sub> selectivity > 73% for T down to 825°C and a GHSV of 20,000h<sup>-1</sup>.

3:50 PM **Tue-GBRE-1550** Hironite-Based Catalyst Series for Tubular Reforming Applications.

**Fernando Morales Cano**, Charlotte Vinding Ovesen and Mads Feddersen, *Haldor Topsøe A/S, Denmark*.

**Short Summary:**

Supported nickel catalysts are widely used in the steam-reforming for industrial scale production of methanol, ammonia, hydrogen or transportation fuels. At HTAS we have developed the new TITAN™ catalyst series for tubular reforming applications, based on a novel hironite-rich carrier, leading to superior catalytic properties compared with other traditional catalysts.

4:10 PM **Tue-GBRE-1610** Direct Electrification of an Rh/Al<sub>2</sub>O<sub>3</sub> Catalyst Washcoated Si-SiC Foam for Methane Steam Reforming.

**Lei Zheng**, Matteo Ambrosetti, Daniele Marangoni, Alessandra Beretta, Gianpiero Groppi and Enrico Tronconi, *Politecnico di Milano, Italy*.

**Short Summary:**

In view of largely available renewable electricity, we report a solution to provide heat for strong endothermic reaction such as methane steam reforming thanks to the direct electrification of an Rh/Al<sub>2</sub>O<sub>3</sub> washcoated SiSiC foam. Test shows high activity and energy efficiency, enabling scale-up for cleaner H<sub>2</sub> production.



4:30 PM **Tue-GBRE-1630** Effects of Oxygen Species in Perovskite Catalysts on Partial Oxidation of Methane in a Low Temperature Plasma Bed. Dongmin Lee<sup>1</sup>, Chaesung Lim<sup>2</sup>, Juchan Kim<sup>1</sup>, Jeong Woo Han<sup>2</sup> and **Kyoung-Su Ha<sup>1</sup>**, (1)*Sogang University, Korea, Republic of (South)*, (2)*Pohang University of Science and Technology (POSTECH), Korea, Republic of (South)*.

**Short Summary:**

For generation of synthesis gas and hydrogen from methane, LaAlO<sub>3</sub> perovskite materials were chosen and studied as a catalyst under non-thermal plasma condition. The perovskite showed increased methane conversion, H<sub>2</sub> selectivity, and CO selectivity due to enhanced oxygen mobility. This performance was greatly improved by doping Sr in La position.

4:50 PM **Tue-GBRE-1650** Impact of Surface Reconstruction of Perovskite Catalysts on CH<sub>4</sub> Conversion and Acid-Base Catalysis.

**Felipe Polo-Garzon<sup>1</sup>**, Zhenghong Bao<sup>1</sup>, Lei Bai<sup>1,2</sup>, Victor Fung<sup>1</sup>, Hanjing Tian<sup>2</sup>, Miaofang Chi<sup>1</sup>, De-en Jiang<sup>3</sup> and Zili Wu<sup>1</sup>, (1)*Oak Ridge National Laboratory, USA*, (2)*West Virginia University, USA*, (3)*University of California, Riverside, USA*.

**Short Summary:**

Surface reconstruction of perovskites, using SrTiO<sub>3</sub> as a model system, can explain performance trends in methane combustion, oxidative coupling of methane, and conversion of 2-propanol. The surface reconstruction of SrTiO<sub>3</sub> was controlled via synthesis and post-synthesis methods, attaining cation segregation and step-sites.

5:10 PM **Tue-GBRE-1710** Carbon-Supported Ni-Cu Catalysts for the Study of Carbon Nanostructure Growth during Thermal Decomposition of Methane.

**Suzan E. Schoemaker**, Tom A.J. Welling, Dennie F.L. Wezendonk, Krijn P. de Jong and Petra E. de Jongh, *Utrecht University, Netherlands*.

**Short Summary:**

Carbon-supported Ni-Cu catalysts were used for the thermocatalytic decomposition of methane to H<sub>2</sub> and carbon. Using a TGA, the carbon deposition was monitored over time. Varying the temperature impacted the catalytic activity and life time. It was found that both carbon nanotubes and fibers formed during the same experiment.

## Grand Ballroom West

### TUESDAY MORNING

#### NO<sub>x</sub> Selective Catalytic Reduction I

**Session Chairs:** Yuejin Li, *BASF Corporation, USA* and Louise Olsson, *Chalmers University of Technology, Sweden*.

9:30 AM **Tue-GBRW-0930** Effect of the Hydrothermal Aging on the NH<sub>3</sub>-SCR Performance and N<sub>2</sub>o Selectivity of Cu-SSZ-39 and Cu-SSZ-13.

**Catarina Simão Marta**, David Berthout, Bogdan Harbuzaru, Stéphane Raux and Christophe Pichon, *IFP Energies Nouvelles, France*.

**Short Summary:**

Commercial fresh and hydrothermally aged SSZ-39 and SSZ-13 (Si/Al ~ 9.5, Cu loading ~ 2 wt. %) were tested in NH<sub>3</sub>-SCR. The catalytic performance of fresh CHA and AEI is identical. The greater presence of Cu<sup>2+</sup>-ZZ species in AEI improves the stability after hydrothermal aging and provides better deNO<sub>x</sub> performance.

9:50 AM **Tue-GBRW-0950** A Unified Reaction Mechanism for the Redox of Active Cu Sites in Cu-SSZ-13 Under SCR and Oxidation Conditions.

**Rohil Daya<sup>1</sup>**, Dhruva J. Deka<sup>2</sup>, Dylan Trandal<sup>1</sup>, Unmesh Menon<sup>1</sup>, Saurabh Joshi<sup>1</sup> and William Partridge<sup>2</sup>, (1)*Cummins Inc., USA*, (2)*Oak Ridge National Laboratory, USA*.

**Short Summary:**

We report on a kinetic model for reduction of Cu<sup>II</sup> sites by NO, NH<sub>3</sub> and NO + NH<sub>3</sub>, along with the re-oxidation of Cu<sup>I</sup> sites by O<sub>2</sub> and NO + O<sub>2</sub> on a state of the art Cu-SSZ-13 catalyst. Transient kinetic experiments are utilized for estimating individual half cycle rates.

10:10 AM **Tue-GBRW-1010** Influence of Zeolite Topology on Cu Ion Mobility and Cu<sup>I</sup>/Cu<sup>II</sup> Redox Kinetics during Low-Temperature NO<sub>x</sub> Selective Catalytic Reduction.

Casey Jones<sup>1</sup>, **Mykela DeLuca<sup>1</sup>**, Siddarth Krishna<sup>1</sup>, Anshuman Goswami<sup>2</sup>, Sichi Li<sup>2</sup>, JohnJoel Sarcis<sup>2</sup>, Subramanian Prasad<sup>3</sup>, Ahmad Moini<sup>3</sup>, William F. Schneider<sup>2</sup> and Rajamani Gounder<sup>1</sup>, (1)*Purdue University, USA*, (2)*University of Notre Dame, USA*, (3)*BASF Corporation, USA*.

**Short Summary:**

Factors governing Cu ion mobility during low temperature NO<sub>x</sub> selective catalytic reduction are interrogated by isolating oxidation and reduction rate constants in Cu-zeolites of varying framework topology. Cu-CHA provides an upper bound on rate constants (per Cu), reflecting benefits conferred by appropriately sized 3D cage-window topologies to utilize mobile Cu.

10:30 AM **Tue-GBRW-1030** A Dual-Site Redox Mechanism for the Reduction Half Cycle of Low-Temperature NH<sub>3</sub>-SCR over Cu-CHA Catalysts.

Wenshuo Hu<sup>1</sup>, Federica Gramigni<sup>2</sup>, Nicole Daniela Nasello<sup>2</sup>, Nicola Usberti<sup>2</sup>, Umberto Iacobone<sup>2</sup>, Maria Elena Azzoni<sup>2</sup>, Shaojun Liu<sup>3</sup>, Xiang Gao<sup>3</sup>, Isabella Nova<sup>2</sup> and **Enrico Tronconi<sup>2</sup>**, (1)*University of California, Berkeley, USA*, (2)*Politecnico di Milano, Italy*, (3)*Zhejiang University, China*.

**Short Summary:**

We combine transient-response methods, in situ/operando spectroscopy and probe reaction experiments with computational approaches to investigate the Low-Temperature redox chemistry of NH<sub>3</sub>-SCR over Cu-CHA. NO pulses to NH<sub>3</sub>-saturated Cu-CHA reveal a quadratic dependence of the Cu-sites reduction rate on Cu<sup>2+</sup>, identifying dinuclear Cu<sup>2+</sup>-NH<sub>3</sub> complexes as the active centers of LT-RHC.

10:50 AM **KEYNOTE Tue-GBRW-1050 Rate Controlling in Low-Temperature Standard NH<sub>3</sub>-SCR: Implications from Reaction Kinetics and in Situ EPR Spectroscopy.** Feng Gao, Yiqing Wu, Yue Ma, Eric D. Walter, Yilin Wang, Kenneth Rappe and Yong Wang, *Pacific Northwest National Laboratory, USA.*

**Short Summary:**

In situ electron paramagnetic resonance (EPR) spectroscopic measurements during steady-state standard NH<sub>3</sub>-SCR reaction reveal remarkable correlation between the loading of Cu-ions and their mobility. With increasing Cu loading, the disappearance of hyperfine and super hyperfine EPR features correlates to high SCR rates, both attributed to high Cu mobility.

11:30 AM **Tue-GBRW-1130 Transient Tests to Assess the Cu Speciation in Cu-CHA Catalysts: Investigating the Hydrothermal Aging Effect.**

**Umberto Iacobone**<sup>1</sup>, Isabella Nova<sup>1</sup>, Enrico Tronconi<sup>1</sup>, Rohil Daya<sup>2</sup>, Krishna Kamasamudram<sup>2</sup>, Dylan Trandal<sup>2</sup>, Unmesh Menon<sup>2</sup>, Ashok Kumar<sup>2</sup> and Aleksey Yezerets<sup>2</sup>, (1)*Politecnico di Milano, Italy*, (2)*Cummins Inc., USA*.

**Short Summary:**

The Cu-CHA catalyst aging is a spontaneous phenomenon active during NH<sub>3</sub>-SCR conditions, which changes the nature of the active Cu<sup>2+</sup> ions. We demonstrate how the transformation can be effectively studied with simple well established transient response methods in alternative to more sophisticated spectroscopic techniques.

## TUESDAY AFTERNOON

### NOx Selective Catalytic Reduction II

**Session Chairs:** Todd J. Toops, *Oak Ridge National Laboratory, USA* and Yuanzhou Xi, *Cummins Emission Solutions, USA*.

1:10 PM **Tue-GBRW-1310 Hydrothermal Stability of Cu-SSZ-39 Compared to Cu-SSZ-13 in NH<sub>3</sub>-SCR of NOx.**

**Mirjam Wenig**, Rachit Khare, Andreas Jentys and Johannes A. Lercher, *Technical University of Munich, Germany*.

**Short Summary:**

The focus of our work was on kinetic studies of the small-pore zeolite SSZ-39 (AEI structure) with different Cu loadings and the influence of hydrothermal ageing on the Cu-species compared to Cu-SSZ-13 (CHA structure). After hydrothermal aging we observed a transformation of the Cu species, resulting in inactive species.

1:30 PM **Tue-GBRW-1330 The NO-N<sub>2</sub>O-SCR Reaction : A Catalytic and Spectroscopic Investigation.**

**Filippo Buttignol**<sup>1,2</sup>, Alberto Garbujo<sup>3</sup>, Pierdomenico Biasi<sup>3</sup>, Oliver Kröcher<sup>1,2</sup> and Davide Ferri<sup>2</sup>, (1)*École Polytechnique Fédérale de Lausanne (EPFL), Switzerland*, (2)*Paul Scherrer Institut, Switzerland*, (3)*CASALE SA, Switzerland*.

**Short Summary:**

The NO-N<sub>2</sub>O-SCR reaction was investigated combining catalytic and transient spectroscopic experiments. We observed that: I) N<sub>2</sub>O promotes NO abatement above 300 °C by enhancing re-oxidation of the Fe sites, II) Fe species are the active centers and NH<sub>3</sub> spill-over from Brønsted sites must occur, III) this latter process is rate-limiting.

1:50 PM **Tue-GBRW-1350 Simple Physical Mixing of Zeolite Prevents Sulfur Deactivation of Vanadia Catalysts for NOx Removal.**

Inhak Song<sup>1</sup>, Hwangho Lee<sup>1</sup>, Se Won Jeon<sup>1</sup>, Joonwoo Kim<sup>2</sup>, Youngchul Byun<sup>2</sup>, Dong Jun Koh<sup>2</sup>, Jeong Woo Han<sup>3</sup> and **Do Heui Kim**<sup>1</sup>, (1)*Seoul National University, Korea, Republic of (South)*, (2)*Research Institute of Industrial Science & Technology, Korea, Republic of (South)*, (3)*Pohang University of Science and Technology (POSTECH), Korea, Republic of (South)*.

**Short Summary:**

This study provided a simple but noble “physical mixing” strategy to achieve excellent sulfur resistance of the vanadia-titania NH<sub>3</sub>-SCR catalyst with high NOx removal ability. It was found that physically mixed zeolite demonstrated ammonium bisulfate (ABS) trapping ability due to interaction between its aluminum sites in zeolite and ABS.

2:10 PM **Tue-GBRW-1410 NH<sub>3</sub> Strategic Dosing Approach for the Minimization of N<sub>2</sub>O Production during NH<sub>3</sub>-SCR Reactions over Cu-CHA Catalysts.**

**Nicole Daniela Nasello**<sup>1</sup>, Federica Gramigni<sup>1</sup>, Isabella Nova<sup>1</sup>, Enrico Tronconi<sup>1</sup>, Frank Hofmann<sup>2</sup>, Marcus Crocoll<sup>2</sup> and Michel Weibel<sup>2</sup>, (1)*Politecnico di Milano, Italy*, (2)*Mercedes-Benz AG, Germany*.

**Short Summary:**

In compliance with stricter environmental regulations, Diesel vehicles are required to further reduce their engine-out harmful emissions. We report an original approach based on the strategic dosing of ammonia aimed at both maximizing NOx conversion and minimizing N<sub>2</sub>O formation in the NH<sub>3</sub>-SCR reactions over Cu-CHA catalysts.

2:30 PM **Tue-GBRW-1430 Field Aging Impact on the NH<sub>3</sub> Selective Catalytic NOx Reduction Redox Half Cycles over a Commercial Cu-SSZ-13 Catalyst.**

**Dhruba J. Deka**<sup>1</sup>, Rohil Daya<sup>2</sup>, Austin Ladshaw<sup>1</sup>, Saurabh Joshi<sup>2</sup>, Krishna Kamasamudram<sup>2</sup> and William Partridge<sup>1</sup>, (1)*Oak Ridge National Laboratory, USA*, (2)*Cummins Inc., USA*.

**Short Summary:**

This study showed that field aging (real-world aging) of Cu-SSZ-13 SCR catalyst degrades its performance by various routes, such as hydrothermal aging, sulfur poisoning, phosphorus poisoning and dealumination. Impact of field aging on the SCR redox half cycles was investigated by transient response experiments and kinetic modeling.

2:50 PM **Tue-GBRW-1450** The Role of Oxide and NH<sub>3</sub> Mobility in Composite Catalysts for Low-Temperature Selective Catalytic Reduction of NO<sub>x</sub> By Ammonia.

Kenneth Rappe<sup>1</sup>, Tahrizi Andana<sup>1</sup>, **Nicholas Nelson**<sup>1</sup>, Feng Gao<sup>1</sup>, Janos Szanyi<sup>1</sup> and Yong Wang<sup>1,2</sup>, (1)*Pacific Northwest National Laboratory, USA*, (2)*Washington State University, USA*.

**Short Summary:**

The presence of oxide in oxide-zeolite composite catalysts is shown to significantly benefit low temperature NO<sub>x</sub> reduction performance. Composite catalyst performance at low temperature derives from a zeolite-to-oxide promotional route involving the oxide phase and zeolite Bronsted acid sites that is reliant upon their adjacency.

## NO<sub>x</sub> Selective Catalytic Reduction III

**Session Chairs:** Feng Gao, *Pacific Northwest National Laboratory, USA* and Unmesh Menon, *Cummins Inc., USA*.

3:30 PM **Tue-GBRW-1530** Consequences of Z<sub>2</sub>-Cu to Z-Cu-OH Hydrolysis for the Low-Temperature NH<sub>3</sub>-SCR on Cu-CHA Catalysts.

Wenshuo Hu<sup>1</sup>, Umberto Iacobone<sup>2</sup>, Federica Gramigni<sup>2</sup>, Yu Zhang<sup>3</sup>, Xiaoxiang Wang<sup>3</sup>, Shaojun Liu<sup>3</sup>, Chenghang Zheng<sup>3</sup>, **Isabella Nova**<sup>2</sup>, Xiang Gao<sup>3</sup> and Enrico Tronconi<sup>2</sup>, (1)*University of California, Berkeley, USA*, (2)*Politecnico di Milano, Italy*, (3)*Zhejiang University, China*.

**Short Summary:**

Hydrolysis of Z<sub>2</sub>Cu to ZCuOH in the presence of NH<sub>3</sub> is both kinetically and thermodynamically favorable, which obscures their differences and renders identical kinetic responses for the two sites in low-temperature NH<sub>3</sub>-SCR reactions over Cu-CHA catalysts.

3:50 PM **Tue-GBRW-1550** Correlating Oxidation Reaction Activities to Extent of Sulfur Poisoning on Cu/SSZ-13 Selective Catalytic Reduction (SCR) Catalysts.

**Yu-Ren Chen**<sup>1</sup>, Ashok Kumar<sup>2</sup>, Di Wang<sup>2</sup> and William Epling<sup>1</sup>, (1)*University of Virginia, USA*, (2)*Cummins Inc., USA*.

**Short Summary:**

Cu/SSZ-13 is a commercially viable selective catalytic reduction (SCR) catalyst, but sulfur poisoning remains a problem. We show that the extent of sulfur poisoning depends on catalyst oxidation ability, which stems from the relative amounts of ZCuOH and Z<sub>2</sub>Cu.

4:10 PM **Tue-GBRW-1610** Combining X-Ray Absorption Spectroscopy and Transient Response Methods for the Kinetic Analysis of the Standard SCR Redox Mechanism over Cu-CHA Catalysts.

**Maria Pia Ruggeri**<sup>1</sup>, Federica Gramigni<sup>2</sup>, Husn Islam<sup>1</sup>, Umberto Iacobone<sup>2</sup>, Nicola Usberti<sup>2</sup>, Nicole Daniela Nasello<sup>2</sup>, Isabella Nova<sup>2</sup>, Roberta Villamaina<sup>1</sup>, Monica Amboage<sup>3</sup>, Loredana Mantarosi<sup>1</sup>, Jillian Collier<sup>1</sup>, David Thompsett<sup>1</sup> and Enrico Tronconi<sup>2</sup>, (1)*Johnson Matthey Technology Centre, United Kingdom*, (2)*Politecnico di Milano, Italy*, (3)*Diamond Light Source, United Kingdom*.

**Short Summary:**

TRM and XAS techniques are demonstrated to be equivalent for the kinetic investigation of the SCR mechanism. According to them the Cu reduction rate exhibits a quadratic dependence on Cu<sup>II</sup> across the investigated T-range (150-250°C), supporting the new dual site pathway recently proposed for the RHC of NH<sub>3</sub>-SCR over Cu-CHA.

4:30 PM **Tue-GBRW-1630** Experimental Investigation of the Oxidation Half-Cycle in Low-T Standard SCR over Cu-CHA: Effect of Gas Phase Composition.

Federica Gramigni, Nicole Daniela Nasello, Nicola Usberti, Umberto Iacobone, **Maria Elena Azzoni**, Isabella Nova and Enrico Tronconi, *Politecnico di Milano, Italy*.

**Short Summary:**

Mechanistic aspects concerning the Oxidation Half Cycle of the low-T Standard SCR reaction over Cu-CHA are addressed by simple transient response methods. We reveal that oxygen alone is able to oxidize the reduced Cu sites.

4:50 PM **Tue-GBRW-1650** Effects of Hydrothermal Aging on the Sulfur Poisoning of a Cu-SSZ-13 SCR Catalyst.

**Yuanzhou Xi**, Changsheng Su, Nathan Ottinger and Z. Gerald Liu, *Cummins Emission Solutions, USA*.

**Short Summary:**

Hydrothermal aging can convert a portion of the ZCuOH sites of Cu-SSZ-13 SCR catalyst to Z<sub>2</sub>Cu, resulting in a more sulfur resistant catalyst. This study provides insights linking catalyst structural and reactivity transformations upon real world aging. It also provides a potential methodology for manufacturing more sulfur tolerant catalyst.

5:10 PM **Tue-GBRW-1710** Aging of Cu-Exchanged Zeolite SCR Catalysts Under Lean, Stoichiometric and Rich Exhaust Relevant to Gasoline Applications.

**Calvin R. Thomas**, Josh A. Pihl, Dhruva J. Deka, Michael J. Lance, Todd J. Toops and Vitaly Y. Prikhodko, *Oak Ridge National Laboratory, USA*.

**Short Summary:**

This presentation will discuss trends in catalyst deactivation for three different Cu-exchanged zeolite formulations as a function of aging temperature and gas composition. The findings will help to define an appropriate operating envelope for Cu-exchanged zeolites in gasoline engine exhaust applications.

## TUESDAY MORNING

### Electro- and Photocatalysis for Organic Transformations

**Session Chairs:** Michal Bajdich, *SLAC National Accelerator Laboratory, USA* and Gianvito Vile, *Politecnico di Milano, Italy*.

9:30 AM **Tue-GRAM-0930** Electrochemical Radical Generation As a Tool for C-C Coupling.

**Haoran Ding** and Marat Orazov, *University of Delaware, USA*.

**Short Summary:**

The Kolbe electrolysis was employed as a tool for C-C coupling. The benign condition and high availability of substrates make the studied reaction a promising synthetic route toward substituted aromatics. The developed pulse technique mitigates the deactivation of electrodes and may be extended to other organic electro-synthesis.

9:50 AM **Tue-GRAM-0950** Fouling of Cu Catalysts during Electrochemical Hydrogenation and Hydrogenolysis of Furfural in Acidic Media.

**Andrew S. May**<sup>1</sup>, Steven M. Watt<sup>1,2</sup> and Elizabeth J. Biddinger<sup>1,2</sup>, (1)*City College of New York, CUNY, USA*, (2)*The Graduate Center of the City University of New York, USA*.

**Short Summary:**

The electrochemical hydrogenation and hydrogenolysis of furfural is impacted by catalyst fouling over copper in acidic media. After extended electrolysis, polymeric substances were observed on the catalyst. This work investigated the mechanism and impact of the fouling using spectroscopic, microscopic and calorimetric techniques.

10:10 AM **Tue-GRAM-1010** Trends in Electrocatalytic Oxidation of Small Organic Molecules at the Buried Interface of Silicon Oxide Encapsulated Platinum Electrodes.

Marissa Beatty and **Daniel Esposito**, *Columbia University, USA*.

**Short Summary:**

This study explores the use of nanoscopic, semipermeable oxide coatings deposited on platinum electrocatalysts to enhance its activity towards oxidation of various organic molecules. Trends in activity and design rules for overlayer structure/composition are reported that may be extended to other electrocatalytic materials and reactions beyond those investigated here.

10:30 AM **Tue-GRAM-1030** Elucidating Thermal and Non-Thermal Effects in Monometallic Plasmonic Catalysts and Their Surrounding Environments.

**Rachel Elias**<sup>1</sup> and Suljo Linic<sup>2</sup>, (1)*University of Michigan-Ann Arbor, USA*, (2)*University of Michigan, USA*.

**Short Summary:**

We provide a comparative study of several monometallic plasmonic catalysts to elucidate the presence and role of macroscopic heating on these materials and their surroundings. We vary the reaction type, catalyst loading, active surface, and support material to examine light-induced effects under different conditions.

10:50 AM **Tue-GRAM-1050** Hybrid Organic-Inorganic Magnetic Supramolecular Composites with Adsorption and Photocatalytic Degradation Capabilities of Antibiotics Under Solar Light.

Bogdan Cojocaru, Razvan Mihailescu, Nicolae Guzo, Octavian D. Pavel, Sabina Ion, Madalina Tudorache, Simona Coman and **Vasile Parvulescu**, *University of Bucharest, Romania*.

**Short Summary:**

The metal-phthalocyanine-LDH-MNPs composites are a promising alternative to quick removal of antibiotics from water by combining an ultrafast absorption and a photocatalytic effect under sun-light irradiation.

11:10 AM **Tue-GRAM-1110** Cerium Carbonate Catalytically Decomposes Reactive Oxygen Species.

Manish Mishra<sup>1</sup>, Juan Callejas<sup>2</sup>, Michaelen Pacholski<sup>2</sup>, Jim Ciston<sup>3</sup>, Alexander Okrut<sup>1</sup>, **Ram Kumar**<sup>1</sup>, Antony Van Dyk<sup>2</sup>, David Barton<sup>2</sup>, James Bohling<sup>2</sup> and Alexander Katz<sup>1</sup>, (1)*University of California, Berkeley, USA*, (2)*The Dow Chemical Company, USA*, (3)*National Center for Electron Microscopy, USA*.

**Short Summary:**

We synthesize and characterize a new class of catalytic antioxidants based on cerium carbonate for the degradation of ROS, which possess unprecedented activity for this purpose.

11:30 AM **Tue-GRAM-1130** Ni Single Atoms on Carbon Nitride for Cross-Coupling Chemistry Under Visible Light Conditions.

**Mark Bajada** and Gianvito Vile, *Politecnico di Milano, Italy*.

**Short Summary:**

Visible light-driven dual catalysis combines photoabsorbers and transition-metal complexes. In our study, we demonstrate the synergistic and sustainable merger of metallic single-atom catalysis and carbon-based photoredox catalysis, in the form of a nickel atom supported carbon nitride material, in order to conduct C-C cross-coupling reactions.

## TUESDAY AFTERNOON

### Selective Oxidation I

**Session Chairs:** Líney Árnadóttir, *Oregon State University, USA* and Weijian Diao, *Villanova University, USA*.

1:10 PM **Tue-GRAM-1310** Nature of Active Sites for Cs, Re and Cl Promoted Supported Ag/ $\alpha$ -Al<sub>2</sub>O<sub>3</sub> Catalysts for Selective Ethylene Epoxidation. Tiancheng Pu<sup>1</sup>, Xuan Tang<sup>2</sup>, Adhika Setiawan<sup>1</sup>, Minghui Zhu<sup>2</sup>, Srinivas Rangarajan<sup>1</sup>, Sheng Dai<sup>2</sup> and **Israel E. Wachs**<sup>1</sup>, (1)*Lehigh University, USA*, (2)*East China University of Science and Technology, China*.

**Short Summary:**

Selective oxidation of ethylene to ethylene oxide (EO) over promoted Ag catalysts has been one of the most significant chemical processes over the past few decades. Herein, HAADF-STEM, *in situ* Raman spectroscopy in combination with computational insights established the structure – activity relationships of promoted supported Ag/ $\alpha$ -Al<sub>2</sub>O<sub>3</sub> catalysts.

1:30 PM **Tue-GRAM-1330** Effects of Pore Condensation on Rates and Barriers for Alkene Epoxidation in Ti-BEA Catalysts.

**Ohsung Kwon**, Zeynep Ayla and David Flaherty, *University of Illinois Urbana-Champaign, USA*.

**Short Summary:**

Condensation of gaseous acetonitrile forms clusters within Ti-incorporated zeolite pores, with densities controlled by manipulating pressures and intrapore silanol densities. This pore condensation leads to significant changes in linear alkene epoxidation rates and activation barriers with hydrogen peroxide due to the structural reorganization during the transition state.

1:50 PM **Tue-GRAM-1350** Impact of Methanol-Water-Silanol Interactions on Alkene Epoxidation Catalysis within Ti-MFI.

**Chris Torres** and David Flaherty, *University of Illinois Urbana-Champaign, USA*.

**Short Summary:**

Solvent molecules interact within Ti-MFI catalysts of varying defect density to stabilize reactive intermediates through excess enthalpic and free energy contributions for 1-hexene epoxidation reaction with aqueous hydrogen peroxide. These findings provide understanding into the design of solvent-surface interfaces to improve rates and selectivities for liquid-phase oxidation catalysis.

2:10 PM **Tue-GRAM-1410** Demonstration of Electronic Impact of Cl on Ethylene Epoxidation over Ag Catalysts Via Kinetic Modeling.

James Harris<sup>1</sup>, Le Wang<sup>2</sup> and **Joseph DeWilde**<sup>2</sup>, (1)*The University of Alabama, USA*, (2)*The Dow Chemical Company, USA*.

**Short Summary:**

We employ kinetic modeling to demonstrate that the surface chlorine content of the relative rates of ethylene epoxidation and ethylene combustion over silver chloride catalysts are unable to be described by ensemble effects alone and chlorine must have some electronic impact on the active energetics.

2:30 PM **Tue-GRAM-1430** Active Site Environments Near Disperse Ti Atoms on Non-Microporous Supports Affect Excess Properties for Alkene Epoxidation.

**Zeynep Ayla**, Darshan Patel, Arzam Harris and David Flaherty, *University of Illinois Urbana-Champaign, USA*.

**Short Summary:**

Differences in rates, selectivities, and apparent barriers for alkene epoxidations over Ti atoms supported on metal oxides reflect the way the chemical identity of the support affects intermolecular interactions in the fluid-phase near the active site and influences excess contributions through those differences.

2:50 PM **Tue-GRAM-1450** Direct Epoxidation of C<sub>3</sub>H<sub>6</sub> Using Molecular O<sub>2</sub> and Novel Ag Catalyst.

**Md Masudur Rahman**<sup>1</sup>, Michael Burkholder<sup>2</sup> and John R. Monnier<sup>1</sup>, (1)*University of South Carolina, USA*, (2)*Virginia Commonwealth University, USA*.

**Short Summary:**

Selective direct epoxidation of propylene to propylene oxide (PO) using molecular oxygen and Ag based catalyst requires an intricate system. In this study role of high levels of gas feed additives, alkali metal promoters and different supports were studied extensively. Fundamental understanding of them is required to improve PO yield.

### Selective Oxidation II

**Session Chairs:** Aditya Bhan, *University of Minnesota, Twin Cities, USA* and Luis Bollman, *Dow*.

3:30 PM **Tue-GRAM-1530** Shaping Catalytic Performance Using Precise Surface-Deposition of Active Elements on Oxidation Catalysts Via ALD.

**Frederik R  ther**<sup>1</sup>, Robert Baumgarten<sup>1</sup>, Fabian Ebert<sup>1</sup>, Michael Geske<sup>1</sup>, Raoul Naumann d'Alnoncourt<sup>1</sup>, Ralph Kraehnert<sup>1</sup>, Annette Trunschke<sup>2</sup>, Robert Schl  gl<sup>2</sup> and Frank Rosowski<sup>1,3</sup>, (1)*Technische Universit  t Berlin, Germany*, (2)*Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany*, (3)*BASF SE, Germany*.

**Short Summary:**

The impact of sub-monolayers of active elements deposited on the surface of oxidation catalysts using atomic layer deposition (ALD) is demonstrated. By precisely adjusting surface-properties, this method is shown to be a versatile tool to enhance catalytic performance in partial oxidation of propane and extract insights into interfacial catalysis.



3:50 PM **Tue-GRAM-1550** Regenerative Stability of Zeolite Supported Ptsn Catalysts for Ethane Dehydrogenation.

**Sara Jacob**, Michael Caulfield, John Gao, Elaine Gomez, Henry Klutse, Randall Meyer, Michele Paccagnini and Aaron Sattler, *ExxonMobil Research and Engineering, USA*.

**Short Summary:**

A high performance catalyst for ethane dehydrogenation must have high thermal stability, high selectivity, long lifetime near equilibrium, low coke yield, and robust regenerability. This work examines factors influencing K-PtSn@MFI performance and its regenerability. Current syntheses result in Pt-Sn segregation following multiple regeneration cycles leading to a loss in performance.

4:10 PM **Tue-GRAM-1610** Ethane ODH on M1-Containing Mixed Metal Oxides. the Role of Te and Nb in Movte(Nb)O Catalysts.

Agustin De ARRIBA<sup>1</sup>, Benjamin Solsona<sup>2</sup>, Ester Garcia-González<sup>3</sup>, Patricia Concepcion<sup>4</sup> and **Jose M. Lopez Nieto**<sup>5</sup>, (1)*CSIC, Spain*, (2)*Universitat de València, Spain*, (3)*Universidad Complutense, Spain*, (4)*Instituto de Tecnología Química (UPV-CSIC), Spain*, (5)*Universitat Politècnica de València, Spain*.

**Short Summary:**

A correlation between the catalytic performance for ethane ODH of MoVO, MoVTeO and MoVTeNbO catalysts, heat-treated at 400 or 600°C, with the physico-chemical properties of catalysts, including adsorption properties, is presented in order to explain the differences in the extent of the over-oxidation of the ethylene formed

4:30 PM **Tue-GRAM-1630** Developing New Insights into Oxidative Methanol Conversion through Operando Interrogation of Both the Near-Surface Gas Phase Above a Catalyst and Its Surface.

Sadi Gurses<sup>1</sup>, Trevor Price<sup>1</sup>, Angie Zhang<sup>2</sup>, Jonathan Frank<sup>2</sup>, Nils Hansen<sup>2</sup>, David Osborn<sup>1,2</sup>, Ambarish Kulkarni<sup>1</sup> and **Coleman Kronawitter**<sup>1</sup>, (1)*University of California, Davis, USA*, (2)*Sandia National Laboratories, USA*.

**Short Summary:**

In the presented studies, a novel approach involving experimental interrogation of both the near-surface gas phase above catalysts and catalyst surfaces is used to provide new mechanistic insights into the oxidative conversion of methanol to C2+ oxygenates.

4:50 PM **Tue-GRAM-1650** The Effect of Cobalt Doping on the Catalytic Properties of Co-Containing Siliceous BEA Zeolite.

Katarzyna Pamin<sup>1</sup>, Jacek Gurgul<sup>1</sup>, Laetitia Valentin<sup>2</sup> and **Stanislaw Dzwigaj**<sup>2</sup>, (1)*Jerzy Haber Institute of Catalysis and Surface Chemistry PAS, Poland*, (2)*Sorbonne Université, France*.

**Short Summary:**

The oxidation of cyclohexane to cyclohexanone and cyclohexanol with molecular oxygen as oxidant is an industrially important chemical process which utilizes cobalt(II) salts as catalysts. One of the aspects of interest is the design of a novel catalytic system which would modify the reaction characteristics.

5:10 PM **Tue-GRAM-1710** Mechanism Investigation of Electrochemical C(sp<sup>3</sup>)-H Oxidation for the Late-Stage Methylation of Complex Molecules.

**Kaida Liu**<sup>1</sup>, Mayank Tanwar<sup>1</sup>, Matthew Neurock<sup>1</sup>, Luiz Novaes<sup>1</sup>, Justin Ho<sup>2</sup>, Kaining Mao<sup>2</sup>, Song Lin<sup>2</sup>, Elisia Villemure<sup>3</sup> and Jack Terrett<sup>3</sup>, (1)*University of Minnesota, Twin Cities, USA*, (2)*Cornell University, USA*, (3)*Genentech, Inc., USA*.

**Short Summary:**

Theoretical results provide important insights to show that the mechanism for the late-stage methylation of protected amines proceeds via a PCET mechanism. A detailed mechanistic understanding will help to guide future developments for improved electrochemical C(sp<sup>3</sup>)-H oxidation protocol, which features broad reaction scope, high functional group compatibility, and operational simplicity.

## Mercury Ballroom

### TUESDAY MORNING

#### Fundamentals of Liquid Phase Catalysis

**Session Chairs:** Martha Arellano-Trevino, *National Renewable Energy Laboratory, USA* and James Harris, *The University of Alabama, USA*.

9:30 AM **Tue-MEBR-0930** Exploiting the Liquid Phase to Enhance Cross-Coupling of Alcohols over Nanoporous Gold Catalysts.

**Nathaniel Eagan**, Mathilde Luneau, Cynthia Friend and Robert Madix, *Harvard University, USA*.

**Short Summary:**

Selectivity in the oxidative cross-coupling of alcohols over Au is found to depend strongly on the phase in which the chemistry is performed. In the liquid phase Au-alkyl van der Waals forces are disrupted, leading to improved cross-coupling versus the gas phase, which favors self-coupling.

9:50 AM **Tue-MEBR-0950** Impact of Interactions between Solvent Structures and Reactive Intermediates on Lewis-Acid Catalyzed Epoxidations.

**David Potts**, Vijay Jeyaraj, Ohsung Kwon, Richa Ghosh, Alexander V. Mironenko and David Flaherty, *University of Illinois Urbana-Champaign, USA*.

**Short Summary:**

Solvent molecules interact with reactive species to influence catalytic reactions. Here, we examine the liquid phase epoxidation of C<sub>6</sub> - C<sub>18</sub> alkenes over zeolite catalysts. We demonstrate that longer alkyl chains must disrupt greater quantities of solvent during transition state formation, which strongly influences epoxidation rates.

10:10 AM **KEYNOTE Tue-MEBR-1010 Promotion of Heterogeneous Catalysis at Solid-Liquid Interfaces with Unconventional Handles.** Yuriy Roman, *Massachusetts Institute of Technology, USA.*

**Short Summary:**

In this presentation, I will discuss recent efforts in our group to use “unconventional” handles, such as confined solvents molecules and interfacial electrostatics, to manipulate the reactivity of heterogeneous catalysts.

10:50 AM **Tue-MEBR-1050 Spontaneous Charge Transfer Reactions Govern Electrostatic Effects in Thermocatalysis at Metal–Liquid Interfaces.**

**Thejas Wesley**, Yuriy Roman and Yogesh Surendranath, *Massachusetts Institute of Technology, USA.*

**Short Summary:**

We show that spontaneous charge transfer reactions, which prevail at *all* solid–liquid interfaces, endow thermocatalytic reactions at metal–liquid interfaces with electrochemical character by controlling the interfacial electrostatic profile and solvent structure. These results reveal unifying concepts across electrochemical and thermochemical catalysis at interfaces.

11:10 AM **Tue-MEBR-1110 Leveraging Polymer-Induced “Solvation Effects” to Modulate Selectivity and Activity of Nitrites Reduction in Aqueous Phase.**

Pengcheng Huang<sup>1</sup>, Aayan Banerjee<sup>1,2</sup>, Leon Lefferts<sup>2</sup> and **Jimmy Faria**<sup>1</sup>, (1)*MESA + Institute for Nanotechnology, Netherlands*, (2)*University of Twente, Netherlands.*

**Short Summary:**

This fundamental research is aimed at developing the designing rules of the catalysts solvation micro-environment for the activation of nitrogen-containing molecules (e.g. nitrates, nitrites, and nitro-organics), which are relevant for closing the nitrogen cycle.

11:30 AM **Tue-MEBR-1130 Confinement- and Solvent-Enabled Control of Reactivity for Liquid-Phase Alcohol Dehydration and Acetone Aldol Condensation.**

**Sungmin Kim**<sup>1</sup>, Feng Chen<sup>1</sup>, Hui Shi<sup>1,2</sup>, Oliver Y. Gutierrez<sup>1</sup>, Donald M. Camaioni<sup>1</sup> and Johannes A. Lercher<sup>1</sup>, (1)*Pacific Northwest National Laboratory, USA*, (2)*Technical University of Munich, Germany.*

**Short Summary:**

We study Brønsted acid-catalyzed dehydration of cyclohexanol and the aldol condensation of acetone in decalin and in water using zeolites with different pore diameters. The intrapore environment allows us to control the reaction rates of C-O bond cleavage and C-C bond formation to steer selectivity in complex reactions.

## TUESDAY AFTERNOON

### Fundamentals of Catalysis: Atomically Dispersed Species I

**Session Chairs:** Jingyue Liu, *Arizona State University, USA* and Ming Yang, *Clemson University, USA.*

1:10 PM **Tue-MEBR-1310 Deciphering the Dynamic CO Oxidation Pathways over Single-Atom Platinum-on-Ceria Catalysts.**

**Dong Jiang**<sup>1</sup>, Berlin Sudduth<sup>1</sup> and Yong Wang<sup>1,2</sup>, (1)*Washington State University, USA*, (2)*Pacific Northwest National Laboratory, USA.*

**Short Summary:**

A dynamic switching between two distinct reaction mechanisms was observed on single-atom Pt<sub>1</sub>/CeO<sub>2</sub> catalysts during lean CO oxidation. Combined kinetics and *in-situ* DRIFTS confirmed that at certain CO/O<sub>2</sub> partial pressures, a LH pathway proceeding through a carbonate intermediate was switched on, showing an increased TOF by an order of magnitude.

1:30 PM **Tue-MEBR-1330 Selective Hydrogenation of Unsaturated Aldehydes Using Single-Atom Alloy Catalysts.**

Yueqiang Cao<sup>1,2</sup>, Tongxin Han<sup>1</sup>, Bo Chen<sup>1</sup>, Yuanyuan Li<sup>3</sup>, Xinggui Zhou<sup>2</sup>, Anatoly Frenkel<sup>3</sup> and **Francisco Zaera**<sup>1</sup>, (1)*University of California, Riverside, USA*, (2)*East China University of Science and Technology, China*, (3)*Stony Brook University, USA.*

**Short Summary:**

Bimetallic CuPt<sub>x</sub>/SBA-15 catalysts were tested for the selective hydrogenation of unsaturated aldehydes. Catalysts with x = 0.001 to 0.05 proved quite selective toward the desired unsaturated alcohol. However, *in situ* adsorption experiments failed to identify any Pt surface atoms. The role of Pt is complex and not fully understood.

1:50 PM **Tue-MEBR-1350 Low Temperature CO Oxidation over Isolated Cobalt Ions in Nitrogen-Doped Carbon.**

**Colby A. Whitcomb**<sup>1</sup>, Raymond R. Unocic<sup>2</sup> and Robert J. Davis<sup>1</sup>, (1)*University of Virginia, USA*, (2)*Oak Ridge National Laboratory, USA.*

**Short Summary:**

Oxidation of CO at low temperature is very rapid over Co atoms loaded onto nitrogen-doped carbon compared to supported Co oxide. Steady-state isotopic transient kinetic analysis revealed a low coverage of intermediates leading to carbon dioxide on the isolated Co atoms and a high intrinsic turnover frequency at 273 K.

2:10 PM **Tue-MEBR-1410 Photolysis for Probing Reaction Mechanisms and Promoting Rates on Atomically Dispersed Rh Catalysts.**

**Emily Schroeder** and Phillip Christopher, *University of California, Santa Barbara, USA.*

**Short Summary:**

The photolysis of Rh-CO bonds on supported atomically dispersed Rh catalysts is explored for promoting catalytic rates of CH<sub>4</sub> conversion to C1 and C2 liquid oxygenates and understanding fast elementary steps in CH<sub>4</sub> oxidation and NO reduction chemistry through observation of ephemeral reaction intermediates by cryogenic *in-situ* FTIR spectroscopy.

2:30 PM **Tue-MEBR-1430** Accelerated Cu<sub>2</sub>O Reduction By Single Pt Atoms at the Metal-Oxide Interface.

Kyle Groden<sup>1</sup>, Alex C. Schilling<sup>2</sup>, Juan Pablo Simonovis<sup>3</sup>, Adrian Hunt<sup>3</sup>, Ryan Hannagan<sup>2</sup>, Iradwikanari Waluyo<sup>3</sup>, E. Charles H. Sykes<sup>2</sup> and **Jean-Sabin McEwen<sup>1</sup>**, (1)Washington State University, USA, (2)Tufts University, USA, (3)Brookhaven National Laboratory, USA.

**Short Summary:**

Ambient-pressure XPS reveals that the presence of a small amount of Pt under the oxide layer can promote the reduction of Cu<sub>2</sub>O by H<sub>2</sub>. We built two density functional theory based models that demonstrate how isolated Pt atoms at the metal/oxide interface helps maintain the reduced state of the catalyst.

2:50 PM **Tue-MEBR-1450** Single Atom Alloys 2.0: Exploiting Undercoordination for Stronger Dissociative CH<sub>4</sub> Chemisorption.

**Debtanu Maiti**, Michael P. Harold and Lars C. Grabow, *University of Houston, USA*.

**Short Summary:**

We explored the role of single atom dopants of transition metals on PGM(211) facets towards C-H bond activation. We elaborate on the segregation behavior of dopants to the edge sites from subsurface and terrace sites and find that locally induced expansive strain on the undercoordinated edge sites improves CH<sub>4</sub> activation.

## Fundamentals of Catalysis: Atomically Dispersed Species II

**Session Chairs:** Phillip Christopher, *University of California, Santa Barbara, USA* and Krijn P. de Jong, *Utrecht University, Netherlands*.

3:30 PM **Tue-MEBR-1530** Theoretical Insights into Ethylene Hydroformylation and Hydrogenation on Atomically Dispersed Rh-Oxide Promoter Pairs on  $\gamma$ -Al<sub>2</sub>O<sub>3</sub>.

**Seungyeon Lee<sup>1</sup>**, Ji Qj<sup>2</sup>, Insoo Ro<sup>2</sup>, Phillip Christopher<sup>2</sup>, Dionisios G. Vlachos<sup>1</sup> and Stavros Caratzoulas<sup>1</sup>, (1)University of Delaware, USA, (2)University of California, Santa Barbara, USA.

**Short Summary:**

We provide mechanistic insights into atomically dispersed Rh-oxide promoter pairs and how the changes in the electronic structure of Rh brought by oxide promoters prompt enhanced hydroformylation activity. We report bifunctional mechanisms at the Rh-W interface via WO<sub>x</sub> reduction, which is crucial for the high activity of this pair site.

3:50 PM **Tue-MEBR-1550** Impact of Nuclearity of Pt Supported on Fe<sub>3</sub>O<sub>4</sub> on Hydrogenation and Aldol Condensation Reactions.

**Honghong Shi<sup>1</sup>**, Shiva Murali<sup>1</sup>, Yubing Lu<sup>2</sup>, Yifeng Zhu<sup>3</sup>, Fan Lin<sup>1</sup>, Johannes A. Lercher<sup>1</sup>, Huamin Wang<sup>1</sup> and Oliver Y. Gutierrez<sup>1</sup>, (1)Pacific Northwest National Laboratory, USA, (2)Lawrence Berkeley National Laboratory, USA, (3)Fudan University, China.

**Short Summary:**

A series of Fe<sub>3</sub>O<sub>4</sub>-supported Pt catalysts with varying nuclearity were tested in CO<sub>2</sub> hydrogenation and aldol condensation of acetone. We provide general structure-activity correlations that apply across dissimilar reactions catalyzed by highly dispersed metal centers. These correlations will help predict catalytic behavior for different, even unexplored, reactions.

4:10 PM **Tue-MEBR-1610** Single-Atom Alloy Catalysts: Born in a Vacuum, Tested in Reactors, and Understood in silico.

**E. Charles H. Sykes**, *Tufts University, USA*.

**Short Summary:**

Single-Atom Alloys represent a promising new class of heterogeneous catalyst in which precious metals are utilized at the ultimate limit of atom efficiency. The simplicity of these active sites makes unambiguous modelling with theory possible, and several recent examples of new single-atom alloy catalysts for (de)hydrogenation reactions will be given.

4:30 PM **Tue-MEBR-1630** Communication between Oxide-Supported Metal Catalysts and TiO<sub>2</sub> Dilutants: The Effects of Metal Migration and Carbon Transfer on the Reverse Water-Gas Shift Reaction.

Linxiao Chen, Nicholas Nelson and **Janos Szanyi**, *Pacific Northwest National Laboratory, USA*.

**Short Summary:**

The rWGS reaction at 673 K results in the transfer of metals onto oxide dilutants leading to increases in catalytic activities while at 523 K brings about an activity decrease. This work elucidates the communication between catalysts and dilutants, which has general implications in catalysis and resolves literature inconsistencies.

## Rendezvous Trianon

### TUESDAY MORNING

#### Transient Approaches for Catalyst Characterization

**Session Chairs:** Michael P. Harold, *University of Houston, USA* and Norbert Kruse, *Pacific Northwest National Laboratory, USA*.

9:30 AM **Tue-RZVS-0930** Application of Frequency Response Methods for Heterogeneous Catalysis: Modulation Excitation Spectrokinetic Analysis (MESKA).

Hongda Zhu, Priya Darshini Srinivasan, Bhagyasha Patil, Alejandra Torres-Velasco and **Juan Bravo Suárez**, *The University of Kansas, USA*.

**Short Summary:**

This work advances frequency response techniques in heterogeneous catalysis for the in situ/operando spectroscopic discrimination of surface intermediate species and to determine reaction rate parameters in elementary steps of catalytic mechanisms.

9:50 AM **Tue-RZVS-0950** Can CO<sub>2</sub> Oxidize Ni? A QXAS Answer.

**Valentijn De Coster**, Nadadur Veeraraghavan Srinath, Parviz Yazdani, Hilde Poelman and Vladimir V Galvita, *Ghent University, Belgium*.

**Short Summary:**

The oxidative effect of CO<sub>2</sub> on Ni remains unclear to date. In situ Quick-XAS and H<sub>2</sub>/CO<sub>2</sub>-redox experiments on Ni/MgAl<sub>2</sub>O<sub>4</sub> and unsupported Ni reveal that strong metal-support interactions can facilitate Ni oxidation by CO<sub>2</sub>. This adds major insight into the redox behavior of Ni-based CO<sub>2</sub> utilization catalysts.

10:10 AM **Tue-RZVS-1010** Time Resolved XAS of Cu-CHA during the Standard SCR Reaction.

**Husn Islam**<sup>1</sup>, Loredana Mantarosie<sup>1</sup>, Roberta Villamaina<sup>1</sup>, Maria Pia Ruggeri<sup>1</sup>, Monica Amboage<sup>2</sup>, Yiyun Liu<sup>3</sup>, Iain Hitchcock<sup>1</sup>, Silvia Alcove Clave<sup>1</sup>, Federica Gramigni<sup>4</sup>, Umberto Iacobone<sup>4</sup>, Nicola Usberti<sup>4</sup>, Nicole Daniela Nasello<sup>4</sup>, Isabella Nova<sup>4</sup>, Enrico Tronconi<sup>4</sup> and Jillian Collier<sup>1</sup>, (1)*Johnson Matthey Technology Centre, United Kingdom*, (2)*Diamond Light Source, United Kingdom*, (3)*University College London, United Kingdom*, (4)*Politecnico di Milano, Italy*.

**Short Summary:**

In this work, X-ray absorption spectroscopy (XAS) was used operando to investigate the evolution of Cu species in Cu-CHA catalysts during the reduction and re-oxidation half cycles of the standard ammonia-SCR reaction.

10:30 AM **Tue-RZVS-1030** Resolving Surface Species and Their Role in Reaction Mechanism By Manipulating the Approach to Equilibrium.

**Rebecca Fushimi**<sup>1</sup>, Yixiao Wang<sup>1</sup>, Sagar Sourav<sup>1,2</sup>, Ross Kunz<sup>1</sup> and Gregory Yablonsky<sup>3</sup>, (1)*Idaho National Laboratory, USA*, (2)*Lehigh University, USA*, (3)*Washington University in St. Louis, USA*.

**Short Summary:**

This work presents a general methodology for resolving different surface species, their surface lifetimes and role in reaction mechanism for diverse catalytic systems by manipulating the approach to equilibrium through controlled pulsing of labeled reactant and product gases.

10:50 AM **Tue-RZVS-1050** A Modified Steady State Isotopic Transient Kinetic Analysis (SSITKA) Instrument to Probe CO Oxidation on Model Pd Catalysts.

**Eric High** and Christian Reece, *Harvard University, USA*.

**Short Summary:**

Pulse-out measurements, in which one or more reactants are temporally removed from the stream, on the modified steady-state isotopic transient kinetic analysis (SSITKA) instrument described in this work demonstrated a unique ability to modulate the state of a model Pd catalyst and rationalize kinetic parameters observed at steady-state.

11:10 AM **Tue-RZVS-1110** In Situ UV-Vis Spectrokinetic Studies for Understanding Gold-Support Interactions in the Catalytic Oxidation of Ethanol. Hongda Zhu, Juan Bravo Suárez, Bhagyesha Patil and **Alejandra Torres-Velasco**, *The University of Kansas, USA*.

**Short Summary:**

This work combines novel analysis methods with insitu spectroscopic measurements to provide relevant kinetic information. We found that absorbance differences decreased with support reducibility. Also spectrokinetic analysis correlating CT with ethanol conversion rate during O<sub>2</sub> modulation leads to hydroperoxides as the most likely active oxygen species involved in ethanol oxidation.

11:30 AM **Tue-RZVS-1130** In Situ Spectroscopy and Kinetic Studies of Vapor Phase Selective Oxidation of Ethanol on Supported Gold Catalysts.

**Bhagyesha Patil**, Priya D. Srinivasan and Juan Bravo Suárez, *The University of Kansas, USA*.

**Short Summary:**

This work focuses on understanding of the effect of supports on vapor phase selective oxidation of ethanol to acetic acid catalyzed by gold catalysts by means of in situ spectroscopic characterization techniques such as ME-PSD-DRIFTS and Au-SPR UV-Vis with the combination of kinetics.

## TUESDAY AFTERNOON

### Electrode-Electrolyte Interaction and Thin Films

**Session Chairs:** Daniel Esposito, *Columbia University, USA* and Astrid Müller, *University of Rochester, USA*.

1:10 PM **Tue-RZVS-1310** Cooperative Site and Electrolyte Design for Optimizing Interfacial Electrokinetics of CO<sub>2</sub> Reduction.

**Tianyou Mou**, Xue Han, Hemanth Somarajan Pillai, Huiyuan Zhu and Hongliang Xin, *Virginia Polytechnic Institute and State University, USA*.

**Short Summary:**

A surface-electrolyte interface model was developed for understanding reaction mechanisms of CO<sub>2</sub> reduction and show that by cooperatively tailoring the active Bi sites via doping and heterocyclic cations of ionic liquids, interfacial electrokinetics of CO<sub>2</sub>RR can be greatly enhanced while suppressing hydrogen evolution.

1:30 PM **Tue-RZVS-1330** The Role of Organic Co-Catalyst in the Electrochemical CO<sub>2</sub> Reduction Reaction.

**Foeroogh Khezeli**, S M Rezwanul Islam and Craig Plaisance, *Louisiana State University, USA*.

**Short Summary:**

This research showed dissociatively adsorption of DMIM to exposed Mo sites of MoS<sub>2</sub> via the C-4 and C-5 carbons in the ring for Electrochemical CO<sub>2</sub>RR. This species can then activate CO<sub>2</sub> on the C-2 carbon to form a -CO<sub>2</sub>H intermediate with a activation free energy barrier of only 0.79 eV.

1:50 PM **Tue-RZVS-1350** Electrocatalytic Hydrogenation of Benzaldehyde in Aqueous Phase – Impact of Electrolyte Composition on Catalyst Performance.

**Philipp Fischer**<sup>1</sup>, Yue Liu<sup>2</sup>, Andreas Jentys<sup>1</sup> and Johannes A. Lercher<sup>1,3</sup>, (1)Technical University of Munich, Germany, (2)East China Normal University, China, (3)Pacific Northwest National Laboratory, USA.

**Short Summary:**

Electrocatalytic hydrogenation (ECH) is a promising, sustainable technology for the ambient reduction of organic molecules. The activity and Faradaic efficiency of noble metal-based catalysts in ECH of biomass-derived feedstocks depends on the electrolyte composition and can be related to changing thermodynamic properties, e.g., binding strength, of electrochemically generated hydrogen.

2:10 PM **Tue-RZVS-1410** Impact of Ionomer Coatings on Catalyst Microenvironments for Electrochemical Reduction of Carbon Dioxide on Copper Catalyst.

**Chanyeon Kim**<sup>1,2</sup>, Justin C. Bui<sup>1,2</sup>, Xiaoyan Luo<sup>2</sup>, Jason K. Cooper<sup>2</sup>, Ahmet Kusoglu<sup>2</sup>, Adam Z. Weber<sup>2</sup> and Alexis T. Bell<sup>1,2</sup>, (1)University of California, Berkeley, USA, (2)Lawrence Berkeley National Laboratory, USA.

**Short Summary:**

Here, we demonstrate how tailored microenvironments can be achieved for selective formation of C<sub>2+</sub> products by layering ionomer coatings on Cu. We also show how this knowledge along with prior knowledge about the effects of pulsed electrolysis enables attainment of exceptionally high C<sub>2+</sub> product formation rates.

2:30 PM **Tue-RZVS-1430** CO<sub>2</sub>RR-to-C<sub>2</sub> Driven By Confined Self-Assembled Monolayer Modulated Metal Interfaces.

**Mingyu Wan**, Zhiyong Gu and Fanglin Che, University of Massachusetts Lowell, USA.

**Short Summary:**

A novel catalyst, aminothiolate self-assembled monolayer (SAM) modulated Cu, was designed to potentially provide hybrid organic-inorganic active sites, hydrogen bond effect, confinement effect, highly localized electric fields and changes in the surface's dipole moment and polarizability, thus promote CO<sub>2</sub> reduction to C<sub>2</sub>.

2:50 PM **Tue-RZVS-1450** Incorporating Electrode-Electrolyte Interfacial Effects on Electrocatalytic Reaction Barriers and Ion Adsorption.

**Naveen Agrawal**, Bolton Tran, Andrew Wong, Sharad Maheshwari and Michael Janik, The Pennsylvania State University, USA.

**Short Summary:**

We demonstrate a new computationally efficient and transferable approach to incorporate interfacial effects on charge transfer energetics that uses DFT calculations to quantify the local electronic structure of electron/ion transition states then combine this with double-layer theory and a force-field molecular dynamics to capture the dynamic effects of the electrolyte/solvent.

## Electrocatalytic CO<sub>2</sub> Reduction

**Session Chairs:** Feng Jiao, University of Delaware, USA and Joshua Schaidle, National Renewable Energy Laboratory, USA.

3:30 PM **Tue-RZVS-1530** Electrosynthesis of Propane Enabled By Imidazolium-Functionalized Transition Metal Phosphide.

**Mohammadreza Esmailirad**, Alireza Kondori, Ahmad Mosen Harzandi and Mohammad Asadi, Illinois Institute of Technology, USA.

**Short Summary:**

A highly efficient electrocatalyst has been developed for eCO<sub>2</sub>RR. Our electrochemical results reveal that this catalyst is mainly selective toward C<sub>3</sub>H<sub>8</sub> production. This catalyst exhibits a remarkable C<sub>3</sub>H<sub>8</sub> current density and turnover frequency of -361.2 mA/cm<sup>2</sup> and 0.29 s<sup>-1</sup>, respectively, at a potential of -0.8 V vs. RHE.

3:50 PM **Tue-RZVS-1550** Asymmetrical C-C Coupling for Electroreduction of CO to Acetate.

**Hao Shen**, Yunzhe Wang, Tim Mueller and Chao Wang, Johns Hopkins University, USA.

**Short Summary:**

We report selective reduction of CO to acetate using Cu-Pd bimetallic electrocatalysts. High activity and selectivity are demonstrated for CO-to-acetate conversion with >200 mA/cm<sup>2</sup> in current density and >65% in Faradaic efficiency. An asymmetrical C-C coupling mechanism is developed to understand the composition-dependent catalytic performance and high selectivity toward acetate.

4:10 PM **Tue-RZVS-1610** Transition Metal Nitrides As Promising Catalyst Supports for Tuning CO/H<sub>2</sub> Syngas Production from Electrochemical CO<sub>2</sub> Reduction.

**Akash Biswas**<sup>1</sup> and Jingguang Chen<sup>1,2</sup>, (1)Columbia University, USA, (2)Brookhaven National Laboratory, USA.

**Short Summary:**

Palladium-modified transition metal nitrides are investigated as electrochemical CO<sub>2</sub> reduction reaction (CO<sub>2</sub>RR) catalysts. Combined in-situ X-ray characterization and density functional theory results demonstrate niobium nitride as an effective support material to enhance CO<sub>2</sub>RR activity. This study provides a comprehensive understanding of how nitride support materials modify catalyst properties and activity.

4:30 PM **Tue-RZVS-1630** 'Microphone' Structured Bismuth/Cuprasulfide Promoting Electrochemical Reduction of CO<sub>2</sub> to Formate.

**Xue Han**, Virginia Polytechnic Institute and State University, USA.

**Short Summary:**

This work highlights a unique interfacial design strategy of *p*-block metal and transition metal chalcogenide (Bi-Cu<sub>2</sub>S) heterostructures to fine tailor active sites for advanced electrocatalysis.



4:50 PM **Tue-RZVS-1650** Ligand-Free Silver Nanoparticles for CO<sub>2</sub> Electrocatalytic Reduction to CO.

**Francesco Mattarozzi**, Petra E. de Jongh and Peter Ngene, *Utrecht University, Netherlands*.

**Short Summary:**

In this work, we report a strategy to synthesize ligand-free silver nanoparticles on high surface area carbon materials via incipient wetness impregnation for the CO<sub>2</sub> electrocatalytic reduction. We correlated specific electrochemistry parameters, such as CO faradaic efficiency and current density, to the particle size and catalyst surface properties.

5:10 PM **Tue-RZVS-1710** Cu-Based Nanoparticles for the Electrochemical Reduction of CO<sub>2</sub>.

**Bokki Min** and Huiyuan Zhu, *Virginia Polytechnic Institute and State University, USA*.

**Short Summary:**

Copper (Cu), as an inexpensive and earth-abundant metal electrocatalyst, converts CO<sub>2</sub> into valuable chemicals and fuels, especially for C<sub>2+</sub> products. We alloyed Cu with nickel (Ni) to promote C-C coupling and investigate the structural evolution during CO<sub>2</sub> reduction reaction.

## Sutton North

### TUESDAY MORNING

#### Catalytic Conversion of Plastics II

**Session Chairs:** Yi Du, *ExxonMobil Research and Engineering, USA* and Cody J. Wrasman, *National Renewable Energy Laboratory, USA*.

9:30 AM **Tue-SUNO-0930** The Essential Effect of Support Acidity on the Tandem Conversion of Polyethylene to Alkylaromatics..

**Jiakai Sun**, Yu-Hsuan Lee, Mahdi M. Abu-Omar and Susannah L. Scott, *University of California, Santa Barbara, USA*.

**Short Summary:**

Model reactions reveal that the catalyst support dramatically affects the activity in the tandem depolymerization of polyolefins. The origin of the effect is proposed to be the strength of the acid sites, which must be present in addition to the metal, and can be used to tune the product distribution.

9:50 AM **Tue-SUNO-0950** Plastic Waste Hydroconversion.

**Pavel Kots**, Brandon Vance and Dionisios G. Vlachos, *University of Delaware, USA*.

**Short Summary:**

We have identified suitable catalysts where the hydroconversion strategy enables high yields of diesel, gasoline, and jet fuel hydrocarbons up to 80% total liquid product yield from polyethylene or polypropylene plastic waste.

10:10 AM **Tue-SUNO-1010** Shape and Size-Controlled ZnO for the Microwave-Assisted Depolymerization of PET.

**Esun Selvam**, Raul F. Lobo and Dionisios G. Vlachos, *University of Delaware, USA*.

**Short Summary:**

Glycolysis has been identified as a promising chemical depolymerization method for the recycling of PET. In this study, we illustrate the use of cheap, non-toxic, and reusable ZnO catalysts for the glycolysis of PET, along with the use of microwaves to achieve this in a cost-effective and energy-efficient fashion.

10:30 AM **Tue-SUNO-1030** Thermodynamic and Kinetic Studies of Model Systems for Polyolefin Upcycling in Acidic Ionic Liquids.

**Lillian Hale**<sup>1</sup>, Lennart Wahl<sup>2</sup>, Wei Zhang<sup>2</sup>, Sungmin Kim<sup>1</sup>, Jian Zhi Hu<sup>1</sup>, Donald M. Camaioni<sup>1</sup>, Oliver Y. Gutierrez<sup>1</sup> and Johannes A. Lercher<sup>1</sup>, (1)*Pacific Northwest National Laboratory, USA*, (2)*Technical University of Munich, Germany*.

**Short Summary:**

We provide a low temperature method to convert polymers into light isoalkanes with acidic ionic liquids, an unprecedented approach towards upcycling. Here we utilize model compounds to understand the elementary steps and the kinetic and thermodynamic handles available to tune the product distribution.

10:50 AM **Tue-SUNO-1050** Assessing Transport Limitations in the Catalytic Cracking of Polypropylene over a Waste Refinery Catalyst.

**Sebastian Rejman**, Ina Vollmer and Bert M. Weckhuysen, *Utrecht University, Netherlands*.

**Short Summary:**

Catalytic cracking is a promising technology to convert polyolefin waste into value-added products, such as aromatics, on a large scale. In this work we show that circumventing the mass transport limitations in the catalytic cracking of polypropylene could decrease the required reaction temperature to < 300°C.

11:10 AM **Tue-SUNO-1110** Molecular Redistribution of Alkanes and the Chemical Upcycling of Low-Density Polyethylene.

**Doyoung Kim**<sup>1</sup>, Zachary R. Hinton<sup>1</sup>, Peng Bai<sup>1,2</sup>, Thomas H. Epps, III<sup>1</sup>, LaShanda T. J. Korley<sup>1</sup> and Raul F. Lobo<sup>1</sup>, (1)*University of Delaware, USA*, (2)*University of Massachusetts Amherst, USA*.

**Short Summary:**

The W/SiO<sub>2</sub>-driven alkane metathesis system demonstrates remarkable potential for the chemical upcycling of low-density polyethylene at 300°C for 3 hours and the capacity to produce solid products of homogenous molecular weight distributions with the greatest reduction in the average molecular weight (Mw) by 99 % and polydispersity over 6-fold.

11:30 AM **Tue-SUNO-1130** Catalytic Depolymerization of Waste Polyolefins By Induction Heating: Selective Alkane/Alkene Production. Bernard Whajah<sup>1</sup>, Natalia da Silva Moura<sup>1</sup>, Justin Blanchard<sup>1</sup>, Scott Wicker<sup>2</sup>, Joseph Heil<sup>3</sup>, Karleigh Gandar<sup>4</sup>, Kerry Dooley<sup>1</sup> and **James Dorman<sup>1</sup>**, (1) *Louisiana State University, USA*, (2) *Rhodes College, USA*, (3) *LeTourneau University, USA*, (4) *Baton Rouge Community College, USA*.

**Short Summary:**

This work uses induction heating to locally heat metal oxide and zeolite-based catalysts for the selective depolymerization of plastic wastes. The iron oxide-catalyst structures generate narrow product distributions with tunability between light gases or light liquids with high depolymerization rates and limited coke/methane formation.

## TUESDAY AFTERNOON

### Catalytic Conversion of Plastics III

**Session Chairs:** Nathaniel Eagan, *Tufts University, USA* and Rebecca Fushimi, *Idaho National Laboratory, USA*.

1:10 PM **Tue-SUNO-1310** Implications of the Presence of Common Additives in Thermal and Catalytic Polyethylene Depolymerization.

**Ana Carolina Jerdy<sup>1</sup>**, Tram Pham<sup>1</sup>, Pascale Atallah<sup>2</sup>, David Soules<sup>2</sup>, Ron Abbott<sup>2</sup>, Lance Lobban<sup>1</sup> and Steven P. Crossley<sup>1</sup>, (1) *University of Oklahoma, USA*, (2) *Chevron Phillips Chemical Company LP, USA*.

**Short Summary:**

Chemical recycling is a promising approach to lessen the environmental impact of plastic waste generation. In this work, we analyze how the presence of four common polymer additives affect chemical upcycling reactions of polyethylene. Further, we show how some of these impurities can deposit and modify acid catalysts.

1:30 PM **Tue-SUNO-1330** Upcycling Polyolefin Plastics to Lighter Alkanes By Hydrogenolysis over Supported Ru Catalysts.

**Linxiao Chen<sup>1</sup>**, Yifeng Zhu<sup>1</sup>, Laura C. Meyer<sup>1</sup>, Lillian Hale<sup>1</sup>, Xavier Isidro Pereira Hernandez<sup>1</sup>, Debora Meira<sup>2</sup>, Libor Kovarik<sup>1</sup>, Mark Engelhard<sup>1</sup>, Johannes A. Lercher<sup>1</sup>, Oliver Y. Gutierrez<sup>1</sup> and Janos Szanyi<sup>1</sup>, (1) *Pacific Northwest National Laboratory, USA*, (2) *Argonne National Laboratory, USA*.

**Short Summary:**

This work demonstrates the upcycling of polypropylene and polyethylene for plastic waste upcycling over supported Ru catalysts. Effects of reaction conditions, catalyst support, and Ru particle size are presented, offering valuable insights into reaction mechanisms and structure-function relationship that instructs future catalyst design.

1:50 PM **Tue-SUNO-1350** Catalytic Upcycling of Oxygenated Plastic Waste.

Andrew Jaeschke, **Michael Royko** and Jochen Lauterbach, *University of South Carolina, USA*.

**Short Summary:**

This work investigates the potential for upcycling of overlooked waste plastics, such as polyols and polyurethanes, using zeolite catalysts. Although this work has demonstrated the capabilities of zeolite catalysts to crack said plastics, there are still ongoing investigations regarding product yield before such a process can be commercially viable.

2:10 PM **Tue-SUNO-1410** Waste Plastic Upcycling By Pt/SrTiO<sub>3</sub> hydrogenolysis Catalysts with Controlled Support Shape, Particle Size, and Catalyst Dispersion.

**Ian Peczak<sup>1,2</sup>** and Kenneth R. Poeppelmeier<sup>1</sup>, (1) *Northwestern University, USA*, (2) *Argonne National Laboratory, USA*.

**Short Summary:**

We report a synthesis for Pt/SrTiO<sub>3</sub> polymer upcycling catalysts with controlled Pt particle size and distribution. These catalyst properties have been studied and modeled to fundamentally understand both the driving forces behind their construction, and their impact on hydrogenolysis of waste polyolefins to highly uniform lubricant products.

2:30 PM **Tue-SUNO-1430** Developing a Mechanistic Framework for Polyolefin Hydroconversion.

**Brandon Vance**, Pavel Kots, Cong Wang and Dionisios G. Vlachos, *University of Delaware, USA*.

**Short Summary:**

Polyolefin hydroconversion is promising for deconstructing polyolefin waste to valuable products. However, there is limited fundamental knowledge available for deconstructing polyolefin substrates. This work establishes mechanistic frameworks for polyolefin hydrocracking and hydrogenolysis by altering the catalyst composition, conducting time-dependent experiments, and comparing the reactivity trends with trends over model alkanes.

2:50 PM **Tue-SUNO-1450** Effects of Branching on the Hydrogenolysis of Heptane Isomers.

**Olajide Bamidele** and Andreas Heyden, *University of South Carolina, USA*.

**Short Summary:**

Hydrogenolysis has been proposed for upcycling of plastic wastes. Pt catalysts are often used for polyolefin processing at both low and high hydrogen pressures, but there is currently only a limited understanding of the active site and how polymer branching affects the reaction, which we computationally investigated from first principles.

## Pyrolysis: Catalysis and Upgrading

**Session Chairs:** Torren Carlson, *Anellotech*, and Siddarth Krishna, *University of Wisconsin, Madison, USA*.

3:30 PM **Tue-SUNO-1530** Low Carbon Transportation Fuel from Lignocellulosic Biomass Via Catalytic Fast Pyrolysis and Hydrotreating.

Kristiina Iisa<sup>1</sup>, Calvin Mukarakate<sup>1</sup>, Huamin Wang<sup>2</sup>, Daniel Santosa<sup>2</sup>, Susan E. Habas<sup>1</sup>, Kinga A. Unocic<sup>3</sup>, Bruce Adkins<sup>3</sup>, Nolan Wilson<sup>1</sup>, Mark Nimlos<sup>1</sup>, Abhijit Dutta<sup>1</sup>, Joshua Schaidle<sup>1</sup> and **Michael B. Griffin<sup>1</sup>**, (1)*National Renewable Energy Laboratory, USA*, (2)*Pacific Northwest National Laboratory, USA*, (3)*Oak Ridge National Laboratory, USA*.

**Short Summary:**

This presentation will feature recent advancements in ex situ CFP with co-fed hydrogen to enable the production of gasoline, diesel, and jet range fuels with a modelled selling price of < \$3.00 GGE and a >70% reduction in greenhouse gas emissions compared to fossil-based pathways.

3:50 PM **Tue-SUNO-1550** Kerr-Gated Raman Spectroscopy to Study Steps in Catalytic Fast Pyrolysis on Zeolite Catalysts.

**Emma Campbell<sup>1,2</sup>**, Andrew M. Beale<sup>3</sup>, Ines Lezcano-Gonzalez<sup>3</sup>, Igor Sazanovich<sup>4</sup>, Michael Watson<sup>5</sup> and Michael Towrie<sup>4</sup>, (1)*Cardiff University, United Kingdom*, (2)*UK Catalysis Hub, United Kingdom*, (3)*University College London, United Kingdom*, (4)*Central Laser Facility, United Kingdom*, (5)*Johnson Matthey Technology Centre, United Kingdom*.

**Short Summary:**

In this work we use a technique known as optical Kerr-gating to cut fluorescence from the detector that usually prevents Raman signals from being detected in such applications. Upgrading of biomass has been studied by operando Kerr-gated Raman spectroscopy, through the conversion of model compounds of biomass on zeolite catalysts.

4:10 PM **Tue-SUNO-1610** Catalytic Fast Pyrolysis on H-ZSM-5 Zeolite: Activity and Stability of N.N.N. Pairs of Al Atoms during Anisole Transformation.

**Nathan Pichot<sup>1</sup>**, Ludovic Pinard<sup>1</sup> and Anthony Dufour<sup>2</sup>, (1)*Université de Poitiers, France*, (2)*Université de Lorraine, France*.

**Short Summary:**

The transformation of the anisole highlights the significant role of the distribution of aluminum in the zeolite framework for the activity and the stability of the catalyst in the context of catalytic fast pyrolysis of biomass, notably of the Next Nearest Neighbour pairs of Al atoms.

4:30 PM **Tue-SUNO-1630** Hydrotreatment of Catalytic Fast Pyrolysis Oil to Renewable Fuels.

**Magnus Stummann<sup>1</sup>**, Christian Ejersbo Strebøl<sup>1</sup>, Jostein Gabrielsen<sup>1</sup>, David Dayton<sup>2</sup> and Ofel Mante<sup>2</sup>, (1)*Haldor Topsøe A/S, Denmark*, (2)*RTI International, USA*.

**Short Summary:**

A toluene extract of a catalytic fast pyrolysis oil was hydrotreated in a pilot plant, which showed that combining fractionation of pyrolysis oil with hydrotreating makes it possible to produce liquid fuels with a low oxygen content (<1 wt %), a high carbon recovery (99 %) in the oil.

4:50 PM **Tue-SUNO-1650** Deactivation By Potassium Accumulation on a Pt/TiO<sub>2</sub> Bifunctional Catalyst for Biomass Catalytic Fast Pyrolysis.

**Fan Lin<sup>1</sup>**, Yubing Lu<sup>1</sup>, Kinga A. Unocic<sup>2</sup>, Susan E. Habas<sup>3</sup>, Michael B. Griffin<sup>3</sup>, Joshua Schaidle<sup>3</sup>, Harry Meyer III<sup>2</sup>, Yong Wang<sup>1,4</sup> and Huamin Wang<sup>1</sup>, (1)*Pacific Northwest National Laboratory, USA*, (2)*Oak Ridge National Laboratory, USA*, (3)*National Renewable Energy Laboratory, USA*, (4)*Washington State University, USA*.

**Short Summary:**

In biomass catalytic fast pyrolysis catalyzed by Pt/TiO<sub>2</sub>, deposition of potassium contaminants from feedstock causes catalyst deactivation. We demonstrate that the deactivation of Pt/TiO<sub>2</sub> by K is caused by sequential poisoning of strong Lewis acid sites followed by metal-support interfacial sites. An approach for regenerating K-deactivated Pt/TiO<sub>2</sub> catalyst was developed.

5:10 PM **Tue-SUNO-1710** Probing Mo<sub>2</sub>C Deactivation during HDO of Biomass Pyrolysis Vapors and Acetic Acid: Correlating Active Sites with Catalytic Activity.

**Matthew M. Yung**, Qiyuan Wu, Susan E. Habas, Joshua Schaidle and Michael B. Griffin, *National Renewable Energy Laboratory, USA*.

**Short Summary:**

Mo<sub>2</sub>C was tested for HDO of acetic acid and biomass pyrolysis vapors. Site titration to probe active sites and in-situ characterization showed coke formation as the main route of deactivation and both metallic and acidic sites decrease at the same relative rates, indicating a site agnostic mechanism.

## Sutton South

### TUESDAY MORNING

## Dynamic and Disordered Catalytic Systems and Catalysis in the Presence of a Liquid Phase

**Session Chairs:** Alyssa Hensley, *Washington State University, USA* and Alexander V. Mironenko, *University of Illinois Urbana-Champaign, USA*.

9:30 AM **Tue-SUSO-0930** Next Generation Quantum Chemistry of Water in Acidic Zeolites.

Henning Windeck<sup>1</sup>, Fabian Berger<sup>1</sup>, Kaido Sillar<sup>2</sup> and **Joachim Sauer<sup>1,3</sup>**, (1)*Humboldt-Universität zu Berlin, Germany*, (2)*University of Tartu, Estonia*, (3)*Charles University, Czech Republic*.

**Short Summary:**

A hybrid QM:QM method is used to get chemically accurate MP2-quality results (OH vibrational frequencies, <sup>1</sup>H-NMR chemical shifts) for different types of bridging OH groups in zeolite H-MFI and their interaction with one and two water molecules (heats of adsorption).

9:50 AM **Tue-SUSO-0950** Mechanistic Investigations at the Alumina/Water Interface.

Jérôme Rey<sup>1</sup>, Paul Clabaut<sup>1</sup>, Romain Réocreux<sup>2</sup>, Etienne Girel<sup>1,3</sup> and **Carine Michel<sup>1</sup>**, (1)Université de Lyon, CNRS, France, (2)University College, United Kingdom, (3)IFP Energies Nouvelles, France.

**Short Summary:**

Combining experiments and ab initio metadynamics, we provide the atomistic mechanism for the early-stage decomposition of  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> in liquid water but also the adsorption/desorption mechanism of (poly)-alcohols at the  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> / water interface. The present achievement constitutes an unprecedented milestone in the understanding of solid/liquid interface transformation.

10:10 AM **Tue-SUSO-1010** Kinetics of Acid-Catalyzed Dehydration of Biomass in Mixed Solvents Modelled By a Combined DFT and Classical MD Approach.

**Bolton Tran**, Michael Janik and Scott Milner, *The Pennsylvania State University, USA.*

**Short Summary:**

We introduce a novel multi-scale computational approach combining DFT with classical MD to model the kinetics of acid-catalyzed dehydration of biomass in mixed solvents. We validated this DFT/MD method by matching the absolute activation free energies to AIMD calculations, as well as relative activation free energies to experimental rate measurements.

10:30 AM **Tue-SUSO-1030** Molecular Simulations of Confined Solvent Dynamics and Its Impact on Catalysis.

**Alexander V. Mironenko**, *University of Illinois Urbana-Champaign, USA.*

**Short Summary:**

A solvent in a confined environment can dramatically alter catalytic reaction kinetics. Synergy between confinement, solvent, and substrate identity remains poorly understood. We carry out grand canonical Monte Carlo and QM/MM calculations to reveal solvent structure in pristine and defected zeolites and quantify its impact on intrinsic alkene oxidation energetics.

10:50 AM **Tue-SUSO-1050** Dynamic Evolution of Atomically Dispersed Catalysts.

**Nicholas Humphrey**, Selin Bac and Shaama Mallikarjun Sharada, *University of Southern California, USA.*

**Short Summary:**

This work studies the diffusion/stability of atomically dispersed catalysts with the use of ab-initio molecular dynamics under experimental conditions. We characterize migration events, coordination environments, hydrogen bonding events, and determine diffusion coefficients of Pt<sub>x</sub>/TiO<sub>2</sub> with simulation of common water-gas shift intermediates: H, O, CO, OH, CO<sub>2</sub>, COOH, CHO, and H<sub>2</sub>O.

11:10 AM **Tue-SUSO-1110** Bayesian Forcefield Driven Monte Carlo and Molecular Dynamics Simulations of O and Cl Promoted Ag Surface Reconstruction.

**Anna Sviripa<sup>1</sup>**, David Flaherty<sup>2</sup> and Christopher Paolucci<sup>1</sup>, (1)University of Virginia, USA, (2)University of Illinois Urbana-Champaign, USA.

**Short Summary:**

We performed Bayesian forcefield driven molecular dynamics and Monte Carlo simulations of oxygen and/or chlorine adsorbed on reconstructed Ag surfaces and observed dioxygen formation, surface and subsurface diffusion of oxygen and chlorine. Here we demonstrate how O and/or Cl affect Ag surface dynamics under ethylene epoxidation reaction conditions.

11:30 AM **Tue-SUSO-1130** Insights into the Electrocatalytic Hydrogen Evolution Reaction Mechanism on Pt<sub>7</sub>/Pt<sub>8</sub> Clusters Supported on ITO: The Role of Metastable Surface States.

**Simran Kumari** and Philippe Sautet, *University of California, Los Angeles, USA.*

**Short Summary:**

We find that Pt<sub>7</sub>H<sub>x</sub>/ITO is more active than Pt<sub>8</sub>H<sub>x</sub>/ITO for H<sub>2</sub> evolution. This activity difference is attributed to the higher number of surface states available for Pt<sub>7</sub> cluster. We go beyond CHE and include the Surface Charging method to define the interaction between species and electrode at specific potential.

## TUESDAY AFTERNOON

### Machine Learning in Catalysis: Applications and Interpretations

**Session Chairs:** Florian Göttl, *The University of Arizona, USA* and Zachary Ulissi, *Carnegie Mellon University, USA.*

1:10 PM **Tue-SUSO-1310** Advancing Catalytic Materials Discovery and Theoretical Knowledge with Interpretable Machine Learning.

**Hongliang Xin**, *Virginia Polytechnic Institute and State University, USA.*

**Short Summary:**

Advancing discovery of novel motifs with desired catalytic properties and scientific knowledge of chemical bonding by learning from data opens up new avenues toward artificial intelligence (AI) in catalysis.

1:30 PM **Tue-SUSO-1330** Development of Machine Learning Ruthenium-Water Interaction Potential.

**Dia Sahseh** and Andreas Heyden, *University of South Carolina, USA.*

**Short Summary:**

Machine learning approaches such as the Behler-Parrinello Neural Network were used to develop an accurate water-Ruthenium interaction potential. This potential can be used together with classical force fields to study solvation effects in heterogeneous catalysis of organic molecules adsorbed on Ru(0001) within our hybrid QM/MM free energy perturbation framework.

1:50 PM **Tue-SUSO-1350** Automated Discovery of Reaction Mechanisms Considering DFT-Based Uncertainties.

**Bjarne Kreitz**<sup>1</sup>, Khachik Sargsyan<sup>2</sup>, Katrín Blöndal<sup>1</sup>, Jongyoon Bae<sup>1</sup>, Emily Mazeau<sup>3</sup>, Richard West<sup>3</sup>, Gregor D. Wehinger<sup>4</sup>, Thomas Turek<sup>4</sup> and Franklin Goldsmith<sup>1</sup>, (1)Brown University, USA, (2)Sandia National Laboratories, USA, (3)Northeastern University, USA, (4)Clausthal University of Technology, Germany.

**Short Summary:**

A method was developed to include DFT-based uncertainties into the Reaction Mechanism Generator framework and applied to the CO<sub>2</sub> methanation on Ni(111). The discovered network and the activity of the catalyst vary significantly in the uncertainty domain, but this procedure provides new insights into the mechanism.

2:10 PM **Tue-SUSO-1410** Machine-Enabled Fast Exploration of Stable and Active Single Atom Catalyst for Oxygen Evolution Reaction.

**Woonghyeon Park**, Juhwan Noh, Geun Ho Gu and Yousung Jung, *Korea Advanced Institute of Science and Technology (KAIST), Korea, Republic of (South).*

**Short Summary:**

This work presents a high-throughput screening framework to accelerate new discovery of stable and active single atom catalysts on various oxides for oxygen evolution reaction in acidic media using machine learning and density functional theory calculations.

2:30 PM **Tue-SUSO-1430** Finding Electronic and Geometric Descriptors of Chemisorption for Alloys Using Unsupervised Machine Learning.

**Jacques Esterhuizen**<sup>1</sup>, Suljo Lincic<sup>2</sup> and Bryan Goldsmith<sup>1</sup>, (1)University of Michigan-Ann Arbor, USA, (2)University of Michigan, USA.

**Short Summary:**

We developed a data-driven workflow that allows us to identify accurate and interpretable electronic-structure-based chemisorption descriptors systematically.

2:50 PM **Tue-SUSO-1450** Electric Fields Accelerated Ammonia Synthesis: A Combination of Multi-Scale Simulation and Deep Learning Study.

**Fanglin Che**<sup>1</sup>, Jaime Notarangelo<sup>1</sup>, Han Yue<sup>2</sup> and Hongfu Liu<sup>2</sup>, (1)University of Massachusetts Lowell, USA, (2)Brandeis University, USA.

**Short Summary:**

This project performed deep-learning assisted DFT calculations and showed that positive electric fields lowered the energetics of ammonia synthesis from N<sub>2</sub> and shifted its mechanism without passing the kinetically unfavorable N<sub>2</sub> dissociation. This project will advance the chemical science and deep-learning model of field-dipole effects on accelerating carbon-free ammonia fuels.

## Porous Material Catalysts

**Session Chairs:** Brandon Bukowski, *Johns Hopkins University, USA* and Raffaele Cheula, *Politecnico di Milano, Italy*.

3:30 PM **KEYNOTE Tue-SUSO-1530 A High-Throughput Theory-Experiment Search for Metal-Organic Frameworks Supported Catalysts.** **Laura**

**Gagliardi**<sup>1</sup>, Daniel King<sup>1</sup>, Katherine McCullough<sup>2</sup>, Saamil Chhedal<sup>3</sup>, Magali Ferrandon<sup>2</sup>, Timothy Goetjen<sup>4</sup>, Zoha Syed<sup>4</sup>, Omar K. Farha<sup>4</sup> and Massimiliano Delferro<sup>2</sup>, (1)University of Chicago, USA, (2)Argonne National Laboratory, USA, (3)University of Minnesota, Twin Cities, USA, (4)Northwestern University, USA.

**Short Summary:**

Modeling single-site metal-oxide catalysts supported on metal-organic frameworks (MOFs) is a challenge and an opportunity. We drive high-throughput experimentation through data-driven algorithms and combine them with density functional theory calculations.

4:10 PM **Tue-SUSO-1610** MD Simulations with Chemical Accuracy – Alkane Reactivity in Acidic Zeolites.

**Fabian Berger**, Joachim Sauer and Marcin Rybicki, *Humboldt-Universität zu Berlin, Germany*.

**Short Summary:**

Standard AIMD simulations suffer from errors connected with the underlying DFT method. By parameterizing the difference between MP2 and DFT, the computational demand for MP2-quality MD is reduced from hundreds of years to a few weeks. This way, chemical accuracy is reached for alkane adsorption and cracking in acidic zeolites.

4:30 PM **Tue-SUSO-1630** Computational Raman Spectroscopy for the Study of Zeolite Self-Assembly to Calcined and As-Made Materials.

**Tongkun Wang**, Wei Fan, Scott M Auerbach and Song Luo, *University of Massachusetts Amherst, USA*.

**Short Summary:**

We computed Raman spectra for zeolites with organic structure directing agents and used Raman features we found to probe intermediate structures in synthesis and revealed possible defects.

4:50 PM **Tue-SUSO-1650** Developing Data-Driven Structure-Entropy Relations for Host-Guest Interactions in Siliceous Zeolites.

**Christopher Rzepa**<sup>1</sup>, Harold Hatch<sup>2</sup>, Vincent Shen<sup>2</sup>, Jeetain Mittal<sup>3</sup>, Daniel Siderius<sup>2</sup> and Srinivas Rangarajan<sup>1</sup>, (1)Lehigh University, USA, (2)National Institute of Standards and Technology, USA, (3)Texas A&M University, USA.

**Short Summary:**

The adsorption entropy of hydrocarbons on catalytic surfaces has been experimentally shown to correlate linearly with the adsorbate's standard gas-phase entropy. Herein, we apply simulations to broaden this dataset and employ data-driven models to understand the important structural and topological factors determining the thermochemistry of the host-guest interactions in zeolites.

5:10 PM **Tue-SUSO-1710** A Kinetic Exploration of the Methane-to-Methanol Energy Landscape for Direct Catalytic Conversion on Metal-Substituted SSZ-13.

Astrid Boje, Unni Engedahl, Henrik Grönbeck, Henrik Ström and **Anders Hellman**, *Chalmers University of Technology, Sweden*.

**Short Summary:**

We use first-principles based microkinetic modelling to investigate the catalytic conversion of methane to methanol. For Cu-SSZ-13, we consider the effect of water on the energy landscape and its implications for activity and degree of rate control. We further study other metal-substituted zeolites, comparing first-principles and scaling-relations based kinetic predictions.



## Trianon Ballroom

### TUESDAY MORNING

#### In Honor of NAM26 Distinguished Woman in Catalysis Edith Flanigen: Microporous Catalysts I

**Session Chairs:** Lin Luo, *The Dow Chemical Company, USA* and Susannah L. Scott, *University of California, Santa Barbara, USA*.

9:30 AM **KEYNOTE Tue-TRBR-0930 Challenges and Opportunities in Developing New Zeolite-Based Catalysts.** Stacey I. Zones, *Chevron Energy Technology Company, USA*.

**Short Summary:**

Zeolites continue to expand their role as important contributors in catalysis. And at present the feedstocks to create fuels and chemicals are changing with the emphasis on renewables and non crude oil sources. I will highlight the increasingly sophisticated catalysis control at the local level in the zeolite crystal.

10:10 AM **Tue-TRBR-1010** On the Route to Shape-Selective, Asymmetric Catalysis Using Chiral Molecular Sieves.

**Youngkyu Park**, Faisal Alshafei and Mark E. Davis, *California Institute of Technology, USA*.

**Short Summary:**

Sn-containing STW-type molecular sieves with high Si content have been synthesized using chiral di-quaternary organic structure-directing agents (OSDAs) prepared via a new synthetic route. Results of triose sugar conversion towards various alkyl lactates will be discussed in terms of shape- and enantio-selectivity using STW-type molecular sieves synthesized with enantiopure OSDAs.

10:30 AM **Tue-TRBR-1030** Identifying and Controlling Defects in Si-LTA Zeolite in Presence of F<sup>-</sup>.

**Song Luo**<sup>1</sup>, Tongkun Wang<sup>1</sup>, Jason Gulbinski<sup>1</sup>, Long Qi<sup>2</sup>, Geoffrey Tompsett<sup>3</sup>, Michael Timko<sup>3</sup>, Scott M Auerbach<sup>1</sup> and Wei Fan<sup>1</sup>, (1)*University of Massachusetts Amherst, USA*, (2)*USDOE Ames Laboratory, USA*, (3)*Worcester Polytechnic Institute, USA*.

**Short Summary:**

The structure-directing role of F<sup>-</sup> for double 4-membered rings during siliceous LTA synthesis was confirmed by utilizing Raman spectroscopy. The amount of F<sup>-</sup> required to synthesize siliceous LTA was substantially reduced by a factor of 6. We also found tetramethylammonium cations can precisely control the number of defects in LTA.

10:50 AM **Tue-TRBR-1050** Surfactant-Assisted Direct Crystallization of CON-Type Zeolites with Particle Size and Acid-Site Location Controlled.

Masato Sawada<sup>1</sup>, Takashi Takeuchi<sup>1</sup>, Takeshi Matsumoto<sup>1</sup>, Ryota Osuga<sup>2</sup>, Shuhei Yasuda<sup>1</sup>, Junko N. Kondo<sup>1</sup>, Hermann Gies<sup>3</sup> and **Toshiyuki Yokoi**<sup>1</sup>, (1)*Tokyo Institute of Technology, Japan*, (2)*Tohoku University, Japan*, (3)*Ruhr University Bochum, Germany*.

**Short Summary:**

We systematically investigated the direct synthesis of [Al, B]-CON borosilicate zeolites from a mother gel containing cetyltrimethylammonium bromide, CTAB. Finally, surfactant-assisted direct crystallization of CON-type zeolites with controlled particle size and acid-site location was achieved.

11:10 AM **Tue-TRBR-1110** A Time-Efficient Non-Corrosive Synthesis Method for Robust and Continuous b-Oriented ZSM-5 Zeolite Membranes on Coated Porous Ceramics of Various Silica-to-Alumina Ratios in Neutral Fluoride Media.

**Romy Riemersma**, Anne-Eva Nieuwelink, Eelco T.C. Vogt and Bert M. Weckhuysen, *Utrecht University, Netherlands*.

**Short Summary:**

During the synthesis of *b*-oriented ZSM-5 membranes, supported on porous coated alumina supports, the support coating delaminates. This was caused by the high alkalinity of the synthesis medium, through hydrolysis and dissolution of the alumina. A new synthesis method at neutral pH was developed to obtain continuous *b*-oriented ZSM-5 membranes.

11:30 AM **Tue-TRBR-1130** Evolution of Framework Al Arrangements in CHA Zeolites during Crystallization Using Organic and Inorganic Structure-Directing Agents.

**Songhyun Lee**<sup>1</sup>, Claire Nimlos<sup>1</sup>, Elijah Kipp<sup>1</sup>, William F. Schneider<sup>2</sup>, Subramanian Prasad<sup>3</sup>, Ahmad Moini<sup>3</sup> and Rajamani Gounder<sup>1</sup>, (1)*Purdue University, USA*, (2)*University of Notre Dame, USA*, (3)*BASF Corporation, USA*.

**Short Summary:**

After bulk crystallization of chabazite (CHA) zeolites has occurred, their framework Al atoms continue to undergo dynamic rearrangement with increasing hydrothermal treatment time. The extent of such rearrangement depends on the organic and inorganic structure directing agents used for crystallization, providing new opportunities to alter active site arrangements in zeolites.

### TUESDAY AFTERNOON

#### Micro- and Meso-porous Catalysts

**Session Chairs:** Zhexi Lin, *Columbia University, USA* and Jonathan Paiz, *Sasol*, .

1:10 PM **Tue-TRBR-1310** Olefins Production from Dimethyl Ether over Zeolites: Material Properties, Products Selectivity, and Catalysts Stability.

**Emanuele Giglio**<sup>1</sup>, Elena Corrao<sup>2</sup>, Giorgia Ferrarelli<sup>1,3</sup>, Fabio Salomone<sup>2</sup>, Massimo Migliori<sup>1</sup>, Samir Bensaid<sup>2</sup>, Raffaele Pirone<sup>2</sup> and Girolamo Giordano<sup>1</sup>, (1)*University of Calabria, Italy*, (2)*Politecnico di Torino, Italy*, (3)*University of Messina, Italy*.

**Short Summary:**

Olefins can be employed in a wide variety of chemical industry application and can be produced in a sustainable way through dimethyl ether-to-olefins (DTO) process. In this work, zeolites with different structure (MFI and FER) and different Si/Al ratio are synthesized and tested to investigate activity, products selectivity and lifetime

1:30 PM **Tue-TRBR-1330** Clarification of Acid Site Location in Mse-Type Zeolites By Spectroscopic Approaches Combined with Catalytic Activity.  
**Ryota Osuga**<sup>1</sup>, Hiroto Toyoda<sup>2</sup>, Yong Wang<sup>2</sup>, Takeshi Matsumoto<sup>2</sup>, Junko N. Kondo<sup>2</sup>, Koji Yazawa<sup>3</sup>, Hermann Gies<sup>2,4</sup>, Christopher J. Gilbert<sup>5</sup>, Bilge Yilmaz<sup>5</sup>, C. P. Kelkar<sup>5</sup> and Toshiyuki Yokoi<sup>2</sup>, (1)Tohoku University, Japan, (2)Tokyo Institute of Technology, Japan, (3)JEOL RESONANCE Inc., Japan, (4) Ruhr University Bochum, Germany, (5)BASF Corporation, USA.

**Short Summary:**

MSE-type aluminosilicate zeolites, UZM-35 and MCM-68, were synthesized. The location of Brønsted acid sites derived from the framework Al atoms was clarified by using <sup>27</sup>Al MQMAS NMR and *in-situ* IR measurements combined with the evaluation of the catalytic activity.

1:50 PM **Tue-TRBR-1350** Structural Insights into Zirconium Metal–Organic Frameworks for Olefin Hydrogenation and Isomerization.

**Kenton Hicks**, Andrew Wolek, Xinyao Liu, Justin Notestein and Omar K. Farha, *Northwestern University, USA*.

**Short Summary:**

Structural variation of metal–organic frameworks through controls the activity and selectivity of zirconium oxide clusters in olefin hydrogenation and isomerization through 1) orientation of adsorption sites and 2) composition of surface ligands.

2:10 PM **Tue-TRBR-1410** Fe Encapsulated in ZSM-5 for CO Hydrogenation.

**Jane Agwara**<sup>1</sup> and Marc Porosoff<sup>2</sup>, (1)Porosoff Lab, University of Rochester, USA, (2)University of Rochester, USA.

**Short Summary:**

Fe supported on ZSM-5 zeolite is encapsulated within a shell ZSM-5 to form a core-shell catalyst (Fe@ZSM-5) for testing the effect of the zeolite shell on CO hydrogenation performance. Fe@ZSM-5 shows higher olefins and C<sub>5+</sub> hydrocarbon selectivities when compared to Fe-supported ZSM-5 catalyst prepared via the traditional impregnation method.

2:30 PM **Tue-TRBR-1430** Mesoporous Silica-Encapsulated Gold Core-Shell Nanoparticles for Active Solvent-Free Benzyl Alcohol Oxidation.

Ellis Hammond-Pereira and **Steven Saunders**, *Washington State University, USA*.

**Short Summary:**

Core-Shell Nanostructures (Au@SiO<sub>2</sub>) were synthesized for the selective oxidation of benzyl alcohol. These structures showed extreme activity and selectivity which can be tuned by adjusting the thickness of the silica shell. Thus suggesting the small pores through the shell aid with in-pore orientation.

2:50 PM **Tue-TRBR-1450** Optimal Supported Cobalt Power-to-Liquids (PtL) Catalysts for Sustainable Aviation Fuel.

**Denzil Moodley**<sup>1</sup>, Thys Botha<sup>1</sup>, Jana Potgieter<sup>1</sup>, Robert Burton<sup>1</sup>, Kobus Visagie<sup>1</sup>, Renier Crous<sup>1</sup>, Dylan Loudon<sup>1</sup>, Michael Claeys<sup>2</sup> and Eric van Steen<sup>2</sup>, (1)Sasol Research & Technology, South Africa, (2)University of Cape Town, South Africa.

**Short Summary:**

The development and scale-up of a best-in class, cobalt PtL catalyst to produce sustainable aviation fuel, to decarbonize the hard-to-abate aviation sector, is described. Understanding of catalyst behavior and catalyst design has been done by Sasol and UCT using an in-situ magnetometer. Catalyst is an enabler for Sasol's eco-FT aspirations.

## Microporous Catalysts II

**Session Chairs:** Griffin Canning, *The Pennsylvania State University, USA* and Bharat Kumar, *Sasol, .*

3:30 PM **Tue-TRBR-1530** Metal Cations As Inorganic Structure-Directing Agents during the Synthesis of Phillipsite and Tobermorite.

**Juan Carlos Vega-Vila**, Advait Holkar, Ross A. Arnold, Samanvaya Srivastava, Gaurav Sant and Dante Simonetti, *University of California, Los Angeles, USA.*

**Short Summary:**

The identity of metal cations influences the polymorphism and structural features of inorganic solids prepared in the absence of organic structure-directing agents. Here, synthesis gels containing sodium and potassium selectively crystallize phillipsite zeolites, whereas synthesis gels crystallize Al-tobermorite silicate hydrates when replacing the cationic content with calcium.

3:50 PM **Tue-TRBR-1550** Cationic Platinum in HZSM-5: Reversible Conversion to Platinum Clusters.

**Noah Felvey**<sup>1</sup>, Jiawei Guo<sup>1</sup>, Bruce Gates<sup>1</sup>, Ambarish Kulkarni<sup>1</sup>, Alexander Katz<sup>2</sup>, Coleman Kronawitter<sup>1</sup> and Ron Runnebaum<sup>1</sup>, *(1)University of California, Davis, USA, (2)University of California, Berkeley, USA.*

**Short Summary:**

By combining EXAFS, XANES, and CO IR spectroscopy, we identified atomically dispersed platinum in the pores of H-ZSM-5 and its reversible conversion into platinum clusters in redox cycles. Adsorptive properties of atomically dispersed cationic platinum and the mechanism of its reduction are discussed.

4:10 PM **Tue-TRBR-1610** Uniform d<sup>8</sup> Cations in Zeolites Reveal New Phenomena in Metal-Zeolite Chemistry and Mechanism of C-H Bond Activation.

**Konstantin Khivantsev**<sup>1</sup>, Nicholas R. Jaegers<sup>2</sup>, Janos Szanyi<sup>1</sup>, Hristiyan Aleksandrov<sup>3</sup> and Georgi Vayssilov<sup>3</sup>, *(1)Pacific Northwest National Laboratory, USA, (2)University of California, Berkeley, USA, (3)University of Sofia, Bulgaria.*

**Short Summary:**

We demonstrate preparation and characterization of uniform d<sup>8</sup> metals for Ni(II), Pd(II), Pt(II) and Ir(I) in zeolite and their new chemistry. Super-electrophile metal cations are shown to exist in zeolites. New phenomena in M-zeolite chemistry described. Individual C-H bond activation (oligomerization) steps of olefins are trapped spectroscopically.

4:30 PM **Tue-TRBR-1630** Thermodynamic and Kinetic Factors Governing the Redispersion of Palladium Nanoparticles to Ion-Exchanged Cations in Zeolites.

**Keka Mandal**<sup>1</sup>, Trevor M. Lardinois<sup>2</sup>, Vamakshi Yadav<sup>2</sup>, Asanka Wijerathne<sup>1</sup>, Brandon K. Bolton<sup>2</sup>, Christina Li<sup>2</sup>, Rajamani Gounder<sup>2</sup> and Christopher Paolucci<sup>1</sup>, *(1)University of Virginia, USA, (2)Purdue University, USA.*

**Short Summary:**

Our findings demonstrate the influence of various factors (gas conditions, particle size and distribution) on the thermodynamics and kinetics of Pd particle redispersion to ion-exchanged cations in CHA zeolites. Smaller sized, monodispersed Pd particles exhibited faster rates of redispersion, while H<sub>2</sub>O promoted formation of PdO agglomerates from ion-exchanged cations.

# Wednesday May 25, 2022

## Grand Ballroom

### WEDNESDAY MORNING

#### Emmett Award Lecture: Beatriz Roldan Cuenya

Session Chairs: Israel E. Wachs, *Lehigh University, USA* and Charles T. Campbell, *University of Washington, USA*

8:00 AM Paul H. Emmett Award Address: From Single Atoms to Clusters and Nanoparticle Catalysts in Energy Conversion.  
**Beatriz Roldan Cuenya**, *Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany*.

## Grand Ballroom East

### Methanol Synthesis and Conversion

Session Chairs: Helena Hagelin-Weaver, *University of Florida, USA* and Dongxia Liu, *University of Maryland - College Park, USA*.

9:30 AM **Wed-GBRE-0930** Cu/ZnO/C As a Promising Model for the Industrial Methanol Catalyst.

**Helene Jakobsen** and Ib Chorkendorff, *Technical University of Denmark, Denmark*.

#### Short Summary:

A Cu/ZnO/C catalyst is tested for its activity towards methanol synthesis in a CO<sub>2</sub>/CO/H<sub>2</sub> gas mixture. By varying the Zn content an interesting trend is found that suggests a possible optimum for the Zn/Cu ratio. Given it performs similarly to the Cu/ZnO/Al<sub>2</sub>O<sub>3</sub> catalyst, Cu/ZnO/C might be a simple model system.

9:50 AM **Wed-GBRE-0950** Silica-Promoted Cu/ZnO/Al<sub>2</sub>O<sub>3</sub>: A New Generation of Exceptionally Stable Methanol Synthesis Catalysts.

**Norman Macleod**, *Johnson Matthey Technology Centre, United Kingdom*.

#### Short Summary:

Optimized Si-doping of ternary CuZnAl methanol synthesis catalysts will be shown to significantly improve sintering resistance, dramatically increasing activity retention over time. Characterization of fresh and aged samples has been used to investigate the origin of the promotional mechanism. This development has application in both conventional and green methanol duties.

10:10 AM **Wed-GBRE-1010** Methanol-to-Olefins Catalysis with CO/H<sub>2</sub> Co-Feeds: Understanding Syngas-to-Olefins Chemistry.

**Zhichen Shi** and Aditya Bhan, *University of Minnesota, Twin Cities, USA*.

#### Short Summary:

Co-feeding high-pressure H<sub>2</sub>, CO, and, syngas are shown here to significantly impact catalyst lifetime and product selectivity during methanol-to-olefins conversion. These effects are attributed to acid-catalyzed hydrogenation and carbonylation reactions that modulate the relative propagation of olefins- and aromatics-based cycles in MTO, as evidenced by kinetic studies and co-feeds experiments.

10:30 AM **Wed-GBRE-1030** DFT Comparison of Pathways for Diene Formation with Methyls and Larger Alkyls during Methanol-to-Olefins in MFI and CHA.

**Lauren Kilburn**<sup>1,2</sup>, Mykela DeLuca<sup>1,2</sup> and David Hibbitts<sup>2</sup>, (1)*Purdue University, USA*, (2)*University of Florida, USA*.

#### Short Summary:

Alkene-mediated and CH<sub>2</sub>O-mediated pathways for the formation of dienes, precursors to deactivation during MTO, are governed by hydride transfers between surface-bound alkyls and C<sub>4</sub>H<sub>8</sub> or CH<sub>3</sub>OH, respectively, in MFI and CHA. Secondary and tertiary alkyls, derived from MTO products, accelerate hydride transfer rates after the MTO induction period.

10:50 AM **Wed-GBRE-1050** Rigorous Modeling of the MTG Synthesis for Operational Optimization of Commercial Plant Performance.

**Martin Soerensen**, *Haldor Topsøe A/S, Denmark*.

#### Short Summary:

A rigorous kinetic model for the methanol to gasoline synthesis is derived from extensive pilot plant tests. The model is used to find the optimal operation conditions for a fixed-bed solution ensuring maximum product yield and stable product composition. The model is finally validated against a commercial reference.

11:10 AM **Wed-GBRE-1110** Identity of Active Sites and Inhibiting Species in the Catalytic Dehydration of Methanol over MIL-100(Cr).

**Mengying Li**, Jacklyn N. Hall, Jiakang Chen and Praveen Bollini, *University of Houston, USA*.

#### Short Summary:

The investigation of well-defined active sites on MIL-100(Cr) provides clear mechanistic insights into Brønsted acid site-mediated methanol dehydration. A range of steady state and transient kinetic data as well as in-situ spectroscopy measurements evidence a sequential mechanism involving methanol-methanol and methanol water dimers as key intermediates and inhibiting species.

11:30 AM **Wed-GBRE-1130** Unraveling the Intricate Relationship between Framework Topology and Acidity on the Light Olefins Selectivities in the Methanol-to-Olefins Reaction.

**Faisal Alshafei**<sup>1</sup>, Youngkyu Park<sup>1</sup>, Stacey I. Zones<sup>2</sup> and Mark E. Davis<sup>1</sup>, (1)*California Institute of Technology, USA*, (2)*Chevron Energy Technology Company, USA*.

**Short Summary:**

Molecular sieves belonging to the following framework types (AEI, CHA, LEV and ERI) were synthesized with variable Si/Al and Si/(Al+P), characterized, and evaluated for their product distribution in MTO, to rationalize the effect of cage structure/size on the olefins product distribution as a function of acid site density and strength.

## WEDNESDAY AFTERNOON

### Fischer-Tropsch Chemistry

**Session Chairs:** Zhenwei Wu, *Shell, USA* and Zili Wu, *Oak Ridge National Laboratory, USA*.

1:10 PM **Wed-GBRE-1310** Manganese As a Promoter Facilitating Oxygen Removal in CO-Hydrogenation at High Conversion.

Chelsea Tucker<sup>1</sup>, Yatheshth Ragoo<sup>1</sup>, Silethukuthula Mathe<sup>1</sup>, Ankur Bordoloi<sup>2</sup> and **Eric van Steen**<sup>1</sup>, (1)*University of Cape Town, South Africa*, (2)*CSIR-Indian Institute of Petroleum, India*.

**Short Summary:**

Manganese as a promoter does improve the activity and the selectivity of Fischer-Tropsch catalysts especially when targeting high conversion. Exploring the role of manganese using DFT by studying the interaction between manganese complexes and various adsorbates showed that these complexes facilitate oxygen removal on Co(111).

1:30 PM **Wed-GBRE-1330** Single-Atom Alloys for Reactive CO/CO<sub>2</sub> Separations.

**Renjie Liu** and Marc Porosoff, *University of Rochester, USA*.

**Short Summary:**

We study a Ru-Co single-atom alloy for reactive CO/CO<sub>2</sub> separations to produce C<sub>5+</sub> hydrocarbons. The catalyst shows a superior FTS activity at 200 °C without converting CO<sub>2</sub>. Interestingly, TEM images show phase changes when the reaction temperature exceeds 200 °C, and the changes transform the catalyst favoring methanation over FTS.

1:50 PM **Wed-GBRE-1350** Rate and Selectivity Oscillations during the Fischer-Tropsch Reaction over a Co/CeO<sub>x</sub> Catalyst.

**Rui Zhang**<sup>1</sup>, Yong Wang<sup>1,2</sup>, Pierre Gaspard<sup>3</sup> and Norbert Kruse<sup>1,2</sup>, (1)*Washington State University, USA*, (2)*Pacific Northwest National Laboratory, USA*, (3)*Université Libre de Bruxelles, Belgium*.

**Short Summary:**

The occurrence of rate-and-selectivity oscillations in syngas conversion over a Co<sub>2</sub>Ce<sub>1</sub> catalyst has been demonstrated for the first time. Long-term oscillations of up to 25 h have been observed at a constant H<sub>2</sub>/CO ratio of 1/1. A possible feedback mechanism for thermokinetic oscillations might involve a reversible reaction-induced catalyst reconstruction.

2:10 PM **Wed-GBRE-1410** Deciphering the Myriad of Reaction Pathways during Fischer-Tropsch Synthesis.

**Iris C. ten Have**<sup>1</sup>, Alexander P. van Bavel<sup>2</sup>, G. Leendert Bezemer<sup>2</sup>, Thomas Hartman<sup>1</sup>, Robert Geitner<sup>3</sup>, Tianbai Huang<sup>4</sup>, Stephan Kupfer<sup>4</sup>, Stefanie Gräfe<sup>4</sup>, Florian Meirer<sup>1</sup> and Bert M. Weckhuysen<sup>1</sup>, (1)*Utrecht University, Netherlands*, (2)*Shell Global Solutions International B.V, Netherlands*, (3)*Technical University Ilmenau, Germany*, (4)*Friedrich Schiller University Jena, Germany*.

**Short Summary:**

Fischer-Tropsch Synthesis (FTS) provides a route to convert municipal waste, biomass, and greenhouse gas CO<sub>2</sub> via CO/H<sub>2</sub> mixtures into fuels and chemicals. In this work, we employ a combination of nanoscale infrared spectroscopy and shell-isolated nanoparticle-enhanced Raman spectroscopy to understand the myriad of mechanisms at play during the cobalt-based FTS.

2:30 PM **Wed-GBRE-1430** High Fischer-Tropsch Synthesis Performance By Iron-Based over SBA-16 Catalysts.

Diogo Pimentel de Sa Silva, Gabriel Garcia Silva, Hidila Souza Teixeira da Silva, Ana Gabriela Martins Silva, Tellys Lins Almeida Barbosa and **Ricardo R. Soares**, *Federal University of Uberlândia, Brazil*.

**Short Summary:**

The Fe/SBA-16 catalyst, no article in the literature, showed excellent activity in the Fisher-Tropsch Synthesis (FTS), providing greater selectivity to gasoline (□ 74.3%) and low CO<sub>2</sub> production. Thus, this study opens a new path to produce biofuels from more selective industrial catalysts.

2:50 PM **Wed-GBRE-1450** Hydroconversion of Fischer-Tropsch Wax into Sustainable Aviation Fuel over Microporous and Mesoporous Catalysts.

**Sundaramurthy Vedachalam**, Biswajit Saha, John Eleeza and Ajay Dalai, *University of Saskatchewan, Canada*.

**Short Summary:**

Bifunctional reforming catalysts were developed for upgrading biosyngas-derived Fischer-Tropsch wax into sustainable aviation fuel. Microporous ZSM-22 and SAPO-11 catalysts resulted in more gasoline-range isoalkanes, whereas jet fuel-range isoalkanes were formed predominantly over mesoporous MCM-41 and TUD-1 catalysts. A clean drop-in substitute for fossil jet fuels was produced from F-T wax.



## Methanation

**Session Chairs:** Prashant Deshlahra, *Tufts University, USA* and Sunitha Tadeballi, *International Flavors and Fragrances, .*

3:30 PM **Wed-GBRE-1530** CO<sub>2</sub> Hydrogenation Activity and Mechanism over Mechano-Chemically Prepared Pd/CeO<sub>2</sub> Catalysts.

**Juan Jimenez**<sup>1</sup>, Maila Danielis<sup>2</sup>, Luis Betancourt<sup>1</sup>, Sara Colussi<sup>2</sup>, Alessandro Trovarelli<sup>2</sup>, Jose A. Rodriguez<sup>1,3</sup> and Sanjaya Senanayake<sup>1</sup>, (1) *Brookhaven National Laboratory, USA*, (2) *University of Udine, Italy*, (3) *Stony Brook University, USA*.

**Short Summary:**

By utilizing the novel mechano-chemical synthesis of Pd/CeO<sub>2</sub>, we developed active catalysts for CO<sub>2</sub> hydrogenation. By probing the catalyst with *in situ* spectroscopic techniques, we were able to discern a novel Pd-C phase that reversibly forms under reaction conditions and a unique CO<sub>2</sub> associative mechanism for Pd/CeO<sub>2</sub> pretreated under O<sub>2</sub>.

3:50 PM **Wed-GBRE-1550** Selectivity Control Using Na Doping for CO<sub>2</sub> Hydrogenation over Ru/ZrO<sub>2</sub> at Low Pressure.

Raimundo Crisostomo Rabelo-Neto<sup>1</sup>, Mayra P. Almeida<sup>1,2</sup>, Martin Ayala<sup>3</sup>, Caleb D. Watson<sup>3</sup>, Jesus Villarreal<sup>3</sup>, Donald C. Cronauer<sup>4</sup>, A. Jeremy Kropf<sup>4</sup>, Michela Martinelli<sup>5</sup>, Fábio Noronha<sup>6</sup> and **Gary Jacobs**<sup>3</sup>, (1) *Instituto Nacional de Tecnologia, Brazil*, (2) *Instituto Militar de Engenharia, Brazil*, (3) *University of Texas at San Antonio, USA*, (4) *Argonne National Laboratory, USA*, (5) *University of Kentucky, USA*, (6) *National Institute of Technology, Brazil*.

**Short Summary:**

CO<sub>2</sub> hydrogenation recycles carbon through the production of either synthetic natural gas or diesel/jet fuels via Fischer-Tropsch synthesis. Na doping of 1%Ru/m-ZrO<sub>2</sub> catalysts containing both water-gas shift and methanation functions allowed selectivity control from 97% CH<sub>4</sub> / 3% CO (without Na) to 16% CH<sub>4</sub> / 84% CO (with 5%Na).

4:10 PM **Wed-GBRE-1610** Particle Size Effects of Nickel on Carbon Catalysts for High Pressure CO<sub>2</sub> Hydrogenation.

**Nienke L. Visser**<sup>1</sup>, Oscar Daoura<sup>1</sup>, Joseph A. Stewart<sup>2</sup>, Jessi E.S. van der Hoeven<sup>1</sup> and Petra E. de Jongh<sup>1</sup>, (1) *Utrecht University, Netherlands*, (2) *TotalEnergies, Belgium*.

**Short Summary:**

Converting CO<sub>2</sub> into valuable fuels could contribute to reducing our carbon footprint. Overall, this work contributes new, valuable insights to the ongoing debate on Ni particle size effects for CO<sub>2</sub> hydrogenation and bridges the gap between low and high pressure methanation studies.

4:30 PM **Wed-GBRE-1630** Alkali Versus Rare-Earth Metal Promoters on Ordered Mesoporous Nickel Alumina Catalysts for CO<sub>2</sub> Methanation.

**Lizbeth Moreno Bravo** and Jan Kopyscinski, *McGill University, Canada*.

**Short Summary:**

This work describes the synthesis of nickel-alumina catalysts, promoted with accessible and affordable metals (e.g., K, Gd, etc.), for application in RNG production via CO<sub>2</sub> methanation. Varying contents of readily available metal promoters are implanted into nickel-alumina structures to boost the support basicity and consequently CO<sub>2</sub> adsorption and conversion.

4:50 PM **Wed-GBRE-1650** Tuning Selectivity of Nickel Methanation Catalysts to Carbon Monoxide: Nickel-Indium Nanoalloys for Reverse Water-Gas Shift.

**Jérôme Simons**, Nikolay Kosinov and Emiel J. M. Hensen, *Eindhoven University of Technology, Netherlands*.

**Short Summary:**

Alloying Ni with In was found to allow steering the selectivity of CO<sub>2</sub> hydrogenation from CH<sub>4</sub> to CO with excellent catalytic activity. The findings in this study provide valuable insights into how to tune the performance of Ni-based catalysts for CO<sub>2</sub> conversion.

5:10 PM **Wed-GBRE-1710** CO<sub>2</sub> Methanation over Ru and Ni Based Catalysts: Towards a Comprehensive Kinetic Model through a Multi-Technique Study.

**Clara Larghi**, Alessandro Porta, Roberto Matarrese, Carlo Giorgio Visconti and Luca Lietti, *Politecnico di Milano, Italy*.

**Short Summary:**

This work provides understanding on the optimal formulation of CO<sub>2</sub> methanation catalysts, as well as on the reaction mechanism and the rate limiting steps: these insights allow to derive a comprehensive kinetic model, which is pivotal for the process industrialization.

## Grand Ballroom West

### WEDNESDAY MORNING

#### Catalytic Oxidation I

**Session Chairs:** Samir Bensaid, *Politecnico di Torino, Italy* and Ming Yang, *Clemson University, USA*.

9:30 AM **KEYNOTE Wed-GBRW-0930 Novel Configured Low-Temperature Diesel Oxidation and Three-Way Catalysts for Emission Control**

**Applications.** Chih Han Liu<sup>1</sup>, Junjie Chen<sup>1</sup>, Todd J. Toops<sup>2</sup>, Cyril Thomas<sup>3</sup>, Michael J. Lance<sup>2</sup>, Stephen Porter<sup>4</sup>, Hien Pham<sup>4</sup>, Abhaya Datye<sup>4</sup>, Jae-Soon Choi<sup>2</sup> and Eleni A. Kyriakidou<sup>1</sup>, (1) *University at Buffalo (SUNY), USA*, (2) *Oak Ridge National Laboratory, USA*, (3) *Sorbonne Université, France*, (4) *University of New Mexico, USA*.

**Short Summary:**

This work illustrates the development of bimetallic Pd,Pt/SiO<sub>2</sub>@Zr DOCs with enhanced durability and low-temperature activity. Pt can be stabilized by forming Pd-Pt alloys and oxide solid solution phases. Decreasing the Pd:Pt ratio led to increased percentages of the metallic phase for both Pd and Pt, resulting to an improved performance.

10:10 AM **Wed-GBRW-1010** CH<sub>4</sub> Conversion By Steam Reforming during Oxidation over Pt + Pd/Al<sub>2</sub>O<sub>3</sub> Monolith Catalysts: Kinetic Model Development.

**Pak Wing Chen**<sup>1</sup>, Kyle Karinshak<sup>1</sup>, Ru-Fen Liu<sup>2</sup>, Lars C. Grabow<sup>1</sup> and Michael P. Harold<sup>1</sup>, (1)University of Houston, USA, (2)CDTi Advanced Materials, USA.

**Short Summary:**

Our study shows the performance and kinetics of the monolith catalysts (PGM+Spinel) during CH<sub>4</sub> conversion by oxidation and steam reforming along with water gas shift in a near-stoichiometric feed. A kinetic model is developed and incorporated into a low-dimensional, dual-layer monolith reactor model for the NGV emission control application.

10:30 AM **Wed-GBRW-1030** Multiscale Imaging and in Situ Analysis of Catalyst Used for Emission Control.

**Monik Panchal**<sup>1,2</sup>, Emma Gibson<sup>2,3</sup>, C. Richard A. Catlow<sup>1,2,4</sup>, Andrew M. Beale<sup>1,2</sup>, Timothy I. Hyde<sup>3</sup>, Manfred Schuster<sup>5</sup>, Andrew York<sup>5</sup> and Paul Collier<sup>5</sup>, (1)University College London, United Kingdom, (2)UK Catalysis Hub, United Kingdom, (3)University of Glasgow, United Kingdom, (4)Cardiff University, United Kingdom, (5)Johnson Matthey Technology Centre, United Kingdom.

**Short Summary:**

This work focused on the role ash accumulation has on Gasoline Particulate Filter (GPF) system, specifically the role ash plays on Pd within the GPF over time after 100 000 km of use. Using a multiscale imaging and operando spectroscopy analysis, the system was understood over a broad length scale.

10:50 AM **Wed-GBRW-1050** Selective Catalytic Oxidation of Ammonia to Nitric Oxide Via Chemical Looping.

**Chongyan Ruan**<sup>1</sup> and Xiaodong Wang<sup>2</sup>, (1)North Carolina State University, USA, (2)Dalian Institute of Chemical Physics, Chinese Academy of Sciences, China.

**Short Summary:**

We proposed for the first time a novel chemical looping ammonia oxidation (CLAO) catalyst and process. The proposed CLAO process exhibited near complete NH<sub>3</sub> conversion and exceptional NO selectivity with negligible N<sub>2</sub>O production using nonprecious V<sub>2</sub>O<sub>5</sub> redox catalyst at a temperature up to 300 °C lower than the existing approach.

11:10 AM **Wed-GBRW-1110** Ni Emergent Nanoparticles As Novel Catalysts for CO Oxidation on High Specific Surface Area Perovskites.

E. Vera, J. Metaouaa, V. Trillaud, Antoinette Boreave, Angel Caravaca, M. Aouine, L. Roiban, P. Steyer and **Philippe Vernoux**, Université de Lyon, CNRS, France.

**Short Summary:**

Redox exsolution offers a new single-step method to tailor and obtain emergent supported active nanoparticles. Here we report Ni exsolution from a large surface area perovskite. The catalytic activity and the stability for CO oxidation of Ni emergent nanoparticles were compared with those of Ni impregnated ones.

11:30 AM **Wed-GBRW-1130** Activation of Lattice and Adatom Oxygen By Highly Stable Ceria-Supported Cu Single Atoms.

**Carlos Eduardo Garcia Vargas**<sup>1,2</sup>, Gregory Collinge<sup>1</sup>, Dongmin Yun<sup>2</sup>, Xavier Isidro Pereira Hernandez<sup>1,2</sup>, Roger Rousseau<sup>1</sup> and Yong Wang<sup>1,2</sup>, (1)Pacific Northwest National Laboratory, USA, (2)Washington State University, USA.

**Short Summary:**

By 2025, EPA Tier 3 exhaust emission regulations will require >90% pollutants abatement at temperatures below 150°C with catalysts of reduced PGM content. This work provides atomic-level insight of the role of thermally stable (non-PGM) Ceria-supported Cu single atoms on the activation of low-temperature lattice oxygen for emissions control.

## WEDNESDAY AFTERNOON

### Catalytic Oxidation and Reduction

**Session Chairs:** Pu-Xian Gao, University of Connecticut, USA and Michael P. Harold, University of Houston, USA.

1:10 PM **Wed-GBRW-1310** Deactivation Mechanisms of FCC SO<sub>x</sub> Additives.

**Xunhua Mo**<sup>1</sup>, Ashish Bambal<sup>1</sup>, Mehdi Allahverdi<sup>1</sup>, Paul Diddams<sup>1</sup>, Yali Tang<sup>1</sup>, Stephen Day<sup>2</sup>, Huw Marchbank<sup>2</sup> and Tuğçe E. Erden<sup>2</sup>, (1)Johnson Matthey, USA, (2)Johnson Matthey Technology Centre, United Kingdom.

**Short Summary:**

This paper reports an ongoing study on the deactivation mechanisms of model sulfur removal additives under Fluid Catalytic Cracking (FCC) conditions. A comprehensive understanding of the deactivation mechanisms will assist the design and development of stable and efficient SO<sub>x</sub> additives. This presentation focuses on deactivation due to steaming.

1:30 PM **Wed-GBRW-1330** Increased Activity and Stability of Pd/Al<sub>2</sub>O<sub>3</sub> Towards Wet Lean CH<sub>4</sub> Oxidation Induced By Pd Structural Changes during Short Reducing Pulses.

**Maneka Roger**<sup>1,2</sup>, Davide Ferri<sup>1</sup>, Tanja Franken<sup>1,3</sup> and Oliver Kröcher<sup>1,2</sup>, (1)Paul Scherrer Institut, Switzerland, (2)École Polytechnique Fédérale de Lausanne (EPFL), Switzerland, (3)Friedrich–Alexander University Erlangen–Nürnberg, Germany.

**Short Summary:**

The activity of Pd/Al<sub>2</sub>O<sub>3</sub> for wet lean CH<sub>4</sub> oxidation was enhanced by applying short reducing pulses compared to static operation, and allowed recovering the degraded activity after thermal aging. From combined of spectroscopic and kinetic data, a practical range of Pd oxidation degree was proposed to preserve high CH<sub>4</sub> conversion.

1:50 PM **Wed-GBRW-1350** Selective Oxidation of NH<sub>3</sub> and CO Emission with Superior N<sub>2</sub> Selectivity By Adding Low Pt Content over Vanadium-Based SCR Catalyst.

**Sang Woo Byun**<sup>1</sup>, Melanie Hazlett<sup>2</sup>, Bekelcha Gadisa<sup>3</sup>, Paul Worn Park<sup>3</sup> and Sung Bong Kang<sup>1</sup>, (1)*Gwangju Institute of Science and Technology, Korea, Republic of (South)*, (2)*Concordia University, Canada*, (3)*NANO Co., Ltd., Korea, Republic of (South)*.

**Short Summary:**

The results of this study will provide a valuable guideline for designing the selective catalytic oxidation catalyst and reducing hazardous NH<sub>3</sub> and CO pollutants from the commercialized SCR process.

2:10 PM **Wed-GBRW-1410** Pt 2D Rafts on Ceria/Alumina for Low Temperature Propane/Propylene Oxidation.

**Hien Pham**<sup>1</sup>, Andrew De La Riva<sup>1</sup>, Eric J. Peterson<sup>1</sup>, Dong Jiang<sup>2</sup>, Yong Wang<sup>2</sup> and Abhaya Datye<sup>1</sup>, (1)*University of New Mexico, USA*, (2)*Washington State University, USA*.

**Short Summary:**

Improved propane/propylene oxidation can be achieved by forming Pt 2D rafts on a ceria/alumina support. The presence of Pt 2D rafts lowers the temperature at which 90% conversion is achieved ( $T_{90}$ ) compared to only single Pt atoms catalysts, and without the need to add Pd, resulting in significant cost savings.

2:30 PM **Wed-GBRW-1430** Development of a Redox Kinetic of Hg<sup>0</sup> Oxidation over a V-Based Catalyst for NH<sub>3</sub>-SCR: Effect of O<sub>2</sub>, NO and NH<sub>3</sub>.

**Aldo Lanza**<sup>1</sup>, Silvia Alcove Clave<sup>2</sup>, Jillian Collier<sup>2</sup>, Luca Lietti<sup>1</sup>, Roberto Matarrese<sup>1</sup> and Alessandra Beretta<sup>1</sup>, (1)*Politecnico di Milano, Italy*, (2)*Johnson Matthey Technology Centre, United Kingdom*.

**Short Summary:**

In this study we present a Redox rate equation for Hg<sup>0</sup> oxidation over V-based catalysts for NH<sub>3</sub>-SCR. The limiting effect of the oxygen coverage at high temperature was described and the individual negative impact of NO and NH<sub>3</sub> were associated to reducing effects via oxidation to NO<sub>2</sub> and N<sub>2</sub>, respectively.

2:50 PM **Wed-GBRW-1450** Particle Deposits and Their Impact on Catalytic Filter Performance: Time-Resolved XRT and Pore-Scale Modeling.

**Petr Koci**<sup>1</sup>, Marie Placha<sup>1</sup>, Martin Isoz<sup>1</sup>, Matthew Jones<sup>2</sup>, David Eastwood<sup>2</sup> and Andrew York<sup>3</sup>, (1)*University of Chemistry and Technology, Czech Republic*, (2)*University of Manchester at Harwell, United Kingdom*, (3)*Johnson Matthey Technology Centre, United Kingdom*.

**Short Summary:**

The work combines advanced characterization techniques with predictive micro-scale models. It provides an insight into evolution of particle deposits inside walls of catalytic filters, and their impact on performance in terms of catalytic conversion, pressure loss and filtration efficiency. The findings provide feedback for optimization of the catalytic coating.

## Low Temperature NO<sub>x</sub> and HC Adsorbers

**Session Chairs:** Yuntao Gu, *General Motors Global R&D, USA* and Sreshtha Sinha Majumdar, *Oak Ridge National Laboratory, USA*.

3:30 PM **Wed-GBRW-1530** Spectroscopic FT-IR Analysis Under Operando Conditions and Reactivity Study of Pd/SSZ-13 Low Temperature NO<sub>x</sub> Adsorbers.

**Roberto Matarrese**<sup>1</sup>, Sara Morandi<sup>2</sup>, Lidia Castoldi<sup>1</sup>, Pierfrancesco Ticali<sup>2</sup> and Luca Lietti<sup>1</sup>, (1)*Politecnico di Milano, Italy*, (2)*University of Turin, Italy*.

**Short Summary:**

The pathways involved in NO adsorption on Pd/SSZ-13 have been investigated by operando FTIR spectroscopy. NO are stored in the form of nitrosyls (anhydrous and hydrated). Nitrates are also formed, especially in the presence of NO<sub>2</sub>. CO and hydrocarbons in the feed compete with NO for adsorption on Pd sites.

3:50 PM **Wed-GBRW-1550** An Examination of the Role of NO<sub>2</sub> in Passive NO<sub>x</sub> Adsorption and Desorption on Pd Loaded Zeolites.

**Robert Pace**, Yaying Ji and Mark Crocker, *University of Kentucky, USA*.

**Short Summary:**

NO<sub>2</sub> is shown to adsorb at partially-hydrolyzed zeolitic aluminum sites, forming nitrate-like adsorbates that desorb at higher temperatures than NO<sup>+</sup> and Pd-nitrosyl complexes. NO<sub>2</sub> also oxidizes Pd at temperatures above 50 °C, resulting in complex desorption behavior in which new Pd-nitrosyl complexes are formed through oxidation of Pd by NO<sub>2</sub>.

4:10 PM **Wed-GBRW-1610** Pd-Based Bi- and Tri-Metallic Compositions for Improved Passive NO<sub>x</sub> Adsorption and Trapping of Hydrocarbons under Industrially Relevant Conditions.

**Pranaw Kunal**<sup>1,2</sup> and Todd J. Toops<sup>2</sup>, (1)*Iowa State University, USA*, (2)*Oak Ridge National Laboratory, USA*.

**Short Summary:**

Platinum group metals are applied across various catalytic processes, however they presents grave economic and sustainability challenges. Our work involves PGM-dilution approaches for synthesizing hybrid high-performance catalysts, also durable under demanding real world conditions containing substrates such as water, and C- and N-oxides, poisonous in nature towards active metallic entities.

4:30 PM **Wed-GBRW-1630** Effect of High Temperature CO/H<sub>2</sub>O Exposure on Pd/BEA Hydrocarbon Traps.

**Ryan Zelinsky** and William Epling, *University of Virginia, USA*.

**Short Summary:**

Pd/Zeolites are currently of interest for automobile exhaust applications including hydrocarbon trapping, NO<sub>x</sub> adsorption, and methane oxidation. Current challenges include Pd characterization, stability, and utilization. In this work, we investigate changes in Pd speciation after high temperature exposure to deactivating agents such as H<sub>2</sub>O and CO.

4:50 PM **Wed-GBRW-1650** Reductant Induced Redox Behavior of Atomically-Dispersed Palladium in Pd-CHA.

**Surya Pratap Solanki**<sup>1</sup>, Mugdha Ambast<sup>1</sup>, Christopher Paolucci<sup>2</sup>, Michael P. Harold<sup>1</sup> and Lars C. Grabow<sup>1</sup>, (1)University of Houston, USA, (2) University of Virginia, USA.

**Short Summary:**

Palladium exchanged zeolites have been identified as passive NO<sub>x</sub> adsorbers (PNA) to store NO<sub>x</sub> at low temperature to control emission during cold-start period. In this study we have used both computational and experimental approaches to investigate underlying reaction mechanisms during NO<sub>x</sub> adsorption with an emphasis on the role of water.

5:10 PM **Wed-GBRW-1710** In Situ FTIR Study for Natural Chabazite for PNA Application.

**Julio C. López Curriel**, María Eugenia Hernández-Terán and Gustavo A. Fuentes, *Universidad Autónoma Metropolitana-Iztapalapa, Mexico.*

**Short Summary:**

Natural chabazite adsorbs a large amount of NO at different temperatures after pretreatment and desorbs NO<sub>x</sub> in the correct range for a Passive No<sub>x</sub> Adsorber. NO adsorption is attributed to the formation of nitrates on the surface and the presence of O<sub>2</sub> promotes NO oxidation and increases the amount adsorbed.

## Gramercy

### WEDNESDAY MORNING

#### Fundamentals of Hydrogenation/Dehydrogenation Catalysis I

**Session Chairs:** Ive Hermans, *University of Wisconsin–Madison, USA* and Aaron Sattler, *ExxonMobil Research and Engineering, USA.*

9:30 AM **Wed-GRAM-0930** Local Brønsted Acid Sites and Acidity Cocatalyze the Selective Hydrogenation of Oxygenates over Supported Metal Catalysts.

**Matthew Neurock**<sup>1</sup>, Guoju Yang<sup>2</sup>, Vineet Maliekkal<sup>1</sup>, Xi Chen<sup>3</sup>, Sebastian Eckstein<sup>3</sup>, Hui Shi<sup>4</sup>, Donald M. Camaioni<sup>5</sup>, Eszter Barath<sup>3</sup>, Gary L. Haller<sup>6</sup>, Johannes Lercher<sup>3</sup> and Yue Liu<sup>7</sup>, (1)University of Minnesota, Twin Cities, USA, (2)Jilin University, China, (3)Technical University of Munich, Germany, (4)Yangzhou University, China, (5)Pacific Northwest National Laboratory, USA, (6)Yale University, USA, (7)East China Normal University, China.

**Short Summary:**

Herein we examine the selective hydrogenation of phenol over Pt-supported on silicalite and within HMFI-zeolites with varying acidity. The results show direct relationship between the local acidity and the hydrogenation rates. Detailed theoretical and experimental studies provide insights into the influence of local Brønsted acidity on the significant rate enhancements.

9:50 AM **Wed-GRAM-0950** Evolution of Chromium Oxide Species in Cr/Al<sub>2</sub>O<sub>3</sub> Propane Dehydrogenation Catalysts during Synthesis and Calcination.

**Adam Hoffman**<sup>1</sup>, Jordan Finzel<sup>1</sup>, Matthew Greaney<sup>2</sup>, Vladimir Fridman<sup>3</sup>, Rong Xing<sup>3</sup>, Claus Lugmair<sup>2</sup> and Simon Bare<sup>1</sup>, (1)SLAC National Accelerator Laboratory, USA, (2)Clariant, USA, (3)Clariant Corporation, USA.

**Short Summary:**

Calcination of physically mixed Cr<sub>2</sub>O<sub>3</sub>/Al<sub>2</sub>O<sub>3</sub> propane dehydrogenation catalysts showed a 100 fold increase in the formation of Cr(VI) species compared to Cr<sub>2</sub>O<sub>3</sub> catalysts. XAS modeling, difference spectra analysis, and FEFF XANES simulations identified the formation of Cr<sub>5</sub>O<sub>12</sub> or Al<sup>3+</sup>Cr<sup>3+</sup><sub>2-x</sub>Cr<sup>6+</sup><sub>3</sub>O<sub>12</sub> species as a result of the Cr<sub>2</sub>O<sub>3</sub>-Al<sub>2</sub>O<sub>3</sub> interaction.

10:10 AM **Wed-GRAM-1010** Electrochemical Insights into Thermochemical Hydrogenations with Metal Oxides.

Yifan Deng, Evan Miu, Götz Vesper and **James McKone**, *University of Pittsburgh, USA.*

**Short Summary:**

Our research team is designing catalysts and chemical processes that leverage the ability of reducible oxides to accept, store, and deliver hydrogen to reactive substrates. This presentation will discuss ongoing investigations directed at using measurements of electrochemical hydrogen intercalation to predict and control the reactivity of hydrogenation catalysts.

10:30 AM **Wed-GRAM-1030** Effect of H<sub>2</sub> Removal on Ethane Dehydrogenation Catalysts Under Simulated Membrane Reactor Conditions.

**Elaine Gomez**, Henry Klutse, Randall Meyer, Sara Jacob and Aaron Sattler, *ExxonMobil Research and Engineering, USA.*

**Short Summary:**

Catalytic dehydrogenation of alkanes using PtSn-K/MFI under conditions designed to simulate hydrogen removal membranes has been assessed employing simulated feeds in a fixed bed configuration. The maximum achievable conversions fall short of those predicted by simple equilibrium assumptions, demonstrating the need for catalyst development to operate under H<sub>2</sub> lean conditions.

10:50 AM **Wed-GRAM-1050** A Mechanistic Study on AlO<sub>x</sub>-Overcoated Pd Catalyst for Selective Hydrogenation.

**Divakar Reddy Airedy** and Kunlun Ding, *Louisiana State University, USA.*

**Short Summary:**

We demonstrate that AlO<sub>x</sub>-ALD improves the alkene selectivity of Pd/Al<sub>2</sub>O<sub>3</sub> in semihydrogenation of acetylene (C<sub>2</sub>H<sub>2</sub>). We also show that AlO<sub>x</sub>-ALD layer is impermeable for C<sub>2</sub>H<sub>2</sub>, O<sub>2</sub>, and CO, but permeable for H<sub>2</sub>. H-D exchange experiment suggested that the dihydrogen dissociation might undergo a heterolytic pathway. These evidence favor hydrogen-spillover mechanism.

11:10 AM **Wed-GRAM-1110** Mechanistic Aspects of CO<sub>2</sub> Hydrogenation over Mono- and Bimetallic Ni-Co Catalysts.

Francisco Villagra, **Sebastián Godoy**, Alejandro Karelovic and Romel Jiménez, *Universidad de Concepción, Chile*.

**Short Summary:**

Kinetic, spectroscopic and isotopic analyses on mono and bimetallic Ni-Co catalysts confirm that CO is formed through the direct CO<sub>2</sub> dissociation without H participation, while CH<sub>4</sub> formation occurs via H-assisted dissociation of the C-O bond of carbonyl species. Weakly adsorbed CO favor the CO<sub>(g)</sub> formation while multi-bound CO\* produce CH<sub>4</sub>.

11:30 AM **Wed-GRAM-1130** Rates and Selectivities for O<sub>2</sub> Reduction with H<sub>2</sub> Reveal Dynamic Structures of Au-Based Bimetallic Nanoparticles.

**Tomas Ricciardulli**<sup>1</sup>, David Flaherty<sup>1</sup>, Jason Adams<sup>1</sup>, Ayman M. Karim<sup>2</sup>, Alexander P. van Bavel<sup>3</sup> and Marco deRidder<sup>3</sup>, (1)*University of Illinois Urbana-Champaign, USA*, (2)*Virginia Polytechnic Institute and State University, USA*, (3)*Shell Global Solutions International B.V, Netherlands*.

**Short Summary:**

Bimetallic PtAu nanoparticles supported on SiO<sub>2</sub> are synthesized with scalable techniques and applied to direct H<sub>2</sub>O<sub>2</sub> synthesis. Rate measurements and characterization results show that Pt single-atoms in Au greatly enhance H<sub>2</sub>O<sub>2</sub> formation rates in comparison to pure Au and selectivity in comparison to pure Pt.

## WEDNESDAY AFTERNOON

### Fundamentals of Oxygen Catalysis

**Session Chairs:** Karl Albrecht, *ADM*, and Yawu-Thomas Chi, *Ascend Performance Materials*, .

1:10 PM **Wed-GRAM-1310** Inverse ZnO/Cu(111) Catalysts for Methanol Synthesis, the Water-Gas Shift and CO Oxidation.

**Jose A. Rodriguez**<sup>1,2</sup>, Mausumi Mahapatra<sup>2</sup>, Jindong Kang<sup>2</sup>, Pedro Ramirez<sup>3</sup>, Ping Liu<sup>2</sup> and Sanjaya Senanayake<sup>2</sup>, (1)*Stony Brook University, USA*, (2)*Brookhaven National Laboratory, USA*, (3)*Universidad Central de Venezuela, Venezuela (Bolivarian Republic of)*.

**Short Summary:**

Experiments performed using HR-TEM have shown the presence of a ZnO overlayer on top of Cu particles when CO<sub>2</sub> hydrogenation is carried out over powder Cu/ZnO/Al<sub>2</sub>O<sub>3</sub> catalysts. Our studies for ZnO/Cu(111) show that this inverse oxide/metal catalyst is active for the synthesis of methanol, the water-gas shift, and CO oxidation.

1:30 PM **Wed-GRAM-1330** Effect of the Size of Pt Particle on Activity of Pt/TiO<sub>2</sub> Catalysts for CO Oxidation.

**Md Raian Yousuf**, Malik Albrahim and Ayman M. Karim, *Virginia Polytechnic Institute and State University, USA*.

**Short Summary:**

We demonstrate, using kinetics analysis, infrared spectroscopy, and temperature-programmed reduction, that CO oxidation activity of metal catalyst supported on a reducible support increases with metal particle size. The results show how reducibility of the support depends on metal size and metal-support interaction which play a crucial role in catalyst activity.

1:50 PM **Wed-GRAM-1350** Spectroscopic Investigations of Active and Selective Oxygen Species in Ethylene Epoxidation on Ag Supported on  $\alpha$ -Al<sub>2</sub>O<sub>3</sub>.

**Shawn Lu**<sup>1</sup>, Jinxun Liu<sup>1</sup>, Shiuann-Bai Ann<sup>1</sup> and Suljo Lincic<sup>2</sup>, (1)*University of Michigan-Ann Arbor, USA*, (2)*University of Michigan, USA*.

**Short Summary:**

A complex distribution of silver-oxygen structures are observed on the Ag surface during ethylene epoxidation reaction conditions. Catalyst activity and product selectivity for ethylene oxide are correlated to the geometry of these surface oxygen species.

2:10 PM **Wed-GRAM-1410** Interpretable Deep Learning Reveals Catalyst Genomes for Oxygen Reduction.

**Noushin Omidvar**, Hemanth Somarajan Pillai, Shih-Han Wang, Yang Huang, Qingmin Mu, Luke E.K. Achenie and Hongliang Xin, *Virginia Polytechnic Institute and State University, USA*.

**Short Summary:**

We developed a rapid screening approach for catalyst discovery based on an interpretable deep learning framework. Utilizing the oxygen reduction reaction (ORR) as an example we showed how this framework can be used to screen for optimal sites and derive physical insights into site reactivity.

2:30 PM **Wed-GRAM-1430** Inadvertent or Intentional Creation of Surface Redox Mediators on Pd Nanoparticles: Evidence, Mechanism, and Opportunity.

Jason Adams<sup>1</sup>, Ashwin Chemburkar<sup>2</sup>, Tomas Ricciardulli<sup>1</sup>, Pranjali Priyadarshini<sup>1</sup>, Vineet Maliekkal<sup>2</sup>, Yubing Lu<sup>3</sup>, Ayman M. Karim<sup>3</sup>, Matthew Neurock<sup>2</sup> and **David Flaherty**<sup>1</sup>, (1)*University of Illinois Urbana-Champaign, USA*, (2)*University of Minnesota, Twin Cities, USA*, (3)*Virginia Polytechnic Institute and State University, USA*.

**Short Summary:**

Adsorption of organic compounds to Pd nanoparticles forms surface bound redox mediators that persist for extended periods during steady-state reactions of O<sub>2</sub> and H<sub>2</sub>. These species improve selectivities to H<sub>2</sub>O<sub>2</sub>, increase rates, and eliminate the need for organic solvents.

2:50 PM **Wed-GRAM-1450** Assessment of Structural and Functional Non-Uniformity of Dispersed VO<sub>x</sub> and O<sub>2</sub> Activation Routes in Mars-Van Krevelen Redox Cycles.

**Nicholas R. Jaegers**<sup>1</sup>, Robert Carr<sup>2</sup> and Enrique Iglesia<sup>1</sup>, (1)*University of California, Berkeley, USA*, (2)*ExxonMobil Research and Engineering, USA*.

**Short Summary:**

Assessment of O<sub>2</sub> activation routes in Mars-van Krevelen redox cycles on supported VO<sub>x</sub> catalysts is complicated by active site non-uniformity, obfuscating extraction of kinetic rate parameters and oxidation half-cycle pathways. A proposed transient dehydrogenation analysis quantifies the intrinsic non-uniformity of VO<sub>x</sub> catalysts and estimates the distribution of ODH rate constants.



## Fundamentals of Hydrogenation/Dehydrogenation Catalysis II

**Session Chairs:** Ive Hermans, *University of Wisconsin–Madison, USA* and Yong Wang, *Pacific Northwest National Laboratory, USA*.

3:30 PM **KEYNOTE Wed-GRAM-1530 Catalytic Roles of Hydrogen Adatoms and Interfacial Protons in Hydrogenation and Hydrogenolysis**

**Reactions.** Junnan Shangguan<sup>1</sup>, Zhenwei Wu<sup>1</sup>, Alyssa Hensley<sup>2</sup>, Haiting Cai<sup>1</sup>, Jean-Sabin McEwen<sup>2</sup> and Ya-Huei (Cathy) Chin<sup>1</sup>, (1)*University of Toronto, Canada*, (2)*Washington State University, USA*.

**Short Summary:**

Our work illustrates how electronic charge of reactive H species on transition metal surfaces dictates their catalytic roles, mechanistic sequence, and reactivity in hydrogenation and hydrodeoxygenation reactions.

4:10 PM **Wed-GRAM-1610 Identification of Determining Factors for Catalytic Hydrogenation of the Furanic Compound over Supported Precious Metal Catalysts.**

**Tae Yong Kim<sup>1</sup>**, Anh Vy Tran<sup>2</sup>, Jayeon Baek<sup>2</sup> and Jeong Woo Han<sup>1</sup>, (1)*Pohang University of Science and Technology (POSTECH), Korea, Republic of (South)*, (2)*Korea Institute of Industrial Technology (KITECH), Korea, Republic of (South)*.

**Short Summary:**

We report DFT and experimental results for catalytic hydrogenation of furanic compound, performed to identify determining factors for reactivity and selectivity. Hydrogen affinity, d-band structures, and van der Waals interaction are the main factors affecting the ring-hydrogenation and ring-opening reactivity.

4:30 PM **Wed-GRAM-1630 Selective Hydrogenation of Acetylene over Thin Film Pd without a Modifying Metal.**

**Zehua Li<sup>1</sup>**, Lukas Thum<sup>1</sup>, Jinhu Dong<sup>1</sup>, Sabine Wrabetz<sup>1</sup>, Jutta Kröhnert<sup>1</sup>, Alexander Steigert<sup>2</sup>, Simone Raoux<sup>2,3</sup>, Daniel Amkreutz<sup>2</sup>, Annette Trunschke<sup>2</sup>, Robert Schlögl<sup>1,4</sup> and Katarzyna Skorupska<sup>1</sup>, (1)*Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany*, (2)*Helmholtz-Zentrum Berlin für Materialien und Energie, Germany*, (3)*Humboldt-Universität zu Berlin, Germany*, (4)*Max Planck Institute for Chemical Energy Conversion, Germany*.

**Short Summary:**

2D thin-film Pd catalysts (3, 11 nm) supported on SiO<sub>2</sub>/Si or ZnO/Si have been synthesized and catalytically tested for acetylene hydrogenation. Without any modifying metal elements, they have very high activity and turnover frequency when compared to single atoms Pd, which provides a new direction for future catalyst development.

4:50 PM **Wed-GRAM-1650 Propane Dehydrogenation to Propylene on Ni and Ni-Sn Catalysts.**

Jason P. Robbins<sup>1</sup>, Lotanna Ezeonu<sup>1</sup>, Ziyu Tang<sup>1</sup>, Xiaofang Yang<sup>2</sup>, Bruce E. Koel<sup>2</sup> and **Simon G. Podkolzin<sup>1</sup>**, (1)*Stevens Institute of Technology, USA*, (2)*Princeton University, USA*.

**Short Summary:**

Propane dehydrogenation to propylene was studied over Ni, Ni-Sn and Sn catalysts. In contrast with low selectivity of Ni and low activity of Sn, Ni-Sn was identified as a highly selective and active catalyst. Effects of Sn addition to Ni were evaluated at the molecular level.

5:10 PM **Wed-GRAM-1710 Palladium Particle Size Effects in Selective Hydrogenation of 1,3-Butadiene.**

**Oscar E. Brandt Corstius<sup>1</sup>**, Jessi E.S. van der Hoeven<sup>1</sup>, Tegan Roberts<sup>2</sup>, Glenn Sunley<sup>2</sup> and Petra E. de Jongh<sup>1</sup>, (1)*Utrecht University, Netherlands*, (2)*BP plc, United Kingdom*.

**Short Summary:**

Increasing selectivity with larger Pd particle sizes in the selective hydrogenation of 1,3-butadiene is explained by in-depth kinetic studies. Reaction order size-dependence indicated stronger binding of butadiene on larger particles, whereas binding of propylene and hydrogen weakened. This rationalizes the decrease of over-hydrogenation and propylene conversion, respectively, with increasing size.

## Mercury Ballroom

### WEDNESDAY MORNING

#### Catalyzed Chemical Transformations I

**Session Chairs:** Líney Árnadóttir, *Oregon State University, USA* and Weijian Diao, *Villanova University, USA*.

9:30 AM **KEYNOTE Wed-MEBR-0930 Ethylene Carbonylation Revisited: Novel Catalysts for the Environmentally Friendly Synthesis of Methyl Methacrylate.** Beata Kilos-Reaume, *The Dow Chemical Company, USA*.

**Short Summary:**

MMA is a specialty monomer to produce polymethylmethacrylate where increasing demand has motivated the industry to develop clean technologies based on leveraging abundant ethylene. We will discuss the synthesis, characterization of novel heterogeneous catalysts for ethylene hydroxy- (Mo(CO)<sub>6</sub>/support) and methoxy-carbonylation (Co<sub>x</sub>S<sub>y</sub>) and the relationships between catalyst properties and catalyst performance.

10:10 AM **Wed-MEBR-1010 Environmentally Friendly Ester Hydrogenation Catalyst for Gas Phase Catalytic Fatty Alcohol Production.**

**Radu Craciun**, *BASF Corporation, USA*.

**Short Summary:**

New and novel Cu-based catalysts used for gas phase catalytic fatty alcohol synthesis. Structural properties are being presented in correlation with their performance, the key technical advantages vs a CuCr based catalyst, emphasizing the role of extrudate's shape and texture in the catalyst bed operation parameters and the catalyst lifetime.

10:30 AM **Wed-MEBR-1030** Spatiotemporal Coke Coupling Enhances Para-Xylene Selectivity in Highly Stable MCM-22 Catalyst.

**Deependra Parmar**<sup>1</sup>, Seung Hyeok Cha<sup>2</sup>, Taha Salavati-fard<sup>1</sup>, Ankur Agrawal<sup>1</sup>, Hsu Chiang<sup>3</sup>, Seth Washburn<sup>3</sup>, Jeremy C. Palmer<sup>1</sup>, Lars C. Grabow<sup>1</sup> and Jeffrey D. Rimer<sup>1</sup>, (1)University of Houston, USA, (2)Korea Research Institute of Chemical Technology, Korea, Republic of (South), (3) ExxonMobil Chemical Company, USA.

**Short Summary:**

Toluene alkylation with methanol (TAM) reaction suffers from low catalyst stability. In this presentation, we will discuss the exceptional catalyst stability of MCM-22 zeolite where the roles different topological features are deconvoluted to introduce a new spatiotemporal coke coupling mechanism for enhanced para-xylene mass-time yield in commercial TAM processes.

10:50 AM **Wed-MEBR-1050** Heterogeneously Supported Single-Atom Lanthanum Catalyzed Borylation of Hydrocarbons.

**Yuting Li**<sup>1</sup>, Long Qi<sup>1</sup> and Aaron Sadow<sup>2</sup>, (1)USDOE Ames Laboratory, USA, (2)Ames Laboratory and Iowa State University, USA.

**Short Summary:**

In this research, we demonstrate a type of novel heterogeneous catalyst through grafting lanthanide borohydride complexes on metal oxide or zeolitic supports. The crystalline microporous support grafted lanthanides present a promising path for borylation of hydrocarbons. More catalysts for C-H activation could be potentially developed using supported rare-earth element catalysts.

11:10 AM **Wed-MEBR-1110** Enhanced Hydrogenation of Oleic Acid By RF Heating of Magnetically Susceptible Nanoparticles.

**Cameron Roman**<sup>1</sup>, Natalia da Silva Moura<sup>1</sup>, Scott Wicker<sup>2</sup>, Kerry Dooley<sup>1</sup> and James Dorman<sup>1</sup>, (1)Louisiana State University, USA, (2)Rhodes College, USA.

**Short Summary:**

Radiofrequency (RF) induction heating is an alternative method of energy transfer whereby dipoles are induced in magnetically susceptible catalysts. For the heterogeneous catalytic hydrogenation of oleic acid, application of RF heating provides has been shown to improve both activity and the selectivity to stearic acid.

11:30 AM **Wed-MEBR-1130** Assessing Lewis Acidity and Confinement for Zeotype-Catalyzed Aldol Condensation between Lower Aldehydes.

**Wenlin He**<sup>1</sup>, Zhongyao Zhang<sup>2</sup>, David Flaherty<sup>2</sup> and Viktor Cybulskis<sup>1</sup>, (1)Syracuse University, USA, (2)University of Illinois Urbana-Champaign, USA.

**Short Summary:**

Framework Lewis acid sites and basic lattice oxygens in zeotype Si-O-M ensembles catalyze C-C coupling between enolizable substrates, such as propionaldehyde, and lower aldehydes lacking  $\alpha$ -C-H bonds, such as benzaldehyde. Second-order rate constants are influenced by functional Lewis strength while confinement effects can steer product selectivity.

## WEDNESDAY AFTERNOON

### Catalysis for Monomers, Oligomers, Polymers and Up-cycling

**Session Chairs:** Rachel Getman, *Clemson University, USA* and Sara Yacob, *ExxonMobil Research and Engineering, USA*.

1:10 PM **Wed-MEBR-1310** Assessing Correlations between the Fragmentation Behavior and the Kinetics of Silica-Supported Ethylene Polymerization Catalysts.

**Maximilian J. Werny**<sup>1,2</sup>, Jelena Zarupski<sup>2,3</sup>, Iris C. ten Have<sup>1</sup>, Alessandro Piovano<sup>2,3</sup>, Coen Hendriksen<sup>4</sup>, Nicolaas H. Friederichs<sup>4</sup>, Florian Meirer<sup>1</sup>, Elena Groppo<sup>3</sup> and Bert M. Weckhuysen<sup>1</sup>, (1)Utrecht University, Netherlands, (2)Dutch Polymer Institute (DPI), Netherlands, (3)University of Turin, Italy, (4)SABIC, Netherlands.

**Short Summary:**

A multiscale microscopy-spectroscopy approach was used to characterize two industrial-grade metallocene-based catalysts, linking the morphological evolution of single catalyst particles to the accessibility and insertion behavior of their active sites. Clear correlations between the catalysts' respective kinetics and their dominant support fragmentation pathways could thus be established.

1:30 PM **Wed-MEBR-1330** Zeolite Catalysis for Cyclic Monomer Synthesis.

**Samuel Meacham** and Russell Taylor, *Durham University, United Kingdom*.

**Short Summary:**

The use of zeolite catalysis to synthesise cyclic monomers from mandelic acid has not yet been reported in the open literature. In this work, the synthesis of lactides and dioxolanones of mandelic acid has been investigated over a range of Brønsted-acidic zeolites.

1:50 PM **Wed-MEBR-1350** Olefin Methylation Reactions over Iron Zeolites: Increasing Reaction Rates and Shifting the Selectivity Towards Olefins.

**Mark LaFollette** and Raul F. Lobo, *University of Delaware, USA*.

**Short Summary:**

Co-feeding olefins over iron zeolites can help overcome low reaction rates commonly seen with these materials in the methanol to hydrocarbon (MTH) reaction. We show that iron-zeolites are, in fact, very selective towards methylation reactions versus other MTH reactions allowing iron zeolites to serve as selective methylation catalysts of olefins.

2:10 PM **Wed-MEBR-1410** Tuning the Hydrophobicity of Lewis Acid Zeolites and Nanozeolites for the Epoxide Ring Opening with Alcohols.

**Nicholas Brunelli**<sup>1</sup>, Nitish Deshpande<sup>1</sup>, Aamena Parulkar<sup>1</sup>, Ambarish Kulkarni<sup>2</sup>, Alexander Spanos<sup>1</sup>, Medha Kasula<sup>1</sup>, Rutuja Joshi<sup>1</sup>, Leah Ford<sup>1</sup> and Sam Holton<sup>2</sup>, (1)The Ohio State University, USA, (2)University of California, Davis, USA.

**Short Summary:**

Nano-zeolites (nano-Sn-Beta) are synthesized, characterized, and tested for catalytic activity in the epoxide ring opening (ERO) of alcohols. Fluoride treatment of the nano-Sn-Beta results in a material with higher catalytic activity, demonstrating that ERO benefits from a hydrophobic reaction environment.

2:30 PM **Wed-MEBR-1430** Ga-Ni Supported Catalytically Active Liquid Metal Solutions (SCALMS) for Selective Alkene Oligomerization.

**Alexander Sogaard**<sup>1</sup>, Annika Schmuker<sup>1</sup>, Ana de Oliveira<sup>2</sup>, Nicola Taccardi<sup>1</sup>, Marco Haumann<sup>1</sup> and Peter Wasserscheid<sup>1,2</sup>, (1)*Friedrich–Alexander University Erlangen–Nürnberg, Germany*, (2)*Forschungszentrum Jülich GmbH, Germany*.

**Short Summary:**

Non-precious metal Supported Catalytically Active Liquid Metal Solutions (SCALMS) display attractive performance in ethylene oligomerization. For Ga-Ni systems on silica it was found that performance strongly depends on the applied Ga/Ni ratio. Ga-rich systems forming liquid alloys exhibit far greater Ni-based catalytic activity than solid intermetallic compounds or Ni nanoparticles.

2:50 PM **Wed-MEBR-1450** Plastic Trash to Monomers and Intermediates – Ptmi.

**Anne Gaffney**<sup>1</sup>, Weijian Diao<sup>2</sup>, Kevin Lynn<sup>3</sup> and Gennaro Maffia<sup>3</sup>, (1)*University of South Carolina, USA*, (2)*Villanova University, USA*, (3)*Manhattan College, USA*.

**Short Summary:**

To address the issue of waste plastics in landfills, a hybrid approach is proposed. This would use low temperature plasma pretreatment followed by catalytic cracking to augment the conversion of waste polyolefins into monomers, intermediates, new polymers and value-added chemicals.

## Catalyzed Chemical Transformations II

**Session Chairs:** Tibor Szilvasi, *University of Alabama, USA* and John Meynard Tengco, *University of South Carolina, USA*.

3:30 PM **Wed-MEBR-1530** N-Heptane Dehydrogenation with Highly Selective and Stable Ruthenium and Molybdenum Phosphide Catalysts.

**Patrick Schuehle**, Robert Stoeber and Oshin Sebastian, *Friedrich–Alexander University Erlangen–Nürnberg, Germany*.

**Short Summary:**

In this work, RuP<sub>2</sub>-MoP catalysts are shown to be highly stable and selective in the dehydrogenation of longer chain alkanes like n-heptane. Furthermore, the active transition metal phosphide is compared to its phosphorous-free RuMo-counterpart. In addition to improving olefin selectivity, incorporation of phosphorous into the RuMo-surface structure avoids catalyst deactivation.

3:50 PM **Wed-MEBR-1550** Implementation of Metal on N-Doped Carbon Electrocatalysts for Thermochemical Aerobic Oxidation of 5-Hydroxymethylfurfural.

Liam O'Connor<sup>1</sup>, Altug Poyraz<sup>2</sup> and **Sourav Biswas**<sup>3</sup>, (1)*University at Buffalo (SUNY), USA*, (2)*Keenesaw State University, USA*, (3)*State University of New York Buffalo State, USA*.

**Short Summary:**

Herein we directly employed electrocatalysts consist of metal on the N doped carbon (M-N/C), which were found to be active in ORR in fuel cells for the aerobic oxidation of 5-hydroxymethylfurfural (HMF) to 2,5-diformylfuran (DFF) in practical reaction conditions used in organic transformations.

4:10 PM **Wed-MEBR-1610** Dynamic Surface Structures of Manganite Perovskite Depending on the Chemical Potential.

**Gregor Koch**<sup>1</sup>, Michael Hävecker<sup>2</sup>, Jinhu Dong<sup>1</sup>, Walid Hetaba<sup>2</sup>, Pierre Kube<sup>1</sup>, Andrey Tarasov<sup>1</sup>, Robert Schlögl<sup>1</sup> and Annette Trunschke<sup>1</sup>, (1)*Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany*, (2)*Max Planck Institute for Chemical Energy Conversion, Germany*.

**Short Summary:**

The potential active sites on the surface of the working AMnO<sub>3</sub> catalyst in oxidative dehydrogenation of propane were identified using operando AP-XPS. Correlations were found between the concentration of defects and electrophilic oxygen species and the selectivity to propene. Thus, many interrelating structural parameters determine catalysis on AMnO<sub>3</sub>.

4:30 PM **Wed-MEBR-1630** Interactions between Free Atom like States of Single Atom Alloys and Frontier Molecular Orbitals of Unsaturated Aldehydes.

**Taylor Spivey** and Adam Holewinski, *University of Colorado Boulder, USA*.

**Short Summary:**

Controlling the selective activation of chemical bonds is a longstanding goal of heterogeneous catalysis. While often difficult to tune for heterogeneous catalysts compared to homogeneous catalysts, single atom alloys present a unique electronic structure well suited to steer toward highly selective adsorption.

## Rendezvous Trianon

### WEDNESDAY MORNING

#### Novel Applications of Reaction Engineering in Catalytic Processes

**Session Chairs:** Ryan Hartman, *New York University, USA* and Kevin Nagy, *Snapdragon Chemistry, USA*.

9:30 AM **Wed-RZVS-0930** Scaling Photocatalytic Reactions in Flow Using Visible Light.

**Eric Moschetta**, *AbbVie, USA*.

**Short Summary:**

This work demonstrates the implementation of a laser-driven CSTR to provide kg/day level throughput for a photocatalytic reaction in a 100 mL reactor using fundamental principles of photocatalytic reactions to inform the design of the flow reactor.

9:50 AM **Wed-RZVS-0950** Combined Experimental and Numerical Approach for the Fundamental Investigation of Transport Properties in Cellular Media.

**Claudio Ferroni**, Federico Sascha Franchi, Matteo Ambrosetti, Mauro Bracconi, Matteo Maestri, Gianpiero Groppi and Enrico Tronconi, *Politecnico di Milano, Italy*.

**Short Summary:**

Lattice materials are envisioned as potential enhanced catalyst substrates for Process Intensification. To enable their rational design, a combined numerical and experimental approach is proposed to fundamentally investigate their transport properties aiming at the derivation of engineering correlations to enable reactor design at the industrial scale.

10:10 AM **Wed-RZVS-1010** Mechanocatalytic Ammonia Synthesis over Metal Nitrides in Transient Microenvironments.

Karoline Hebisch<sup>1</sup>, Andrew Tricker<sup>1</sup>, Erin Phillips<sup>1</sup>, Marco Buchmann<sup>2</sup>, Yu-Hsuan Liu<sup>1</sup>, Marcus Rose<sup>2</sup>, Eli Stavitski<sup>3</sup>, Andrew J. Medford<sup>1</sup>, Marta Hatzell<sup>1</sup> and **Carsten Sievers**<sup>1</sup>, (1)*Georgia Institute of Technology, USA*, (2)*Technische Universität Darmstadt, Germany*, (3)*Brookhaven National Laboratory, USA*.

**Short Summary:**

Ammonia is synthesized mechanocatalytically from nitrogen and hydrogen at nominally ambient conditions over metal nitrides. Catalytic activity of TiN continuously increases with milling time for at least 12 h. Ammonia synthesis is proposed to follow a transient Mars-van Krevlen mechanism, where N<sub>2</sub> activation and ammonia formation under different conditions.

10:30 AM **Wed-RZVS-1030** Enhanced Catalytic Turnover By Non-Linear Thermal Frequency Response.

**Cameron Armstrong**, Fatou Diop and Andrew Teixeira, *Worcester Polytechnic Institute, USA*.

**Short Summary:**

By applying an input waveform to a reactor system, we have observed rate enhancement effects over its isothermal counterpart. We show here that these effects are due to the applied waveforms resonating with inherent catalytic phenomena (i.e. TOF) which enhances bottlenecks that traditionally limit a reaction.

10:50 AM **Wed-RZVS-1050** Microwave Heating of Liquid-Liquid Biphasic Systems.

**Montgomery Baker-Fales**<sup>1</sup>, Tai-Ying Chen<sup>1</sup>, Himanshu Goyal<sup>2</sup> and Dionisios G. Vlachos<sup>1</sup>, (1)*University of Delaware, USA*, (2)*Indian Institute of Technology Madras, India*.

**Short Summary:**

Microwaves can enable the intensification of chemical manufacturing. They've been applied to various unit separations, but the understanding of MW-heated liquid-liquid biphasic systems related to extraction is limited. This work measures the temporal and spatial temperature difference between an aqueous and an organic phase in batch and continuous microfluidic modes.

11:10 AM **Wed-RZVS-1110** Implementation of Fluid-Solid Mass and Heat Transfer in Particle Resolved CFD Simulations of Catalytic Fixed Beds.

**Martin Kutscherauer**<sup>1,2</sup>, Scott Anderson<sup>2</sup>, Gerhard Mestl<sup>1</sup>, Sebastian Boecklein<sup>1</sup>, Thomas Turek<sup>2</sup> and Gregor D. Wehinger<sup>2</sup>, (1)*Clariant AG, Germany*, (2)*Clausthal University of Technology, Germany*.

**Short Summary:**

Particle resolved CFD simulation is the most established detailed modeling approach for catalytic fixed bed reactors. In this work a novel computationally efficient approach is presented to couple the fluid flow through the void in the packed bed with transport and reaction inside the porous catalyst particle.

11:30 AM **Wed-RZVS-1130** Mechanistic Modeling of the Pd-Catalyzed Amidation Reaction Used in the Synthesis of ABT-530.

**Eric Sacia**, Daniel Caspi, Moiz Diwan, Jean-Christophe Califano, Daniel Mack and Shashank Shekhar, *AbbVie, USA*.

**Short Summary:**

Process development in the pharmaceutical industry requires elucidating the impact of the reaction environment on yield and formation of impurities that are particularly challenging to separate. The kinetic modeling performed in this work has enabled the production of ABT-530 by constraining the operating space and ensuring a robust manufacturing process.

## WEDNESDAY AFTERNOON

### Catalysis and Reaction Engineering for a Greener Future

**Session Chairs:** Eric Hukkanen, *Alkermes, USA* and Joshua Pacheco, *Zeolyst International, USA*.

1:10 PM **Wed-RZVS-1310** Effect of Membrane Properties on the Direct Conversion of CO<sub>2</sub> to Dimethyl Ether in a Fixed Bed Membrane Reactor.

Maria Fernanda Neira Dangelo, **Serena Poto** and Fausto Gallucci, *Eindhoven University of Technology, Netherlands*.

**Short Summary:**

The work addresses the direct conversion of CO<sub>2</sub> to dimethyl ether, i.e., a key CO<sub>2</sub> recycling solution, in a membrane reactor to abate thermodynamic limitations. Using phenomenological modelling, the work shows the effects of membrane properties on coupling reaction with in-situ water and heat removal, and thereby on reactor performance.

1:30 PM **KEYNOTE Wed-RZVS-1330** Developing Process Technologies for a Sustainable Future. **Stanley Frey**, *Honeywell UOP, USA*.

**Short Summary:**

Several examples are shown that illustrate the implementation of sustainable biomass conversion and plastic upcycling technologies. The maturation of these technologies is enabled by the integration of commercial experience and scientific knowledge contributions from both the academic and industrial technical communities.

2:10 PM **Wed-RZVS-1410** Design of an Innovative Compartmented Heterogeneous Reactor Dedicated to Hemicelluloses Valorization.  
**Victoria Dias da Silva Freitas**, Maxime Pichou, Léa Vilcocq, Régis Philippe and Pascal Fongarland, *Université de Lyon, CNRS, France*.

**Short Summary:**

In order to study the coupling reaction/separation/reaction of sugar alcohols synthesis from hemicelluloses, xylan hydrolysis, xylan/xylose membrane separation and ex-hemicellulose sugars hydrogenation were studied in continuous mode. Individual simulation models are being developed to provide enough information to establish the innovative reactor model, which will also be tested experimentally.

2:30 PM **Wed-RZVS-1430** Pd-CHA Catalysts As Passive NO<sub>x</sub> Adsorbers (PNA): Kinetic Modeling of Transient Adsorption Tests.

Djamela Bounechada<sup>1</sup>, **Donna Liu**<sup>2</sup>, Umberto Iacobone<sup>3</sup>, Roberta Villamaina<sup>1</sup>, Isabella Nova<sup>3</sup>, Enrico Tronconi<sup>3</sup>, Maria Pia Ruggeri<sup>1</sup>, Loredana Mantarosie<sup>1</sup>, Jillian Collier<sup>1</sup> and David Thompsett<sup>1</sup>, (1)*Johnson Matthey Technology Centre, United Kingdom*, (2)*Johnson Matthey, USA*, (3)*Politecnico di Milano, Italy*.

**Short Summary:**

Transient kinetic analysis of NO<sub>x</sub> storage over Pd-CHA as PNA material validates a storage mechanism based on redox processes where NO<sub>x</sub> are stored primarily on Pd<sup>0</sup>. Pd<sup>0</sup> can be reduced to Pd<sup>I</sup> by NO itself and more efficiently by CO: indeed, CO presence determines greater NO storage capacity.

2:50 PM **Wed-RZVS-1450** Spatiotemporal Features of NO<sub>x</sub> + Hydrocarbon Trapping and Conversion in a Sequential Monolith Configuration.

**Abhay Gupta** and Michael P. Harold, *University of Houston, USA*.

**Short Summary:**

In this study we utilize the spatially-resolved mass spectrometry experiments to resolve the spatiotemporal features of the Lean Hydrocarbon NO<sub>x</sub> Trap (LHCNT) comprising of PNA (Passive NO<sub>x</sub> Adsorber), HCT (HC trap) and OC (oxidation catalyst) functions to devise an operating strategy towards meeting emission performance targets.

## Reaction Engineering for Fuels and Petrochemicals

**Session Chairs:** Jennifer Lee, *Harvard University, USA* and Bjorn Moden, *Zeolyst International, USA*.

3:30 PM **Wed-RZVS-1530** Sharpening Spatial Temperature of Millisecond Catalytic Wall Reactor for Selective Nonoxidative Coupling of Methane.

**Sichao Cheng** and Dongxia Liu, *University of Maryland - College Park, USA*.

**Short Summary:**

An autothermal millisecond wall reactor achieved self-sustaining nonoxidative methane conversion reaction with tunable hydrocarbon product selectivity and negligible coke formation. This reactor design enables high local temperature for methane activation as well as sharpening spatial temperature and short methane contact time to effectively suppress coke formation.

3:50 PM **Wed-RZVS-1550** A Tailored Multi-Functional Catalyst for Efficient Alkenylbenzene Production Under a Cyclic Redox Scheme.

**Junchen Liu**<sup>1</sup>, Xing Zhu<sup>2</sup>, Yunfei Gao<sup>1</sup>, Xijun Wang<sup>1</sup>, Vasudev Pralhad Haribal<sup>1</sup>, Luke Neal<sup>1</sup> and Fanxing Li<sup>1</sup>, (1)*North Carolina State University, USA*, (2)*Kunming University of Science and Technology, China*.

**Short Summary:**

We report a redox oxidative dehydrogenation to produce styrene with (Ca/Mn)<sub>1-x</sub>O@KFeO<sub>2</sub>. This catalyst auto-thermally converts ethylbenzene to styrene with >90% single-pass yield. *in-situ* XRD, XPS and TEM indicate the lattice-oxygen donation from (Ca/Mn)<sub>1-x</sub>O core stabilizes the KFeO<sub>2</sub> shell. Aspen Plus process modeling indicates a potential 82% energy savings.

4:10 PM **Wed-RZVS-1610** Development of a Novel Reactor for the Production of Sustainable Aviation Fuel.

Jay Clarkson and **Dan Enache**, *Johnson Matthey Technology Centre, United Kingdom*.

**Short Summary:**

The development of novel reactor enhancement device (CANS<sup>tm</sup>) for the efficient production of sustainable aviation fuels. This device containing sub mm catalyst particles, is inserted into a traditional tubular fixed bed reactor to increase the productivity per unit volume of reactor.

4:30 PM **Wed-RZVS-1630** Breakthrough Fixed-Bed Catalytic Reactors Based on Packed-Structured Cellular Internals for Intensified Heat Transfer in Compact Applications: A Pilot-Scale Demonstration.

**Carlo Giorgio Visconti**, Gianpiero Groppi and Enrico Tronconi, *Politecnico di Milano, Italy*.

**Short Summary:**

Through a pilot-scale study, we demonstrate that structuring tubular reactors with highly conductive engineered cellular internals, and packing catalysts micro-pellets within those internals, represents a game-changing solution to enhance the radial heat transfer in compact reactors, where convective heat transport is poor, paving the way to intensified catalytic reactors technologies.

4:50 PM **Wed-RZVS-1650** Heat Management in the Catofin Process.

**Alexander Nijhuis**, Ewa Gebauer Henke and Aaron Vandeputte, *SABIC, Netherlands*.

**Short Summary:**

A pilot scale study, combined with kinetic and reactor modeling, into the dynamics of the Catofin process for the dehydrogenation of light alkanes is presented. It is shown how heat management, coke formation and changing catalyst oxidation state in this cyclic process significantly affect its performance.



5:10 PM **Wed-RZVS-1710** Sustainable Green Hydrogen Production Via Sorption Enhanced Steam Reforming of Bio-Based and Waste Streams. Abdelrahman Mostafa, Matteo Romano, Alessandra Beretta and **Gianpiero Groppi**, *Politecnico di Milano, Italy*.

**Short Summary:**

This work discusses the integration between bio-refineries and a novel hydrogen production unit based on the sorption enhanced reforming concept aiming to valorize the biorefinery by-products and waste streams. A computational model developed and results verify a potential benefit for such integration leading to overall cost reduction of the biofuels.

## Sutton North

### WEDNESDAY MORNING

#### Catalytic Conversion of Biomass to Fuels and Chemicals I

**Session Chairs:** Madelyn R. Ball, *West Virginia University, USA* and Derek Butler, *Archer Daniels Midland, ; Archer Daniels Midland, .*

9:30 AM **Wed-SUNO-0930** Improved Biofuel Cracking in a Refinery FCC Unit Via Mechanistic Insights from Isotopic Labeling.

**Joel E. Schmidt**, Matthew Hurt and Tengfei Liu, *Chevron Technical Center, USA*.

**Short Summary:**

Using biobased feedstocks for fuels is being increasingly seen as the only method to quickly decarbonize. We present the catalytic cracking of a <sup>13</sup>C labelled triglyceride using a unit operating at one millionth refinery scale, with subsequent cracking mechanism insight from high resolution GC-MS analysis of the products.

9:50 AM **Wed-SUNO-0950** Redefining Catalyst and Process Development in Fluid Catalytic Cracking for Chemical Recycling and Renewable Feedstock Integration.

Marius Kirchmann and **Simon Wodarz**, *hte GmbH, Germany*.

**Short Summary:**

A novel, more affordable FCC catalyst testing procedure based on the Micro Downflow Unit (MDU) redefines catalyst and process development in fluid catalytic cracking for chemical recycling and renewable feedstock integration. It provides realistic cracking conditions, closely simulating the gradients in temperature, partial pressure and contact time of commercial FCC.

10:10 AM **Wed-SUNO-1010** Co-Processing of Hydrothermal Liquefaction Bio-Crude for the Production of Liquid Transportation Fuels.

**Venu Babu Borugadda**, Rishav Chand and Ajay Dalai, *University of Saskatchewan, Canada*.

**Short Summary:**

This research is significant to co-process the bio-crude produced from HTL in existing refineries in order to meet the Canada's Renewable Fuel Standards and Low Carbon Emission Standards.

10:30 AM **Wed-SUNO-1030** Pathways, Kinetics, and Reactor Design for Upgrading of Wet Waste-Derived Volatile Fatty Acids to Sustainable Aviation Fuel.

**Jacob H. Miller**, Nabila A. Huq, Glenn R. Hafenstine, Hannah Nguyen and Derek R. Vardon, *National Renewable Energy Laboratory, USA*.

**Short Summary:**

We present a strategy for upgrading waste-derived carboxylic acids into aviation fuel blendstock which meets ASTM criteria using catalytic ketonization, aldol condensation, and hydrodeoxygenation. Kinetics and deactivation phenomena of carboxylic acid ketonization over ZrO<sub>2</sub> are studied thoroughly; results of these studies are used to simulate an industrial-scale packed bed reactor.

10:50 AM **Wed-SUNO-1050** Heterogeneous Organoacid Catalysts for Biofuel Production.

**Cameron Alexander Price** and Christopher Parlett, *University of Manchester, United Kingdom*.

**Short Summary:**

This work demonstrates the effectiveness of solid organoacid catalysts for free fatty acid conversion to methyl esters, with the surprising finding that carboxylic acids offer the best activities; demonstrating that acid strength does not equate to better performance in this reaction, when compared to analogous or industrially available materials

11:10 AM **Wed-SUNO-1110** Co-Processing Renewable/Recyclable Feedstocks in FCC.

**Jian Shi**, James Fu, Lucas Dorazio, C. P. Kelkar, Vasileios Komvokis and Bilge Yilmaz, *BASF Corporation, USA*.

**Short Summary:**

Co-processing renewable/recyclable crude oil (RCO) in an FCC unit is a new and developing area. A wide variety of RCO (waste plastic & biogenic source) were evaluated in ACE unit. The impacts of co-feeding on products yields and chemistry in FCC process were discussed.

11:30 AM **Wed-SUNO-1130** Deoxygenation of Fatty Acid to Aviation Biofuel Via Ketonization-McLafferty Rearrangement without External H<sub>2</sub>.

Tosapol Maluangnont and **Tawan Sooknoi**, *King Mongkut's Institute of Technology Ladkrabang, Thailand*.

**Short Summary:**

Bio-jet fuels, C<sub>9</sub>-C<sub>14</sub> hydrocarbons, can be obtained from deoxygenation of palmitic acid via ketonization-McLafferty scission over the basic layered alkali titanate catalysts without externally fed H<sub>2</sub>.

## WEDNESDAY AFTERNOON

### Catalytic Conversion of Biomass to Fuels and Chemicals II

**Session Chairs:** Michael M. Nigra, *University of Utah, USA* and Jun Wang, *SABIC, USA*.

1:10 PM **Wed-SUNO-1310** Accelerating the Catalyst and Process Development Cycle for Bioenergy Applications.

**Joshua Schaidle**, *National Renewable Energy Laboratory, USA*.

**Short Summary:**

Biomass presents a near-term opportunity to produce renewable fuels with low carbon intensity, yet, as a complex, heterogeneous feedstock, it introduces a number of challenges for catalytic processing. This work describes a Design-Build-Test-Learn cycle for catalyst and process development for bioenergy applications and demonstrates a 4x acceleration in this cycle.

1:30 PM **Wed-SUNO-1330** Catalytic Hydroconversion of HTL Micro-Algal Bio-Oil into Biofuel.

**Bruno Magalhaes**, Ruben Checa, Chantal Lorentz, Pavel Afanasiev, Dorothée Laurenti and Christophe Geantet, *Université de Lyon, CNRS, France*.

**Short Summary:**

Catalytic HDT can be used for the upgrading of HTL micro-algal bio-oil, producing more than 60% of biofuel in the diesel range. Sulfided catalyst performed better than nitride and phosphide systems. However, catalyst performances can be increased or may be associated with a second treatment stage to reduce less-reactive N-components.

1:50 PM **Wed-SUNO-1350** Enhancing the Conversion of Wet Waste to Jet Fuels with Atomic Layer Deposition-Coated Catalysts.

**W. Wilson McNeary**<sup>1</sup>, Jacob H. Miller<sup>1</sup>, Jonathan Travis<sup>2</sup>, Gabriella Lahti<sup>1</sup>, Tuğçe E. Erden<sup>3</sup>, Luke Tuxworth<sup>3</sup>, Michael Watson<sup>3</sup>, Arrelaine Dameron<sup>2</sup> and Derek R. Vardon<sup>1</sup>, (1)*National Renewable Energy Laboratory, USA*, (2)*Forge Nano, USA*, (3)*Johnson Matthey Technology Centre, United Kingdom*.

**Short Summary:**

We report herein the development of highly-active catalysts for hydrodeoxygenation of wet waste-derived ketones into sustainable aviation fuel. TiO<sub>2</sub> overcoats synthesized via atomic layer deposition were found to promote up to a 5-fold increase the alkane selectivity of supported Pt catalysts, with maximum alkane production observed at low Pt loadings.

2:10 PM **Wed-SUNO-1410** Co-Processing Bio-Crudes with Petroleum Gas Oil in Hydrotreating: Kinetics of Heteroatom Removal and Incorporation of Biogenic Carbon in Produced Fuels.

**Huamin Wang**, Daniel Santosa, Cheng Zhu, Igor Kutnyakov and Matthew Flake, *Pacific Northwest National Laboratory, USA*.

**Short Summary:**

Co-processing of liquid intermediates, such as bio-oil and bio-crudes from biomass and waste, with petroleum gas oil demonstrate high biogenic carbon incorporation and simultaneous removal of heteroatoms. Understanding the kinetics of hydrotreating of the new heteroatom-containing species in bio-crudes greatly help the design of improved catalysts and process.

2:30 PM **Wed-SUNO-1430** A Two-Step Approach for Catalytic Conversion of 2,3-Butanediol to n-C4-C5 Rich Olefins Fuel Precursors.

**Martin Affandy**<sup>1</sup>, Libor Kovarik<sup>1</sup>, Steven Phillips<sup>1</sup>, Richard Elander<sup>2</sup> and Vanessa Dagle<sup>1</sup>, (1)*Pacific Northwest National Laboratory, USA*, (2)*National Renewable Energy Laboratory, USA*.

**Short Summary:**

We present a new process for upgrading of 2,3-butanediol fermentation broth to hydrocarbon fuels that does not require 2,3-BDO separation from water.

2:50 PM **Wed-SUNO-1450** Transforming Biological Feedstocks to Renewable Fuels and Base Oils Via Novel Technologies.

**Cong-Yan Chen**<sup>1,2</sup>, Yalin Hao<sup>1</sup> and Alexander Kuperman<sup>1</sup>, (1)*Chevron Technical Center, USA*, (2)*University of California, Davis, USA*.

**Short Summary:**

In this paper we will present the latest results from our R&D on transforming lipids to renewable jet/diesel fuels and lubricant base oils via novel technologies. Furthermore, we will report the new role of paraffin disproportionation in improving the properties of jet/diesel fuels.

### Biomass to Chemicals I: Surfaces and Supports

**Session Chairs:** Bin Liu, *Kansas State University, USA* and Manoj Koranne, *Grace*, .

3:30 PM **Wed-SUNO-1530** Carbon Nanotube Hydrogen Highways to Decouple Active Sites Responsible for Selective C-O Cleavage.

Laura A. Gomez, Tram Pham, Reda Bababrik, Lawrence Barrett, Taiwo Omotoso, Nicholas Briggs, Don Jones, Han Chau and **Steven P. Crossley**, *University of Oklahoma, USA*.

**Short Summary:**

We discuss a method of separating the kinetic relevance of prospective sites at the metal-support interface from promoter effects for C-O bond activation on reducible supports. This is accomplished by depositing metals such as Pt and reducible oxides such as TiO<sub>2</sub> or MoO<sub>3</sub> on opposing ends of carbon nanotubes.

3:50 PM **Wed-SUNO-1550** Mesoporous Silica Nanospheres Supported Ru Catalyst for the Hydrogenation of Levulinic Acid to Gamma-Valerolactone. **Antonio Torres López**<sup>1,2,3</sup>, Christopher Parlett<sup>1,2,3</sup> and Arthur Garforth<sup>1</sup>, (1)University of Manchester, United Kingdom, (2)Diamond Light Source, United Kingdom, (3)UK Catalysis Hub, United Kingdom.

**Short Summary:**

The coupling of Ru nanoparticles and mesoporous silica nanospheres, via ethylene glycol assisted impregnation, yields a catalyst that permits the efficient conversion of levulinic acid into  $\gamma$ -valerolactone, with high activity and selectivity. Operando XAS/DRIFTS/MS has revealed the critical role of ethylene glycol in preventing Ru sintering during thermal processing.

4:10 PM **Wed-SUNO-1610** Steering the Oxophilicity and Hydrogenation Ability of Transition Carbide Catalysts for Deoxygenation of Stearic Acid.

**Marlene Fuhrer**, J.H. (Harry) Bitter and Tomas Haasterecht, van, *Wageningen University & Research, Netherlands*.

**Short Summary:**

We highlighted the potential of bimetallic molybdenum and tungsten carbides as viable replacement for noble metal catalysts. We propose that the Mo/W ratio in bimetallic carbide based-catalysts influences the oxophilicity and hydrogenation power of the catalyst which in turn effects the selectivity of the catalysts towards oxygenates, alkenes or alkanes.

4:30 PM **Wed-SUNO-1630** Assessing the Role of Interfacial and Metal Sites in Pt/TiO<sub>2</sub>-Catalyzed Acetic Acid Hydrodeoxygenation.

**Sean Tacey** and Carrie Farberow, *National Renewable Energy Laboratory, USA*.

**Short Summary:**

Effective hydrodeoxygenation (HDO) catalysts are needed to create more-stable bio-oil products following the catalytic fast pyrolysis of biomass. Acetic acid, a carboxylic acid model compound, HDO reaction pathways were modeled through DFT at Pt-metal and Pt-anatase-interface sites. The results indicate Pt-metal and Pt-anatase-interface sites prefer decarboxylation and deoxygenation products, respectively.

4:50 PM **Wed-SUNO-1650** Effects of Pore Topology and Polarity on Rates and Selectivities for Aldol Condensation on Ti-Silicates.

**Zhongyao Zhang**, Claudia Berdugo-Díaz, Matthew Jacobson, Hongbo Zhang, Daniel Bregante and David Flaherty, *University of Illinois Urbana-Champaign, USA*.

**Short Summary:**

The results suggest topology and polarity of Ti-silicates affect the stability of reactive intermediates for aldol condensation and esterification by excess interactions, which change primary reaction rates, decrease the tendency for rates to be inhibited by water vapor, and improve selectivities to aldol condensation products, especially C<sub>4</sub> species.

5:10 PM **Wed-SUNO-1710** Promoted Molybdenum Oxide for the Deoxygenation of Carboxylic Acids: Kinetics and Mechanism.

**Laura A. Gomez**, Caleb Q. Bavlnka, Tianhao E. Zhang and Steven P. Crossley, *University of Oklahoma, USA*.

**Short Summary:**

Promoted MoO<sub>3</sub> shows high activity and selectivity for the conversion of pentanoic acid to aldehyde at low temperatures (<350°C). This study provides an insight into the mechanism by using a pulse reactor. The active sites at the interface were investigated by a controlled distance on a conductive carbon nanotubes support.

## Sutton South

### WEDNESDAY MORNING

#### Catalyst Characterization with Synchrotron and Lab-based X-ray Sources

**Session Chairs:** Viktor Cybulskis, *Syracuse University, USA* and Robert J. Davis, *University of Virginia, USA*.

9:30 AM **Wed-SUSO-0930** Resolving Mechanistic Aspects of Non-Oxidative Methane Upgrading on Fe/Zeolite Catalysts By Operando XRD and Photoelectron Photoion Coincidence Spectroscopy.

**Hao Zhang**, Nikolay Kosinov and Emiel J. M. Hensen, *Eindhoven University of Technology, Netherlands*.

**Short Summary:**

Through operando XRD and photoelectron photoion coincidence spectroscopy, we provide mechanistic insights into the formation and evolution of confined hydrocarbon species and gas-phase intermediates over Fe@MFI and Fe@CHA catalysts during methane non-oxidative coupling reaction.

9:50 AM **Wed-SUSO-0950** The Synergy of Lab- and Synchrotron-X-Ray Absorption Spectroscopy: Operando Studies of Multi-Metal Solid CO<sub>2</sub> Hydrogenation Catalysts.

**Nina S. Genz**<sup>1</sup>, Antti-Jussi Kallio<sup>2</sup>, Ramon Oord<sup>1</sup>, Matteo Monai<sup>1</sup>, Florian Meirer<sup>1</sup>, Simo Huotari<sup>2</sup> and Bert M. Weckhuysen<sup>1</sup>, (1)Utrecht University, Netherlands, (2)University of Helsinki, Finland.

**Short Summary:**

Gaining insight into the synergistic effects of multi-metal catalysts is key for the rational design of improved catalysts. We used the synergy of operando X-ray absorption spectroscopy in the laboratory and at a synchrotron to unravel metal- and metal ratio-dependent differences in multi-metal CO<sub>2</sub> hydrogenation catalysts on multiple time scales.

10:10 AM **KEYNOTE Wed-SUSO-1010 Science from the Front Lines of a Catalysis Operando X-Ray Absorption Spectroscopy Operation at SsrI.** Simon Bare<sup>1</sup>, Adam Hoffman<sup>1</sup>, Jiyun Hong<sup>1</sup>, Jorge Perez-Aguilar<sup>1</sup>, Rachita Rana<sup>2</sup>, Ambarish Kulkarni<sup>2</sup> and Fernando Vila<sup>3</sup>, (1)SLAC National Accelerator Laboratory, USA, (2)University of California, Davis, USA, (3)University of Washington, USA.

**Short Summary:**

Synchrotron *operando* catalyst characterization provides critical structural and electronic information on the nature of the working catalyst. New methods and approaches continue to evolve providing even more detailed insight. Success of these challenging experiments demands the collaboration from a team of dedicated researchers, with researchers located at the synchrotron facility.

10:50 AM **Wed-SUSO-1050 Quantexafs: A Theory-Guided Approach for Quantitative Characterization of Atomically Dispersed Catalysts.**

Rachita Rana<sup>1</sup>, Yizhen Chen<sup>2</sup>, Bruce Gates<sup>1</sup>, Simon Bare<sup>3</sup> and Ambarish Kulkarni<sup>1</sup>, (1)University of California, Davis, USA, (2)University of Science and Technology of China, China, (3)SLAC National Accelerator Laboratory, USA.

**Short Summary:**

Presenting a novel EXAFS analysis workflow combining density functional theory with automated EXAFS analysis. 'QuantEXAFS', emphasizes the quantitative nature of fitting based on hundreds of structures derived from DFT. This is instrumental in predicting the atomistic mechanisms associated with the formation of active sites and their evolution under reaction conditions.

11:10 AM **Wed-SUSO-1110 Surprise and Shine: The Untold Capabilities of Benchtop Bragg Diffraction in Characterizing Ultrasmall, Not-so-Noble Supported Nanoparticles.**

Jeremiah Lipp<sup>1</sup>, Ritubarna Banerjee<sup>1</sup>, Nirmalendu Patra<sup>2</sup>, M. D. Fakhruddin Patwary<sup>1</sup>, Anhua Dong<sup>1</sup>, Frank Girgsdies<sup>3</sup>, Simon Bare<sup>2</sup> and John R. Regalbuto<sup>1</sup>, (1)University of South Carolina, USA, (2)SLAC National Accelerator Laboratory, USA, (3)Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany.

**Short Summary:**

We demonstrate the capabilities of benchtop Bragg diffraction (XRD) in characterizing ultra-small (< 2nm) nanoparticles by examining six silica-supported "noble" metals under ambient conditions. Surprisingly, Bragg diffraction is capable of shining light on this difficult-to-characterize size region – revealing the propensity of these metal nanoparticles to oxidize at room temperature.

11:30 AM **Wed-SUSO-1130 Electrophilic Oxygen in Alkene Epoxidation.**

Emilia Carbonio<sup>1,2</sup>, Frederic Sulzmann<sup>2</sup>, Alexander Klyushin<sup>1,2</sup>, Michael Hävecker<sup>2,3</sup>, Simone Piccinin<sup>4</sup>, Axel Knop-Gericke<sup>2,3</sup>, Robert Schlögl<sup>2,3</sup> and Travis Jones<sup>2</sup>, (1)Helmholtz-Zentrum Berlin für Materialien und Energie, Germany, (2)Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany, (3)Max Planck Institute for Chemical Energy Conversion, Germany, (4)Istituto Officina dei Materiali (CNR-IOM) c/o SISSA, Italy.

**Short Summary:**

We identify the nature of electrophilic oxygen on silver catalyst by combining NAP-XPS and DFT. This species is identified as an adsorbed SO<sub>x</sub> species whose coverage correlates with ethylene epoxide selectivity. Consistent with a lower epoxide selectivity, we show the SO<sub>x</sub> species is not present under steady-state propylene epoxidation conditions.

## WEDNESDAY AFTERNOON

### Operando Approaches for Catalyst Characterization

**Session Chairs:** Brad Fingland, *Spartan Innovations*, and Moniek Tromp, *University of Groningen, Netherlands*.

1:10 PM **Wed-SUSO-1310 Combining Operando Studies and Model Supports to Unravel the Nature of the Promotion of Supported Cu Catalysts for High Pressure Syngas Conversion.**

Petra E. de Jongh, Remco Dalebout and Laura Barberis, *Utrecht University, Netherlands*.

**Short Summary:**

We show that the use of carbon model supports allows to unravel the nature of the relevant fraction of promoter species using X-Ray Spectroscopy under working conditions. We illustrate this using supported Cu catalysts promoted with ZnO and MnO for high pressure methanol synthesis from syngas or by CO<sub>2</sub> hydrogenation.

1:30 PM **Wed-SUSO-1330 Atomically Dispersed Indium Ions in Monoclinic ZrO<sub>2</sub> Catalyze Efficiently CO<sub>2</sub> Hydrogenation to Methanol: Evidence from Operando X-Ray Absorption Spectroscopy.**

Athanasia Tsoukalou, Paula Macarena Abdala, Elena Willinger, Andac Armutlulu, Alexey Fedorov and Christoph Müller, *ETH Zürich, Switzerland*.

**Short Summary:**

*Operando* X-ray absorption spectroscopy identifies the monoclinic solid solution m-ZrO<sub>2</sub>:In as a superior catalyst for the direct conversion of CO<sub>2</sub> to methanol. This catalyst contains active In–V<sub>o</sub>–Zr surface species that are significantly more stable towards reduction than In–V<sub>o</sub>–In sites in bixbyite-type In<sub>2</sub>O<sub>3</sub>.

1:50 PM **Wed-SUSO-1350 Cu-Al-Oxo Clusters As Active Site in Mordenite for the Direct Methane to Methanol Reaction.**

Lei Tao<sup>1</sup>, Maricruz Sanchez-Sanchez<sup>2</sup> and Johannes A. Lercher<sup>1,3</sup>, (1)Technical University of Munich, Germany, (2)Technische Universität Wien, Austria, (3)Pacific Northwest National Laboratory, USA.

**Short Summary:**

The combination of XANES simulations with experimental spectra and catalytic data of a series of CuMOR prepared under controlled conditions has led to identifying two different active sites for CH<sub>4</sub> oxidation to CH<sub>3</sub>OH. The presence of extra-framework Al leads to the formation of a new highly active Al-containing Cu-oxo nanocluster.

2:10 PM **KEYNOTE Wed-SUSO-1410** Elucidating the Origin of Catalyst Activation and Deactivation with Operando Spectroscopy and Microscopy.

**Bert M. Weckhuysen**, *Utrecht University, Netherlands.*

**Short Summary:**

Catalytic performance is usually assessed on the basis of activity, selectivity and stability. In this lecture, advances in the development of operando spectroscopy and microscopy for probing catalyst activation and deactivation processes will be presented. This will be done by using four different showcases from our own work.

2:50 PM **Wed-SUSO-1450** A Paradigm Shift in the Nature of the Active Surface of the Bismuth Molybdate Catalyst during the Selective Oxidation of Propylene.

**Bar Mosevitzky Lis**<sup>1</sup>, Yunfei Gao<sup>2</sup>, Eric D. Walter<sup>3</sup>, Michael E. Ford<sup>1</sup>, Jih-Mirn Jehng<sup>4</sup> and Israel E. Wachs<sup>1</sup>, (1)*Lehigh University, USA*, (2)*North Carolina State University, USA*, (3)*Pacific Northwest National Laboratory, USA*, (4)*National Chung Hsing University, Taiwan*.

**Short Summary:**

Bulk  $\alpha$ -Bi<sub>2</sub>(MoO<sub>4</sub>)<sub>3</sub> used for propylene selective oxidation was studied *in situ*, the results indicating that the reaction takes place on a mostly oxidized, molybdenum enriched surface where only molybdenum participates in the reaction by undergoing redox (Mo<sup>6+</sup>→Mo<sup>5+</sup>), while bismuth remains fully oxidized possibly promoting the reaction via a ligand effect.

## Catalyst Characterization One Molecule or Particle at a Time

**Session Chairs:** Konstantinos Goulas, *Oregon State University, USA* and Lucun Wang, *Idaho National Laboratory, USA*.

3:30 PM **Wed-SUSO-1530** Unravelling Channel Structure–Diffusivity Relationships in Zeolite ZSM-5 at the Single-Molecule Level.

**J.J. Erik Maris**, Donglong Fu, Katarína Stančíaková, Nikolaos Nikolopoulos, Onno van der Heijden, Laurens Mandemaker, Marijn E. Siemons, Desiree Salas Pastene, Lukas C. Kapitein, Freddy T. Rabouw, Florian Meirer and Bert M. Weckhuysen, *Utrecht University, Netherlands*.

**Short Summary:**

Diffusion of single molecules is tracked in the straight and sinusoidal channels of the ZSM-5 zeolites using a combination of single-molecule localization microscopy and uniformly oriented zeolite thin films. Quantification of diffusion heterogeneities shows that the geometry of zeolite channels dictates the mobility and motion behavior of the guest molecules.

3:50 PM **Wed-SUSO-1550** Revealing Early-Stage Ethylene Polymerization Versus Catalyst Fragmentation By Using a Spherical Cap Ziegler-Type Model Catalyst.

Laurens Mandemaker<sup>1</sup>, Koen Bossers<sup>1</sup>, **Nikolaos Nikolopoulos**<sup>1</sup>, Marcus Rohnke<sup>2</sup>, Peter de Peinder<sup>1</sup>, Bas Terlingen<sup>1</sup>, Yuanshuai Liu<sup>1</sup>, Felix Walther<sup>2</sup> and Bert M. Weckhuysen<sup>1</sup>, (1)*Utrecht University, Netherlands*, (2)*Justus Liebig University, Germany*.

**Short Summary:**

In this work, a model spherical LaOCl catalyst, patterned on a substrate, was used to characterize and link early stage ethylene polymerization versus catalyst fragmentation using a broad toolbox of micro-spectroscopic techniques.

4:10 PM **Wed-SUSO-1610** Fluorescent Probe Molecules Assay for Space-Resolved Chemical Characterization of Shaped Catalyst Bodies.

**Matteo Monai**, Erik Maris, Nikolaos Nikolopoulos, Luke Parker, Caroline Versluis, Sophie H. van Vreeswijk, Silvia Zanoni, Florian Meirer and Bert M. Weckhuysen, *Utrecht University, Netherlands*.

**Short Summary:**

To translate fundamental knowledge to industrial-scale applications, structure-activity relationships should be extended to complex, technical catalysts. For this, spatially resolved, chemically sensitive and fast screening techniques are needed. Here, we introduce bioscience-inspired fluorescent probe assays for fast and space-resolved (100 nm) chemical characterization of shaped catalysts using confocal fluorescent microscopy.

4:30 PM **Wed-SUSO-1630** Diffusion Phenomena at the Single Catalyst Particle Level As Evaluated within a Multiplexed Microfluidic Chip with Fluorescence Microscopy.

**Alessia Broccoli**<sup>1</sup>, Luca Carnevale<sup>1</sup>, Rafael Mayorga Gonzalez<sup>2</sup>, Bert M. Weckhuysen<sup>2</sup>, Wouter Olthuis<sup>1</sup>, Mathieu Odijk<sup>1</sup> and Florian Meirer<sup>2</sup>, (1)*University of Twente, Netherlands*, (2)*Utrecht University, Netherlands*.

**Short Summary:**

A method to evaluate the accessibility of catalysts at the single-particle level is proposed. A microfluidic device is used to evaluate the uptake of fluorescent molecules in porous particles over time. The device allows parallel experiments performance, enabling the comparison of the diffusion in different particles under the same conditions.

4:50 PM **Wed-SUSO-1650** Catalysis for Mapping Nanoscale Cooperative Ligand Adsorption.

**Rong (Rocky) Ye** and Peng Chen, *Cornell University, USA*.

**Short Summary:**

We use catalysis to map the adsorption of small-molecule/ion/polymer ligands on gold nanoparticles of various morphologies *in situ* under ambient solution conditions. We differentiate at nanometer resolution their adsorption affinities among different sites on the same nanoparticle and uncover positive/negative adsorption cooperativity, both essential for understanding adsorbate-surface interactions.

5:10 PM **Wed-SUSO-1710** Argon Isotherms and Simulations Define Sites in Zeolites.

**James Crawford**<sup>1</sup>, Ryther Anderson<sup>2</sup>, Diego Gomez-Gualdrón<sup>2</sup> and Moises Carreon<sup>2</sup>, (1)*National Renewable Energy Laboratory, USA*, (2)*Colorado School of Mines, USA*.

**Short Summary:**

Confined copper clusters in zeolites are active for biomimetic methane oxidation to methanol. Conventional characterization includes X-ray absorption and chemisorption implying the location and site nuclearity. Cryogenic argon adsorption coupled with computational adsorption, reported here, provides access to unique information on the location and abundance of sites.



## Trianon Ballroom

### WEDNESDAY MORNING

#### Catalyst Design

**Session Chairs:** Matthew Montemore, *Tulane University, USA* and Christopher Paolucci, *University of Virginia, USA*.

9:30 AM **Wed-TRBR-0930** Stability and Catalytic Activity of Non-Stoichiometric Overlayers in Bimetallic Systems.

**Trenton Wolter**, Roberto Schimmenti and Manos Mavrikakis, *University of Wisconsin-Madison, USA*.

**Short Summary:**

In this talk, we discuss non-stoichiometric overlayer structures in bimetallic catalysts. We utilize moiré patterns to identify stable non-stoichiometric structures for Cu, Ir, Ni, Pd, Pt, Rh, and Ru supported on Au(111). We then determine ORR activity and stability descriptors for stoichiometric and non-stoichiometric overlayer structures.

9:50 AM **Wed-TRBR-0950** Oxygen Induced Surface Dynamics of Bimetallic Catalysts for Selective Activation of CO<sub>2</sub> and Light Alkanes.

Haoyue Guo<sup>1</sup>, Xuelong Wang<sup>1</sup>, Jingguang Chen<sup>2</sup> and **Ping Liu**<sup>1</sup>, (1)*Brookhaven National Laboratory, USA*, (2)*Columbia University, USA*.

**Short Summary:**

Bimetallic catalysts typically feature distinct chemical and electronic properties. Hereby, we conducted Density Functional Theory (DFT) investigation of a wide range of bimetallic-derived catalysts, in particular the surface dynamics under oxidative chemical environments, which provided a strategy to guide the design of bimetallic catalysts for target catalytic reactions.

10:10 AM **Wed-TRBR-1010** Computational Modelling of Ni-in Intermetallic Catalysts for Selective Hydrogenation of Acetylene to Ethylene.

**Zahra Almisbaa**<sup>1</sup>, Hassan Aljama<sup>2</sup>, Luigi Cavallo<sup>3</sup> and Philippe Sautet<sup>1</sup>, (1)*University of California, Los Angeles, USA*, (2)*Research & Development Center, Saudi Arabia*, (3)*King Abdullah University of Science and Technology (KAUST), Saudi Arabia*.

**Short Summary:**

DFT-based modelling is used to describe the key hydrogenation and oligomerization reactions for acetylene on Ni-In intermetallic compounds. The promotional effect of introducing In to metallic Ni is evaluated against monometallic Ni surface. This investigation aims to unravel the characteristics of some novel intermetallic catalysts during selective hydrogenation of alkynes.

10:30 AM **Wed-TRBR-1030** Computational Evidence for Promoted Chemicals Production Enabled By Bifunctional Catalysts.

**Bin Liu**, Narges Manavi and Hao Deng, *Kansas State University, USA*.

**Short Summary:**

Unambiguous evidence regarding promoted NH<sub>3</sub> synthesis was obtained using well-defined bifunctional models. This finding will enable us to pursue sophisticated catalytic materials for both NH<sub>3</sub> or other key chemicals production.

10:50 AM **Wed-TRBR-1050** Rationalization of Promoted Reverse Water Gas Shift Reaction By Pt<sub>3</sub>Ni Alloy: Essential Contribution from Ensemble Effect.

**Hong Zhang**<sup>1</sup>, Xuelong Wang<sup>2</sup>, Anatoly Frenkel<sup>2</sup> and Ping Liu<sup>2</sup>, (1)*Stony Brook University, USA*, (2)*Brookhaven National Laboratory, USA*.

**Short Summary:**

We studied the superior catalytic behavior of Pt<sub>3</sub>Ni nanowire during the reverse Water Gas Shift reaction using Density Functional Theory and identified a unique Ni-Pt hybrid ensemble at the 110/111 edge of Pt<sub>3</sub>Ni nanowire, the synergy between Pt and Ni shows selective binding-tuning property and promotion of catalytic activity.

11:10 AM **Wed-TRBR-1110** Programmable Catalysts: A Kinetic Strategy for Enhancing Catalyst Activity and Product Selectivity.

**Sallye R. Gathmann**, M. Alexander Ardagh and Paul J. Dauenhauer, *University of Minnesota, Twin Cities, USA*.

**Short Summary:**

Dynamic catalysis, implemented via programmable catalysts, is an alternate catalyst design strategy that can enhance turnover rates and control reaction selectivity. We explore the parameter space of a model A-to-B reaction with a ratchet-like energy profile to elucidate how selectivity can be tuned, and propose a predictive descriptor.

11:30 AM **Wed-TRBR-1130** Assessing the Role of Surface Carbon on the Surface Stability and Reactivity of  $\beta$ -Mo<sub>2</sub>C Catalysts.

Sean Tacey, Matthew Jankousky and **Carrie Farberow**, *National Renewable Energy Laboratory, USA*.

**Short Summary:**

The surface energy of  $\beta$ -Mo<sub>2</sub>C facets is systematically computed as a function of carbon chemical potential and surface-carbon coverage. The results illustrate the role of surface-carbon on predicted surface thermodynamics and reactivity of metal carbides and provides more realistic active-site models for simulating the reactivity of promising, low-cost  $\beta$ -Mo<sub>2</sub>C catalysts.

## WEDNESDAY AFTERNOON

### Reaction Modeling: Applications and Approaches

**Session Chairs:** David Hibbitts, *University of Florida, USA* and Tibor Szilvasi, *University of Alabama, USA*.

1:10 PM **Wed-TRBR-1310** Enhancement of Power-to-Gas Via Multi-Catalyst Reactors Tailoring reaction Rate and Heat Exchange.

**Emanuele Moioli**, *Paul Scherrer Institut, Switzerland*.

**Short Summary:**

A new multi-stage reactor for highly-efficient CO<sub>2</sub> methanation with waste heat recovery was manufactured and tested in field

1:30 PM **Wed-TRBR-1330** Catalytic Methanol Synthesis Mechanism Development Using the Reaction Mechanism Generator.

**Christopher Blais**<sup>1</sup>, Sevy Harris<sup>1</sup>, Emily Mazeau<sup>1</sup>, Bjarne Kreitz<sup>2</sup>, Oscar Diaz-Ibarra<sup>3</sup>, Eric Hermes<sup>3</sup>, Cosmin Safta<sup>3</sup>, Habib Najm<sup>3</sup>, Eric Bylaska<sup>4</sup>, Judit Zádor<sup>3</sup>, Franklin Goldsmith<sup>2</sup> and Richard West<sup>1</sup>, (1)*Northeastern University, USA*, (2)*Brown University, USA*, (3)*Sandia National Laboratories, USA*, (4)*Pacific Northwest National Laboratory, USA*.

**Short Summary:**

The Reaction Mechanism Generator (RMG) was used to generate a microkinetic model for methanol synthesis over Cu(111). The mechanism was scrutinized using CSP and sensitivity analysis in Cantera, refined with DFT, and the thermodynamic uncertainty was assessed. The resulting model shows qualitative agreement with prior theoretical models.

1:50 PM **Wed-TRBR-1350** Quantification and Utilization of Uncertainties in Transient Kinetic Experiments.

**Adam Yonge**<sup>1</sup>, Ross Kunz<sup>2</sup>, Rebecca Fushimi<sup>2</sup> and Andrew J. Medford<sup>1</sup>, (1)*Georgia Institute of Technology, USA*, (2)*Idaho National Laboratory, USA*.

**Short Summary:**

**Transient approaches, like the Temporal Analysis of Products (TAP), provide data that is sensitive to a broad range of elementary steps in a catalytic process. Through the development and application of uncertainty quantification methods to transient data, investigators can have greater confidence in their results and identify parameters needing improvement.**

2:10 PM **Wed-TRBR-1410** Coupling Kmc Models into Macroscopic Reactor Models through Machine Learning Techniques.

**Mauro Bracconi** and Matteo Maestri, *Politecnico di Milano, Italy*.

**Short Summary:**

A design procedure of the training data for Machine Learning algorithms able to reduce the number of data points up to 80% without any penalization on the function approximation accuracy is proposed. The procedure is assessed in the context computationally-expensive 1p-kinetics at the level of kMC simulations.

2:30 PM **Wed-TRBR-1430** Estimation of Thermochemical Properties Using Group Additivity for Species Involved in Coke Formation on Pt(111) during Ethane Dehydrogenation.

**Jinwoong Nam**, Charanyadevi Ramasamy, Daniel E. Raser, Gustavo L. Barbosa Couto and Fuat E. Celik, *Rutgers, The State University of New Jersey, USA*.

**Short Summary:**

Thermochemical properties of a large number of gaseous and surface hydrocarbons and molecular fragments involved in carbon chain growth during ethane dehydrogenation are investigated on a model on Pt(111) surface using a combination of computational methods including density functional theory, automated reaction network generation, and group additivity theory.

2:50 PM **Wed-TRBR-1450** Spatially-Resolved Insights into Local Activity and Structure of Ni-Based CO<sub>2</sub> Methanation Catalyst in Fixed-Bed Reactors.

Rinu Chacko, **Akash B. Shirsath**, Mariam L. Schulte, Marc-André Serrer, Matthias Stehle, Sofia Angeli, Hendrik Gossler, Erisa Saraçi, Jan-Dierk Grunwaldt and Olaf Deutschmann, *Karlsruhe Institute of Technology (KIT), Germany*.

**Short Summary:**

For reliable implementation of P2X solutions, understanding the effect of concentration and temperature gradients on the catalyst structure is imperative. Here, automated numerical simulations (DETCHEM<sup>PBR</sup> and CaRMEN) with various experimental techniques to examine the local activity and structure of Ni-based methanation catalysts in a fixed-bed reactor (PBR) are explored.

### Development and Applications of New Methods and Strategies

**Session Chairs:** Craig Plaisance, *Louisiana State University, USA* and Srinivas Rangarajan, *Lehigh University, USA*.

3:30 PM **Wed-TRBR-1530** Degree of Rate Control and Sensitivity Analysis By Automatic Differentiation.

Yilin Yang, Siddarth Achar and **John R. Kitchin**, *Carnegie Mellon University, USA*.

**Short Summary:**

We show how to use automatic differentiation to compute the degree of rate control and sensitivity analysis in complex reaction mechanisms in both transient and steady state conditions.

3:50 PM **Wed-TRBR-1550** Development and Implementation of a Non-Linear and Non-Local Implicit Electrolyte Model in the Vienna Ab-Initio Simulation Package.

**S M Rezwanul Islam**, Forough Khezeli and Craig Plaisance, *Louisiana State University, USA*.

**Short Summary:**

Solvation models with linear approximations cannot describe highly polar surfaces in presence of strong electric fields that invoke a highly nonlinear response. The model proposed in this work extends the capabilities of widely used self-consistent solvation model, VASPsol, to capture the non-local non-linear responses of both dielectric and ionic screening.

4:10 PM **Wed-TRBR-1610** High Throughput Computing of Structure-Sensitive Catalytic Reactions.

**Xue Zong**<sup>1,2</sup> and Dionisios G. Vlachos<sup>1</sup>, (1)*University of Delaware, USA*, (2)*RAPID Manufacturing Institute, University of Delaware, USA*.

**Short Summary:**

We have developed a novel structure-dependent kinetic model by use of generalized coordination number as the structure descriptor. Based on this, we can predict the kinetic performances on arbitrary surfaces and design the optimal catalyst structure for the given reaction.

4:30 PM **Wed-TRBR-1630** Uncertainty Quantification of Stability Metrics of Nanoparticle Catalysts from First Principles.

**Jaideep S. Soodan**<sup>1</sup>, Asmee Prabhu<sup>1</sup>, Verena Streibel<sup>2</sup>, Joakim Halldin Stenlid<sup>2</sup>, Frank Abild-Pedersen<sup>2</sup> and Tej S. Choksi<sup>1</sup>, (1)*Nanyang Technological University, Singapore*, (2)*SLAC National Accelerator Laboratory, USA*.

**Short Summary:**

Using a coordination-based approach, we estimate the accuracy of stability metrics of catalytic nanoparticles. We show that the ratios of surface energies and densities of active sites are well described by DFT. Errors in cohesive energies of nanoparticles are systemic and can be mitigated with calibrations to experiments.

# Thursday May 26, 2022

## Grand Ballroom

### THURSDAY MORNING

#### Panel Discussion: Future of Catalysis for Sustainable Manufacturing

Session Chairs: Stuart Soled, *ExxonMobil Research and Engineering, USA*

8:00 AM Future of Catalysis for Sustainable Manufacturing.

**Deirdre Dunne**<sup>1</sup>, Nils Bottke<sup>2</sup>, Nagore Sabio<sup>3</sup> and Viviane Schwartz<sup>4</sup>, (1)*Elsevier, Netherlands*, (2)*BASF, Germany*, (3)*ExxonMobil, USA*, (4)*US Department of Energy, USA*.

## Grand Ballroom East

### CO<sub>2</sub> Hydrogenation to Methanol

Session Chairs: Aditya Bhan, *University of Minnesota, Twin Cities, USA* and Dongxia Liu, *University of Maryland - College Park, USA*.

9:30 AM **Thu-GBRE-0930** The Promotion of CO<sub>2</sub> Hydrogenation to CH<sub>3</sub>OH on Cu Nanoparticles Supported on Y-Containing Oxides.

**Gina Noh**, Zachariah Berkson, Erwin Lam, Petr Šot, Enzo Brack and Christophe Copéret, *ETH Zürich, Switzerland*.

#### Short Summary:

The identity, role, and nature of active sites is assessed for copper nanoparticles supported on mixed yttria-zirconia oxides, as catalysts for CO<sub>2</sub> hydrogenation to methanol. A surface organometallic chemistry approach, used to synthesize model catalysts, allows molecular understanding. The utility of solid-state NMR to characterize materials is also demonstrated.

9:50 AM **Thu-GBRE-0950** Particle Size Effects for Copper-Catalyzed CO<sub>2</sub> hydrogenation to Methanol.

**Laura Barberis**<sup>1</sup>, Amir H. Hakimioun<sup>2</sup>, Joseph A. Stewart<sup>3</sup>, Felix Studt<sup>2</sup> and Petra E. de Jongh<sup>1</sup>, (1)*Utrecht University, Netherlands*, (2)*Karlsruhe Institute of Technology (KIT), Germany*, (3)*TotalEnergies, Belgium*.

#### Short Summary:

In this work, we report that the CO<sub>2</sub> hydrogenation to methanol reaction exhibits clear particle size effects. Small nanoparticles give the lowest CO<sub>2</sub> conversions but the highest MeOH selectivity, these trends are related to changes in the fraction of surface atoms and coverage of reaction intermediates with particle size.

10:10 AM **Thu-GBRE-1010** First-Principles Study of Photocatalytic CO<sub>2</sub> Reduction Reactions on a 2D Ferroelectric Surface.

**Mo Li** and Joshua Young, *New Jersey Institute of Technology, USA*.

#### Short Summary:

The ferroelectric property of the 2D Y<sub>2</sub>CO<sub>2</sub> MXene material provided a promising solution for increasing the selectivity of the desired product and the activity of the CO<sub>2</sub> reduction reaction.

10:30 AM **Thu-GBRE-1030** Conversion of CO<sub>2</sub> to Methanol over Bi-Functional Basic-Metallic Catalysts.

Andreas Jentys, Johannes A. Lercher and **Jakub Pazdera**, *Technical University of Munich, Germany*.

#### Short Summary:

Efficient carbon capture and utilization (CCU) is a key process for a sustainable carbon neutral economy. In this presentation we discuss the role of the dual functionality of base and metal groups in a sorbent and catalyst, which can be applied for sorption and direct hydrogenation of CO<sub>2</sub> to methanol.

10:50 AM **Thu-GBRE-1050** Ni Clusters As the Active Sites for CO<sub>2</sub> Hydrogenation to Methanol in Ni/In<sub>2</sub>O<sub>3</sub> Catalysts.

**Francesco Cannizzaro**, Ivo Filot and Emiel J. M. Hensen, *Eindhoven University of Technology, Netherlands*.

#### Short Summary:

Ni promotion of CO<sub>2</sub> hydrogenation to methanol on In<sub>2</sub>O<sub>3</sub> was investigated with density functional theory. Small Ni clusters catalyze H<sub>2</sub> dissociation on the Ni cluster, CO<sub>2</sub> adsorption on oxygen vacancies and subsequent methanol formation. Single atoms of Ni adsorbed on or doped into the In<sub>2</sub>O<sub>3</sub> surface mainly catalyze CO formation.

11:10 AM **Thu-GBRE-1110** Bimetallic Ru-Based Alloy Nanoparticles: Unravelling the Effects of In Addition on Methanol Synthesis from CO<sub>2</sub>.

**Feiyang Geng** and Jason C. Hicks, *University of Notre Dame, USA*.

#### Short Summary:

This work investigated the effects of alloying In with Ru for CO<sub>2</sub> hydrogenation. Our results provide insight into the role of the promotor on the inhibition of methanation and promotion of methanol formation, as well as detailed results regarding the synthesis, characterization and performance of these materials.

11:30 AM **Thu-GBRE-1130** Catalytic Hydrogenation of CO<sub>2</sub> to Methanol Enabled By the Metal-Lewis Acid Interfaces in Metal Organic Frameworks (MOFs) UiO-66.

**Huy Nguyen**<sup>1</sup>, Matthew Neurock<sup>1</sup>, Johannes A. Lercher<sup>2</sup>, Donald G. Truhlar<sup>1</sup> and Jingyun Ye<sup>1,3</sup>, (1)University of Minnesota, Twin Cities, USA, (2) Pacific Northwest National Laboratory, USA, (3)Clarkson University, USA.

**Short Summary:**

MOF UiO-66 with Copper nanoparticles loaded between Zirconia nodes effectively catalyzes CO<sub>2</sub> hydrogenation to Methanol. DFT calculations identify the interfacial Zr-Cu as active sites. Methanol is formed through HCOO Pathway, while CO is formed via COOH Pathway. The isostructural Hf-UiO-66 is predicted to have the same mechanistic and energetic behaviors.

## THURSDAY AFTERNOON

### Tandem/Bifunctional/Multiple Catalysts

**Session Chairs:** Ping Liu, Brookhaven National Laboratory, USA and Jacob H. Miller, National Renewable Energy Laboratory, USA.

1:10 PM **Thu-GBRE-1310** Direct CO<sub>2</sub> hydrogenation to Aromatics over Bifunctional ZnZrOx/ZSM-5: Effect of Zeolite Morphology to Product Distribution.

**Mansoor Ali**, Faisal Zafar and Jong Wook Bae, Sungkyunkwan University, Korea, Republic of (South).

**Short Summary:**

The ZSM-5 morphologies were found to be crucial to control activity and product distributions for direct CO<sub>2</sub> hydrogenation to aromatics. The bifunctional ZnZr/ZSM-5 with nano and hierarchical nano structures on the ZnZr/N-ZSM-5 and ZnZr/HN-ZSM-5 exhibited higher CO<sub>2</sub> conversion and aromatic selectivity due to abundant stronger Brønsted acid sites.

1:30 PM **Thu-GBRE-1330** Direct Conversion of Syngas to Ethanol Via Tandem Catalysis.

**Martin Konrad**<sup>1</sup>, Julia Bauer<sup>1</sup>, Michael Geske<sup>1</sup>, Phil Preikschas<sup>1</sup>, Robert Baumgarten<sup>1</sup>, Piyush Ingale<sup>1</sup>, Chiara Boscagli<sup>2</sup>, Manuel Gentzen<sup>3</sup>, Ralph Kraehnert<sup>1</sup> and Frank Rosowski<sup>3,4</sup>, (1)BasCat – UniCat BASF JointLab: Technische Universität Berlin, Germany, (2)hte GmbH, Germany, (3)BASF SE, Germany, (4)Technische Universität Berlin, Germany.

**Short Summary:**

A tandem catalyst concept was employed for the direct conversion of syngas to ethanol. By combining a Rh-catalyst with a Cu-catalyst in one reactor, functionalities required for the complex reaction are divided. Interactions of both catalysts, intermediates and reaction pathways were investigated to understand and utilize synergetic effects.

1:50 PM **Thu-GBRE-1350** Direct Synthesis of Branched Hydrocarbons from CO<sub>2</sub> Hydrogenation over Composite Catalysts in a Single Reactor.

**Anh To**, Daniel Ruddy, Connor Nash and Martha Arellano-Trevino, National Renewable Energy Laboratory, USA.

**Short Summary:**

Direct synthesis of a versatile branched hydrocarbon mixture through non-Fischer-Tropsch CO<sub>2</sub> hydrogenation in a single reactor with high selectivity (over 94% C-selectivity in hydrocarbon products) is advantageous for valorizing waste CO<sub>2</sub> by subsequent upgrading to gasoline, diesel, marine, or jet fuels.

2:10 PM **Thu-GBRE-1410** Determining Bifunctionality of Mesoporous Co/Zeolite Catalyst for Direct Synthesis of Liquid Fuel By Fischer-Tropsch Reaction.

**Sungtak Kim**, Chungnam National University, Korea, Republic of (South).

**Short Summary:**

Porous Co/HZSM-5 were synthesized to investigate the effect of porosity and acidity on the performance of Fischer-Tropsch reaction for the production of liquid fuel. Mesoporosity was advantageous to the dispersion of Co nanoparticles. Hydrocracking and isomerization were determined by the number of acid site of the zeolite.

2:30 PM **Thu-GBRE-1430** Cu-Zn-Al@Ferrierite Core-Shell Catalysts for Directly Converting CO<sub>2</sub> and H<sub>2</sub> into Dimethyl-Ether.

**Fabio Salomone**<sup>1</sup>, Elena Corrao<sup>1</sup>, Emanuele Giglio<sup>2</sup>, Micaela Castellino<sup>1</sup>, Raffaele Pirone<sup>1</sup> and Samir Bensaïd<sup>1</sup>, (1)Politecnico di Torino, Italy, (2) University of Calabria, Italy.

**Short Summary:**

This work focuses on the development of CuZnAl@Ferrierite core-shell catalysts for directly converting CO<sub>2</sub> and H<sub>2</sub> into methanol and DME by means of a one-step process, enhancing the CO<sub>2</sub> conversion and the DME productivity with the engineered structure of the catalytic pellets.

2:50 PM **Thu-GBRE-1450** Direct Conversion of CO<sub>2</sub>-Rich Syngas to High-Octane Gasoline in a Single Reactor.

**Claire Nimlos**, Connor Nash, Anh To, Daniel Dupuis and Daniel Ruddy, National Renewable Energy Laboratory, USA.

**Short Summary:**

Here we used a single reactor to convert syngas to hydrocarbons, exploiting overlapping process conditions and commercial catalysts with a Cu/BEA zeolite catalyst. Process intensification and co-conversion of CO<sub>2</sub> with syngas to hydrocarbons provides an opportunity to improve carbon efficiency in a biorefinery to produce high-value hydrocarbons from renewable sources.



## CO<sub>2</sub> Conversion

**Session Chairs:** Hai-Ying Chen, *Oak Ridge National Laboratory, USA* and Prasanna Dasari, *SABIC, USA*.

3:30 PM **Thu-GBRE-1530** Catalytic and Aging Studies on Dual Function Materials (DFM) for CO<sub>2</sub> Capture and Hydrogenation.

**Alessandro Porta**, Roberto Matarrese, Carlo Giorgio Visconti and Luca Lietti, *Politecnico di Milano, Italy*.

**Short Summary:**

This work provides novel insights on the mechanism of cyclic CO<sub>2</sub> storage and reduction at simulated flue gases conditions, by means of microreactor experiments, FTIR operando and aging tests, aiming at the rational design of DFMs and Ru-based catalysts.

3:50 PM **Thu-GBRE-1550** Packed Bed Membraneless Electrolyzers for Electrochemical CO<sub>2</sub> Conversion.

**Xueqi Pang** and Daniel Esposito, *Columbia University, USA*.

**Short Summary:**

In this work, we present a packed bed membraneless electrolyzer (PBME) concept based on porous flow-through electrodes to convert CO<sub>2</sub> into value-added fuels and chemicals. PBMEs are well-suited for incorporation into a CO<sub>2</sub> capture system. Enhanced CO<sub>2</sub>RR performance was observed when running multiple pairs of electrodes simultaneously in a PBME.

4:10 PM **Thu-GBRE-1610** Electrochemical CO<sub>2</sub> Reduction over Cu-Based Catalysts.

**Piaoping Yang**<sup>1</sup> and Zhi-Jian Zhao<sup>2</sup>, (1)*University of Delaware, USA*, (2)*Tianjin University, China*.

**Short Summary:**

Linkage correlations were established between the atomic structure of active sites and their catalytic activities for specific products in CO<sub>2</sub>RR over OD-Cu catalysts, where  $\Sigma 3$  grain boundary like planar-square sites and convex-square sites are responsible for ethylene production while step-square sites, i.e. n(111)  $\times$  (100), favor alcohols generation.

4:30 PM **Thu-GBRE-1630** One-Pot CO<sub>2</sub> Hydrogenation to Lower-Olefins.

**Chiara Coffano**<sup>1</sup>, Alessandro Porta<sup>1</sup>, Carlo Giorgio Visconti<sup>1</sup>, Francesca Rabino<sup>2</sup>, Guido Franzoni<sup>2</sup>, Barbara Picutti<sup>2</sup> and Luca Lietti<sup>1</sup>, (1)*Politecnico di Milano, Italy*, (2)*Tecnimont, Italy*.

**Short Summary:**

The one-pot conversion of CO<sub>2</sub> into olefins is here investigated using physical mixtures comprising methanol synthesis catalysts and MTO zeolites. The runs carried out under different operating conditions and with different catalysts combinations provided valuable mechanistic information useful for the design of improved catalytic systems.

4:50 PM **Thu-GBRE-1650** Tungsten Carbides As Active Catalysts for CO<sub>2</sub> Hydrogenation.

**Mitchell Juneau** and Marc Porosoff, *University of Rochester, USA*.

**Short Summary:**

Tungsten carbides are low-cost substitutes for noble metal catalysts for CO<sub>2</sub> hydrogenation but prone to agglomeration during synthesis. Tungsten particles are encapsulated in silica, preserving particle size (~10 nm), and confirmed as tungsten carbides via XRD and XPS. Increased CO<sub>2</sub> uptake compared to incipient-wetness-synthesized controls suggests greater active site availability.

5:10 PM **Thu-GBRE-1710** Non-Thermal Plasma-Assisted Catalytic CO<sub>2</sub> Hydrogenation to Hydrocarbons.

Jiajie Wang<sup>1,2</sup>, Xiaoxing Wang<sup>1</sup>, Mohammad AlQahtani<sup>1</sup>, Sean Knecht<sup>1</sup>, **Sven Bilén**<sup>1</sup>, Chunshan Song<sup>1,3</sup> and Wei Chu<sup>2</sup>, (1)*The Pennsylvania State University, USA*, (2)*Sichuan University, China*, (3)*Chinese University of Hong Kong, China*.

**Short Summary:**

A strong synergy was observed when combining DBD plasma and Co catalyst for CO<sub>2</sub> hydrogenation, where plasma enhanced CO<sub>2</sub> conversion and CH<sub>4</sub> formation rate. By changing the catalyst-bed configuration, much higher C<sub>2</sub>+ hydrocarbon selectivity can be achieved. The present work demonstrates the promise of plasma-catalysis for effective CO<sub>2</sub> utilization.

## Grand Ballroom West

### THURSDAY MORNING

#### Catalytic Oxidation II

**Session Chairs:** Gianpiero Groppi, *Politecnico di Milano, Italy* and Philippe Vernoux, *Université de Lyon, CNRS, France*.

9:30 AM **Thu-GBRW-0930** Tuning the Reactivity of Pd/CeO<sub>2</sub> Catalysts for Low-Temperature CO Oxidation By Changing the Size of CeO<sub>2</sub> Support.

Valerii Muravev, Nikolay Kosinov and **Emiel J. M. Hensen**, *Eindhoven University of Technology, Netherlands*.

**Short Summary:**

Single-atom Pd/CeO<sub>2</sub> catalysts made by flame spray pyrolysis display high catalytic activity towards low-temperature CO oxidation. By tuning the size of CeO<sub>2</sub> support in Pd/CeO<sub>2</sub> catalysts the activity can be further improved. Control over the size of the support expands the toolbox for the design of novel environmental catalysts.

9:50 AM **Thu-GBRW-0950** Low-Temperature Oxidation of Methane on Pd-Based Monolith Catalysts for Efficient ICE Emission Control.

**Vittoria Troisi**, Alessandra Beretta and Gianpiero Groppi, *Politecnico di Milano, Italy*.

**Short Summary:**

In this work, a spatially resolved sampling technique is applied to achieve new evidences on the complex behavior of methane oxidation over Palladium based catalysts. The experimental data show the presence of a critical oxygen concentration below which methane conversion rate is increased by almost one order of magnitude.

10:10 AM **Thu-GBRW-1010** Understanding the Aging Phenomena of Diesel Oxidation Catalysts.

**Miren Agote Aran** and Davide Ferri, *Paul Scherrer Institut, Switzerland*.

**Short Summary:**

A diesel oxidation catalyst extracted from a truck was analysed to understand its aging phenomena. The sintering and poisoning gradients observed were then simulated in a fresh catalyst using a dedicated lab-scale reactor. The results highlight the importance of mimicking such gradients for more accurate catalyst durability predictions.

10:30 AM **Thu-GBRW-1030** Experimental and Theoretical Studies on Diesel Oxidation Catalysis over Bimetallic PdCu Catalysts.

**Stephen Kristy**<sup>1</sup>, Yuying Song<sup>2</sup>, Adam Hoffman<sup>3</sup>, Tanmayi Bathena<sup>1</sup>, Scott Svadlenak<sup>1</sup>, Yu Liu<sup>2</sup>, Simon Bare<sup>3</sup>, Lars C. Grabow<sup>2</sup> and Konstantinos Goulas<sup>1</sup>, (1)*Oregon State University, USA*, (2)*University of Houston, USA*, (3)*SLAC National Accelerator Laboratory, USA*.

**Short Summary:**

PdCu alloys outperform industry-standard PdPt catalysts in diesel oxidation catalysis. The formation of adjacent CO\* and O\* binding sites alleviates poisoning by CO and NO at low temperatures.

10:50 AM **Thu-GBRW-1050** Effect of Low Index Ceria Surfaces on Pd/CeO<sub>2</sub> Methane Oxidation Catalysts.

**Maïla Danielis**<sup>1</sup>, Sara Colussi<sup>1</sup>, Jordi Llorca<sup>2</sup> and Alessandro Trovarelli<sup>1</sup>, (1)*University of Udine, Italy*, (2)*Universitat Politècnica de Catalunya, Spain*.

**Short Summary:**

The effect of undercoordinated ceria surfaces on the nature of supported Pd species was experimentally investigated on Pd/CeO<sub>2</sub> methane oxidation catalysts. Preliminary results evidenced a correlation between the stability of the supported Pd species with the observed catalytic performance, as well as with the effectiveness of the milling technique.

11:10 AM **Thu-GBRW-1110** Microkinetic Analysis of Low Temperature Nitrous Oxide Formation on Pt: Understanding the Role of Catalyst Surface Structure and Coverage.

**Sugandha Verma** and Christopher Paolucci, *University of Virginia, USA*.

**Short Summary:**

The formation of N<sub>2</sub>O on diesel oxidation catalyst(DOC) is expected to depend on oxygen coverage, nature of hydrocarbons in diesel blend, and catalyst surface structure. We perform microkinetic modeling for identification of reaction intermediates and surfaces responsible for N<sub>2</sub>O formation; this information will aid in reducing N<sub>2</sub>O emissions from DOC.

11:30 AM **Thu-GBRW-1130** The Role of Redox Properties and Acid-Base Sites in Defining the Soot Oxidation Mechanisms for Aliovalently-Doped Ceria Nanocatalysts.

Enrico Sartoretto, Chiara Novara, Fabrizio Giorgis, Marco Piumetti, **Samir Bensaïd**, Nunzio Russo and Debora Fino, *Politecnico di Torino, Italy*.

**Short Summary:**

Highly active ceria-based oxides containing La, Nd or Pr were compared as oxidizing catalysts. The structure, morphology, defectiveness, surface acidity/basicity and chemical/redox properties were investigated with different techniques. The influence of these features on the catalytic activity towards soot oxidation was assessed in different conditions, unveiling the reaction mechanisms involved.

## THURSDAY AFTERNOON

### Environmental Catalysis in Aqueous Phase

**Session Chairs:** Rohil Daya, *Cummins Inc., USA* and Christopher L. Muhich, *Arizona State University, USA*.

1:10 PM **Thu-GBRW-1310** Electrocatalytic Nitrate Reduction to Ammonia on Metals and Binary Alloys.

Jinxun Liu, Zixuan Wang, Samuel Young, Danielle Richards, Nirala Singh and **Bryan Goldsmith**, *University of Michigan-Ann Arbor, USA*.

**Short Summary:**

Electrocatalytic nitrate reduction (NO<sub>3</sub>RR) is a promising route to remediate nitrate while generating value-added products such as ammonia. We identified fundamental activity and selectivity trends for NO<sub>3</sub>RR on metals and generated theoretical volcano plots. Based on computational predictions, we demonstrated that Pt<sub>78</sub>Ru<sub>22</sub>/C is six times more active than Pt/C.

1:30 PM **Thu-GBRW-1330** Broad-Spectrum Photocatalytic Degradation of Perfluorooctanoic Acid on Boron Nitride/Titanium Oxide.

**Bo Wang**<sup>1</sup>, Lijie Duan<sup>2,3</sup>, Kimberly Heck<sup>1</sup>, Chelsea Clark<sup>1</sup>, Jinshan Wei<sup>2,3</sup>, Minghao Wang<sup>2,3</sup>, Jordin Metz<sup>1</sup>, Gang Wu<sup>4</sup>, Ah-Lim Tsai<sup>4</sup>, Sujin Guo<sup>1</sup>, Jacob Arredondo<sup>1</sup>, Aditya D. Mohite<sup>1</sup>, Thomas Senftle<sup>1</sup>, Paul Westerhoff<sup>5</sup>, Pedro Alvarez<sup>1</sup>, Xianghua Wen<sup>3</sup>, Yonghui Song<sup>2,3</sup> and Michael S. Wong<sup>1</sup>, (1)*Rice University, USA*, (2)*Chinese Research Academy of Environmental Sciences, China*, (3)*Tsinghua University, China*, (4)*University of Texas-Medical School at Houston, USA*, (5)*Arizona State University, USA*.

**Short Summary:**

Novel photocatalyst is required to efficiently degrade PFAS. Herein, we synthesized a BN/TiO<sub>2</sub> composite and tested it for PFOA degradation under UV-C, UV-A, and sunlight. To explain its unique activity, we characterized the material to develop a band diagram and performed EPR and scavenging experiments to explain possible reaction pathways.

1:50 PM **Thu-GBRW-1350** Unraveling the Ability of Neighboring Pd Single Atom Catalyst to Selectively Degrade Organohalide Contaminants.

**Srishti Gupta** and Christopher L. Muhich, *Arizona State University, USA*.

**Short Summary:**

Metal nanoparticles are non-selective for halo-aromatic hydrodehalogenation. We investigated single atom and neighboring atom catalysts for Cl-/F-phenol degradation using DFT. Neighboring Pd atoms improve selectivity and activity by inhibiting side reactions and lowering competitive water and product desorption barriers. This enables a path for remediating “forever” halogenated chemicals like PFAS.

2:10 PM **Thu-GBRW-1410** Kinetic Analysis of Iron-Based Metal-Organic Frameworks (MOFs) in Aqueous Pollutant Degradation.

**Samuel Moore** and Michele Sarazen, *Princeton University, USA*.

**Short Summary:**

This work shows that between two polymorphic, iron-based MOFs, MIL-101(Fe) outperforms MIL-88B(Fe) in the degradation of the model pollutant methylene blue in a wider effort to establish structure-functional relationships to inform Fe-MOF use in wastewater treatment applications.

2:30 PM **Thu-GBRW-1430** On the Dual Role of the Reactant during Aqueous Phase Hydrodechlorination of Trichloroethylene (HDC of TCE) Using Pd Supported on Swellable Organically Modified Silica (SOMS).

**Anagha Hunoor**<sup>1</sup>, Saurabh Ailawar<sup>1</sup>, Benjamin Rudzinski<sup>1</sup>, Gokhan Celik<sup>1</sup>, Laurence Burel<sup>2</sup>, Millet Jean-Marc<sup>2</sup>, Jeffrey T. Miller<sup>3</sup>, Paul Edmiston<sup>4</sup> and Umit S. Ozkan<sup>1</sup>, (1)*The Ohio State University, USA*, (2)*Université de Lyon, CNRS, France*, (3)*Davidson School of Chemical Engineering, Purdue University, USA*, (4)*The College of Wooster, USA*.

**Short Summary:**

Swellable organically modified silica (SOMS), an animated, hydrophobic material was used as a catalyst support to overcome slow kinetics of hydrodechlorination in aqueous phase and product inhibition due to HCl. As SOMS swells in presence of organics, the role of trichloroethylene both as a reactant and swelling agent was investigated.

2:50 PM **Thu-GBRW-1450** Computational Insights of Two-Dimensional Materials in Photocatalysis.

Taha Salavati Fard, Tong Mou and **Bin Wang**, *University of Oklahoma, USA*.

**Short Summary:**

In this study we apply DFT calculations to reveal the mechanism of perfluorocarboxylic acids (PFCAs) degradation over hexagonal boron nitride (h-BN) and show the necessity of oxygen dopants to activate h-BN for photocatalytic reactions and more importantly, their ability to facilitate activation of C-F bond.

## Fundamentals of Catalysis: Theoretical Insights

**Session Chairs:** Prashant Deshlahra, *Tufts University, USA* and Philippe Sautet, *University of California, Los Angeles, USA*.

3:30 PM **Thu-GBRW-1530** Active Site Dynamics in Heterogeneous Catalysis.

Geng Sun, Anastassia Alexandrova and **Philippe Sautet**, *University of California, Los Angeles, USA*.

**Short Summary:**

The determination of active site structure is key for the design of efficient catalysts. With a novel method to explore the configuration of active sites that provide the lowest barrier, we show that the capability of a Pt cluster catalyst to reconstruct simultaneously during reaction controls the catalytic activity.

3:50 PM **Thu-GBRW-1550** Developing a Physics Based Model to Predict the Chemisorption Energy on Surface Alloys.

**Shikha Saini**<sup>1,2</sup>, Joakim Halldin Stenlid<sup>1,2</sup> and Frank Abild-Pedersen<sup>1</sup>, (1)*SLAC National Accelerator Laboratory, USA*, (2)*Stanford University, USA*.

**Short Summary:**

All the approximation methods for predicting chemisorption energy (e.g., Newns-Anderson model, d-band model, coordination number based models) have neglected the induced effects on the surface by adding the atom or molecule. We present a physics-based model based on geometric and electronic structure that captures adsorbate-induced effects on the surface-site.

4:10 PM **Thu-GBRW-1610** Decoupling Geometric and Electronic Effects during C–O Hydrogenolysis on Transition Metal Phosphides.

**Hansel Montalvo-Castro**, Conor Waladt and David Hibbitts, *University of Florida, USA*.

**Short Summary:**

The incorporation of P into Ni materials causes shifts in selectivity toward cleavage of sterically hindered C–O bonds in 2-methyltetrahydrofuran (MTHF). We explore structure-function relationships on Ni<sub>x</sub>P<sub>y</sub> isostructural materials to decouple electronic and geometric effects to provide rationale for the role of P in transition metal phosphide catalysts.

4:30 PM **Thu-GBRW-1630** Iron Surface Dynamics and Reactivity for Ammonia Synthesis.

**Daniela Polino**<sup>1</sup>, Luigi Bonati<sup>2</sup>, Cristina Pizzolitto<sup>3</sup>, Pierdomenico Biasi<sup>3</sup>, Rene Eckert<sup>4</sup>, Stephan Reitmeier<sup>4</sup>, Robert Schloegl<sup>5</sup> and Michele Parrinello<sup>2</sup>, (1)*University of applied sciences and arts of southern Switzerland - SUPSI, Switzerland*, (2)*Italian Institute of Technology, Italy*, (3)*CASALE SA, Switzerland*, (4)*Clariant Produkte (Deutschland) GmbH, Germany*, (5)*Max Planck Institute for Chemical Energy Conversion, Germany*.

**Short Summary:**

An ab-initio quality potential constructed with machine-learning was used to describe iron surface dynamics, while ab-initio metadynamics was adopted to investigate N<sub>2</sub> dissociation and hydrogenation. With these simulations we understood how surface dynamics affects the reactions and the structural and electronic contributions to activity for iron-based ammonia synthesis catalysts.

4:50 PM **Thu-GBRW-1650** The Effect of Water on Thermal Decomposition of Acetic Acid on Pd(111), a Combined DFT and AP-XPS Study.  
Hoan Nguyen, Kingsley Chuckwu and **Líney Árnadóttir**, *Oregon State University, USA*.

**Short Summary:**

Chemical processes involving fatty acids often operate in water as solvent, which are driven by decomposition of oxygenates and acids. Here, we use combined experimental and computational study on how water affects different bond cleavages and overall selectivity, using acetic acid as model oxygenate on Pd (111).

5:10 PM **Thu-GBRW-1710** Clean Experimental Data for Artificial Intelligence - a Key to Decoding Material Genes in Heterogeneous Catalysis.

**Lucas Foppa**<sup>1</sup>, Luca Ghiringelli<sup>1</sup>, Matthias Scheffler<sup>1</sup>, Spencer J. Carey<sup>1</sup>, Frank Girgsdies<sup>1</sup>, Michael Hävecker<sup>1</sup>, Maike Hashagen<sup>1</sup>, Pierre Kube<sup>1</sup>, Peter Kraus<sup>1</sup>, Andrey Tarasov<sup>1</sup>, Frederik Rütger<sup>2</sup>, Michael Geske<sup>3</sup>, Raoul Naumann d'Alnoncourt<sup>3</sup>, Frank Rosowski<sup>2</sup>, Robert Schlögl<sup>1</sup> and Annette Trunschke<sup>1</sup>, (1)*Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany*, (2)*Technische Universität Berlin, Germany*, (3)*BasCat – UniCat BASF JointLab: Technische Universität Berlin, Germany*.

**Short Summary:**

By applying data science methods based on experimental results obtained according to rigorous protocols (handbooks), correlations between the few most important material properties and the catalytic performance could be found in complex reactions, contributing to the understanding of the underlying physicochemical processes and accelerating the development of catalysts.

## Gramercy

### THURSDAY MORNING

#### Ligand and Support Interactions I

**Session Chairs:** Wes Sattler, *ExxonMobil, USA* and Jun Wang, *SABIC, USA*.

9:30 AM **Thu-GRAM-0930** Empowering Catalyst Supports – Unleashing the Potential of Promoters.

Motlokoa Khasu<sup>1</sup>, Wijnand Marquart<sup>1</sup>, Alexander J. Mayer<sup>2</sup>, Sandie Dann<sup>2</sup>, Simon A. Kondrat<sup>2</sup>, Michael Claeys<sup>1</sup> and **Nico Fischer**<sup>1</sup>, (1)*Catalysis Institute and c\*change (DSI-NRF Centre of Excellence in Catalysis), University of Cape Town, South Africa*, (2)*Loughborough University, United Kingdom*.

**Short Summary:**

Perovskites were synthesized, incorporating K and Mn in their crystal structure. As such, the materials do not only fulfil the physical role of a catalyst support but also provide promotional functionality. This novel design concept was demonstrated for the iron based Fischer-Tropsch synthesis outperforming classic promotional techniques.

9:50 AM **Thu-GRAM-0950** Synthetic Control over Ternary Metal Phosphides Enable Pathway Selectivity in Hydrodeoxygenation of Biomass-Derived Model Compounds.

**Nicole LiBretto**, Sean Tacey, Carrie Farberow, Daniel Ruddy and Susan E. Habas, *National Renewable Energy Laboratory, USA*.

**Short Summary:**

The role of geometry on catalytic reactivity can be investigated on the materials in the Ni<sub>2-x</sub>Rh<sub>x</sub>P system because they have a electronic structure. Therefore, changes in selectivity during the *m*-cresol HDO reaction are thought to be due to changes in the arrangement of metal atoms with increasing Rh concentration.

10:10 AM **Thu-GRAM-1010** Direct Reduction of Esters to Ethers Using H<sub>2</sub> over Supported Pd Catalysts: Importance of Brønsted Acid Sites on Ether Formation.

**Yangsik Yun**<sup>1</sup>, Claudia Berdugo-Díaz<sup>1</sup>, Jing Luo<sup>2</sup>, David Barton<sup>2</sup>, Ida Chen<sup>2</sup>, Jieun Lee<sup>1</sup> and David Flaherty<sup>1</sup>, (1)*University of Illinois Urbana-Champaign, USA*, (2)*The Dow Chemical Company, USA*.

**Short Summary:**

Bifunctional catalysts for direct ester reduction to ether in heterogeneous catalysis

10:30 AM **Thu-GRAM-1030** Selective Hydrogenation/Hydrogenolysis over Pd Based Catalysts Doped with Alkene-Type Carbon Species.

Jianghao Zhang<sup>1</sup>, **Wenda Hu**<sup>1</sup>, Binbin Qian<sup>2</sup>, Berlin Sudduth<sup>1</sup>, Mark Engelhard<sup>3</sup>, Jian Zhi Hu<sup>3</sup>, Junming Sun<sup>1</sup>, Lian Zhang<sup>2</sup> and Yong Wang<sup>3</sup>, (1)*Washington State University, USA*, (2)*MONASH University, Australia*, (3)*Pacific Northwest National Laboratory, USA*.

**Short Summary:**

A homogeneous-like surface Pd-alkene metallacycle was created on the heterogeneous Pd nanoparticle catalyst for selective hydrogenolysis and selective hydrogenation reactions, which sheds a light on the controlled synthesis of selective heterogeneous hydrogenation via mimicking the homogeneous analogues.

10:50 AM **Thu-GRAM-1050** Selective Hydrogenation of Acetylene over Well-Defined Nanocrystals: The Effects of Support Interactions and Single-Site Active Centers.

**Huiyuan Zhu**, *Virginia Polytechnic Institute and State University, USA*.

**Short Summary:**

In this work, we will discuss our recent efforts in optimizing Pd performance for semihydrogenation of acetylene (C<sub>2</sub>H<sub>2</sub>) by tuning the support interactions between Pd and transition metal oxides (TMO) and single-site active centers of Pd in transition metal (TM) hosts.

11:10 AM **Thu-GRAM-1110** Measuring the Influence of Surface Defects during Methanol Oxidative Dehydrogenation over Nanoshaped V/CeO<sub>2</sub> Catalysts.

**Berlin Sudduth**<sup>1</sup>, Junming Sun<sup>1</sup> and Yong Wang<sup>1,2</sup>, (1)Washington State University, USA, (2)Pacific Northwest National Laboratory, USA.

**Short Summary:**

Grafting less redox-active silica onto the defects of CeO<sub>2</sub> is shown to mitigate the overwhelming influence of these defects, providing nanoparticles with increased homogeneity in active sites. This study highlights the impact of defects on methanol's interaction with (100) and (111) CeO<sub>2</sub> facets and the relative activity associated with defects.

11:30 AM **Thu-GRAM-1130** Exploraton of Catalyst Structure-Activity Correlations By Pulsed Laser Defect Engineering in Liquids.

**Sven Reichenberger**, Swen Zerebecki and Stephan Barcikowski, *University of Duisburg-Essen, Germany.*

**Short Summary:**

Pulsed laser defect engineering of spinel cobaltites with single laser pulses enables a gradual tuning of materials properties and catalytic activity in electro- and oxidation catalysis. During laser processing, the size, surface area, and spinel phase are maintained allowing to study related structure-activity correlations.

## THURSDAY AFTERNOON

### Ligand and Support Interactions II

**Session Chairs:** Karl Albrecht, *ADM*, and Juan Henao, *ExxonMobil*, .

1:10 PM **Thu-GRAM-1310** Tuning Catalyst Nuclearity and Local Coordination at Interfaces to Control CO<sub>2</sub> Hydrogenation.

Yifeng Zhu<sup>1</sup>, Jian Zheng<sup>2</sup>, John Fulton<sup>2</sup>, Johannes A. Lercher<sup>2,3</sup> and **Oliver Y. Gutierrez**<sup>2</sup>, (1)*Fudan University, China*, (2)*Pacific Northwest National Laboratory, USA*, (3)*Technical University of Munich, Germany.*

**Short Summary:**

Tuning the properties of supported metals was studied for the reduction of CO<sub>2</sub>. Coverages and barriers for hydrogenation and C-O bond cleavage are controlled by interfaces and nuclearity of metal sites. We describe how to tune the activity and selectivity for producing CO or methanol.

1:30 PM **Thu-GRAM-1330** Monolayer Support Control and Precise Colloidal Nanocrystals Demonstrate Metal-Support Interactions in Heterogeneous Catalysts.

**Arun Asundi**<sup>1</sup>, Emmett Goodman<sup>2</sup>, Adam Hoffman<sup>1</sup>, Karen Bustillo<sup>3</sup>, Jonathan Stebbins<sup>2</sup>, Simon Bare<sup>1</sup>, Stacey Bent<sup>2</sup> and Matteo Cargnello<sup>2</sup>, (1)*SLAC National Accelerator Laboratory, USA*, (2)*Stanford University, USA*, (3)*Lawrence Berkeley National Laboratory, USA.*

**Short Summary:**

We develop a combined atomic layer deposition and colloidal synthesis method of preparing supported nanoparticle catalysts with precise control over the physical structure and chemical properties of the active phase and support. We apply this method to study the metal support interactions governing methane combustion rates in well-defined Pd/Al<sub>2</sub>O<sub>3</sub>/SiO<sub>2</sub> catalysts.

1:50 PM **Thu-GRAM-1350** Organic-Ligand Control of Grafted Ti(IV)-on-Silica Catalysts.

Franck Ulm<sup>1</sup>, Sonjong Hwang<sup>2</sup>, John Arnold<sup>1</sup> and **Alexander Katz**<sup>1</sup>, (1)*University of California, Berkeley, USA*, (2)*California Institute of Technology, USA.*

**Short Summary:**

Using a surface polymerization and crosslinking strategy to add robustness to supported molecular catalysts for liquid phase reactions, we synthesized a grafted Ti molecular catalyst for MPV reduction. Our results demonstrate an unusually large organic-ligand effect, which controls catalysis, while the conventional Ti-on-silica catalyst is completely inactive.

2:10 PM **Thu-GRAM-1410** Targeted Modulation of the Electronic Structure of Metal Cationic Centers in Non-Stoichiometric Mixed Metal Oxides for Enhanced Electrochemical Oxygen Reduction Activity.

**John Carl Camayang**, Samji Samira, Xiangkui Gu, Krishna Patel and Eranda Nikolla, *Wayne State University, USA.*

**Short Summary:**

In this work, we demonstrate that non-stoichiometric oxides such as perovskites can be used as frameworks for modulating the electronic properties of highly dispersed, active metal cationic sites for enhanced electrocatalytic performance. This approach could be applied for designing catalytic properties of non-stoichiometric mixed metal oxides for other electrocatalytic reactions.

2:30 PM **Thu-GRAM-1430** Modulating the Structure and Hydrogen Evolution Reactivity of Metal Chalcogenide Complexes through Ligand Exchange Onto Colloidal Au Nanoparticles.

**Vamakshi Yadav**, Jeffrey Lowe, Alexander Shumski, Eric Liu, Jeffrey Greeley and Christina Li, *Purdue University, USA.*

**Short Summary:**

We utilize colloidal ligand exchange methods to synthesize thin monolayers of metal chalcogenides on Au nanoparticles. Strong interactions between the MoS<sub>4</sub> complexes and Au nanoparticle surface leads to enhanced and stabilized HER catalytic turnover.

2:50 PM **Thu-GRAM-1450** Harnessing the Support's Electronic Properties to Enhance the Performance of Pd/C Catalysts for the Hydrogenation of Multifunctional Chemicals.

**Hamed Bateni**<sup>1,2</sup>, Laura M. Snyder<sup>1,2</sup>, Ting-Hung Chu<sup>1,2</sup>, Marco Nazareno Dell'Anna<sup>1,2</sup>, Jaeryul Park<sup>1,2</sup>, Luke T. Røling<sup>1</sup> and Jean-Philippe Tessonnier<sup>1,3</sup>, (1)*Iowa State University, USA*, (2)*Center for Biorenewable Chemicals (CBiRC), USA*, (3)*NSF-ERC Center for Biorenewable Chemicals (CBiRC), USA.*

**Short Summary:**

Electronic metal-support interactions (EMSIs) play an important role in regulating the performance of carbon-supported catalysts. We show that engineering the electronic properties of the carbon support (i.e., bandgap and workfunction) represents a viable strategy to control EMSIs and consequently the performance of Pd/C for the liquid-phase hydrogenation of multifunctional chemicals.



## Catalysts with Differently Sized and Shaped Nanoparticles

**Session Chairs:** Konstantinos Goulas, *Oregon State University, USA* and Megan Witzke, *University of Illinois at Urbana-Champaign, USA*.

3:30 PM **Thu-GRAM-1530** Role of Interface for the Water-Gas Shift Reaction over Size-Controlled Supported Metal Catalysts: A Combined Theoretical and Experimental Study.

**Dongjae Shin**, Rui Huang, Seokhyun Choung, Youngbi Kim, Kiheon Sung and Jeong Woo Han, *Pohang University of Science and Technology (POSTECH), Korea, Republic of (South)*.

**Short Summary:**

Metal-support interface of supported metal catalysts has been reported to facilitate H<sub>2</sub>O dissociation, which is an essential step in water-gas shift reaction (WGS). However, an origin of the promoted H<sub>2</sub>O dissociation has not been clearly revealed yet. Herein, the origin was theoretically studied for Pd/Co<sub>3</sub>O<sub>4</sub>, followed by experimental validations.

3:50 PM **Thu-GRAM-1550** Reversible Atomization and Nano-Clustering of Pt As a Strategy for Designing Ultra-Low Metal Loading Catalyst.

**Thomas Erik Lyck Smitshuysen**, Debasish Chakraborty, Christian Danvad Damsgaard and Ib Chorkendorff, *Technical University of Denmark, Denmark*.

**Short Summary:**

Reversible atomization and nano-clustering of Pt through oxidizing and reducing treatment is characterized and understood. Furthermore a very active and ultra-low loading Pt catalyst is achieved using a twentieth part of what is conventionally needed. This ultra-low loading catalyst is based on preparing the catalyst solely with nano-clusters.

4:10 PM **Thu-GRAM-1610** Explaining the Shape Selectivity of High-Index NiO Particles Produced By Molten Salts Synthesis.

Raffaele Cheula<sup>1</sup>, Mariano D. Susman<sup>2</sup>, David West<sup>3</sup>, Sivadinarayana Chinta<sup>3</sup>, Jeffrey D. Rimer<sup>2</sup> and **Matteo Maestri**<sup>1</sup>, *(1)Politecnico di Milano, Italy, (2)University of Houston, USA, (3)SABIC, USA*.

**Short Summary:**

We show for the first time that localized ordering of salts behaves as capping agents that regulate the anisotropic growth rates of a metal oxide.

4:30 PM **Thu-GRAM-1630** Effect of Pretreatment on Metal Dispersion in Carbon Supported Catalysts.

**MD Fakhruddin Patwary**<sup>1</sup>, Alaba Ojo<sup>1</sup>, Manuel A. Nieto<sup>2</sup> and John R. Regalbuto<sup>1</sup>, *(1)University of South Carolina, USA, (2)University of Illinois, USA*.

**Short Summary:**

In this study nanoparticles of Pt and Pd on two different carbon supports were examined. The growth in particle size, under several reduction temperatures, heating rates and humidity conditions, was investigated. In most cases a trend of increasing particle size with increasing reduction temperature or humidity was observed.

4:50 PM **Thu-GRAM-1650** Designing Stable, Active, and Selective Low-Dimensional Gold-Heterostructures for CO<sub>2</sub> Reduction to C<sub>1</sub> Products.

**Lavie Rekhi**<sup>1</sup>, Quang T. Trinh<sup>1,2</sup>, Asmee Prabhu<sup>1</sup>, Luan Q. Le<sup>1</sup> and Tej S. Choksi<sup>1,2</sup>, *(1)Nanyang Technological University, Singapore, (2)Cambridge Centre for Advanced Research and Education, Singapore*.

**Short Summary:**

We present generalized principles to design stable, active, and selective gold-heterostructure catalysts with active site precision using CO<sub>2</sub> reduction as a probe reaction. We demonstrate the role of charge transfer in dictating the structure sensitivity of supported catalysts, and in tuning the selectivity to various C<sub>1</sub> products.

5:10 PM **Thu-GRAM-1710** Tuning the Reactivity of Propane Dehydrogenation Catalysts By Using Well-Defined, Single-Phase Pt-Sn Nanocrystals.

**Baraa Werghi**<sup>1</sup>, Liheng Wen<sup>1</sup>, Amani Ebrahim<sup>2</sup>, Miaofang Chi<sup>3</sup>, Simon Bare<sup>2</sup> and Matteo Cargnello<sup>1</sup>, *(1)Stanford University, USA, (2)SLAC National Accelerator Laboratory, USA, (3)Oak Ridge National Laboratory, USA*.

**Short Summary:**

Controlled synthesis of well-defined PtSn based nano-catalysts from single phase nanocrystal precursors with competing catalytic performance for the PDH reaction. The selective formation of specific active phases insures the stability of the catalyst with deactivation rate 10 times less than the classical impregnated Pt and PtSn catalytic systems.

## Mercury Ballroom

### THURSDAY MORNING

## Lignin II: Catalysts and Reactions

**Session Chairs:** George Huber, *University of Wisconsin-Madison, USA* and Theodore Walker, *Great Lakes Bioenergy Research Center, USA*.

9:30 AM **Thu-MEBR-0930** Continuous Hydrodeoxygenation of Lignin to Jet-Range Aromatic Hydrocarbons.

Michael L. Stone<sup>1</sup>, **Matthew S. Webber**<sup>1</sup>, William P. Mounfield<sup>1</sup>, Earl Christensen<sup>2</sup>, Ana R. C. Morais<sup>2</sup>, Yanding Li<sup>1</sup>, Eric Anderson<sup>1</sup>, Gregg T. Beckham<sup>2,3</sup> and Yuriy Roman<sup>1</sup>, *(1)Massachusetts Institute of Technology, USA, (2)National Renewable Energy Laboratory, USA, (3)Center for Bioenergy Innovation, USA*.

**Short Summary:**

Selective deoxygenation of lignin oil using Mo<sub>2</sub>C produces renewable jet-range aromatic hydrocarbons with high atom economy.

9:50 AM **Thu-MEBR-0950** Catalytic Valorization of Brazilian Sugar Cane Lignin to Produce Value-Added Chemicals..

Danielle Fragoso<sup>1</sup>, Henrique Goulart<sup>2</sup>, Euzebio Goulart<sup>2</sup> and **S. David Jackson<sup>1</sup>**, (1)University of Glasgow, United Kingdom, (2)Universidade Federal de Alagoas, Brazil.

**Short Summary:**

Sugar-cane bagasse can be used to generate a range of fine chemicals such as 4-methylphenol and 4-(2-hydroxyethyl)-2,6-dimethoxyphenol. These, and other molecules, can be tuned dependent upon the catalyst used.

10:10 AM **Thu-MEBR-1010** Effect of Copper on Hydrodeoxygenation and Hydrodesulfurization Coprocessing of Phenol and DBT for a Ru/TiO<sub>2</sub>-ZrO<sub>2</sub> Catalyst.

Jessica Torres, Reyna Rios and Jose Antonio De los Reyes, *Universidad Autónoma Metropolitana-Iztapalapa, Mexico*.

**Short Summary:**

The effect of copper on the catalytic properties of a Ru/TiO<sub>2</sub>-ZrO<sub>2</sub> catalyst was investigated on hydrodeoxygenation and hydrodesulfurization coprocessing of phenol and DBT. The results showed that Cu on Ru catalysts improves catalytic activity and their resistance to sulfur related to a change in acidity and structure.

10:30 AM **Thu-MEBR-1030** Catalyst Development for Reductive Liquefaction of Sulfur-Containing Lignin.

Pouya Rezaei, Derek Creaser and **Louise Olsson**, *Chalmers University of Technology, Sweden*.

**Short Summary:**

Lignin is a renewable material which could be utilized for the production of fuels and chemicals. This is the first study using rhenium sulfide catalysts for the conversion of kraft lignin, showing that sulfided Re/Al<sub>2</sub>O<sub>3</sub> is a highly efficient catalyst for suppressing char formation in a lignin liquefaction process.

10:50 AM **Thu-MEBR-1050** Tertiary Amines from Lignin Using Commercial Cu Catalyst.

Dieter Ruijten and Bert F. Sels, *KU Leuven, Belgium*.

**Short Summary:**

Lignin model compounds are successfully converted to tertiary amines by commercial Cu catalyst following a hydrogen borrowing pathway. Various tertiary amines were obtained in high yield. Catalyst reuse experiments and ToF-SIMS analysis provided important insights into major deactivation pathways.

11:10 AM **Thu-MEBR-1110** Multi-Pass Flow-through Reductive Catalytic Fractionation.

Jun Hee Jang<sup>1</sup>, David G. Brandner<sup>1</sup>, Yuriy Roman<sup>2</sup> and Gregg T. Beckham<sup>1</sup>, (1)National Renewable Energy Laboratory, USA, (2)Massachusetts Institute of Technology, USA.

**Short Summary:**

Flow-through reductive catalytic fractionation (FT-RCF) enables physical separation of biomass and catalyst, but operates at high solvent-to-biomass ratios. Here, we demonstrate that methanol can be recycled after FT-RCF without lignin removal, and that the delignification extent and monomer yields are additive, significantly reducing overall solvent usage in the RCF process.

11:30 AM **Thu-MEBR-1130** Platinum Catalysts for the Lignin Conversion into Phenolics As Bio-Based Resource for Phenolic Resins.

Gisa Meissner<sup>1</sup>, Hendrik Spod<sup>1</sup>, Raphaela Süß<sup>2</sup> and Birgit Kamm<sup>2</sup>, (1)Heraeus Deutschland GmbH & Co. KG, Germany, (2)Wood K plus, Austria.

**Short Summary:**

Using Platinum-based catalysts ensures the access to important organic building blocks as sustainable products made from biomass to realize its total utilization. The full avoidance of any coke formation allows the application of the obtained phenolics as starting material for phenolic resins.

## THURSDAY AFTERNOON

### Biomass to Chemicals II: Oxides as Catalysts

**Session Chairs:** Robert Harding, *Grace*, and Juan Bravo Suárez, *The University of Kansas, USA*.

1:10 PM **Thu-MEBR-1310** Conversion of Ethanol to C<sub>5</sub>+ Ketones over Pd Promoted Mixed Oxide Catalyst.

Karthikeyan Ramasamy<sup>1</sup>, Mond Guo<sup>1</sup>, Senthil Subramaniam<sup>1</sup>, Tanmayi Bathena<sup>2</sup> and Konstantinos Goulas<sup>2</sup>, (1)Pacific Northwest National Laboratory, USA, (2)Oregon State University, USA.

**Short Summary:**

Single step ethanol conversion to C<sub>5</sub>+ ketones, building blocks for lubricants and sustainable aviation fuels from ethanol was achieved over stable Pd-promoted ZnO-ZrO<sub>2</sub> catalyst. The formation of a Pd-Zn alloy in situ was identified to be the critical factor in maintaining high selectivity to C<sub>5</sub>+ ketones and the catalyst stability.

1:30 PM **Thu-MEBR-1330** New Insights into the Activity & Stability of Sulfated Metal Oxide Catalysts for Vapor-Phase Ketonisation of Volatile Fatty Acids.

Gunjan Deshmukh, Alexandre Goguet and **Haresh Manyar**, *Queen's University Belfast, United Kingdom*.

**Short Summary:**

The effect of sulfation of ceria zirconia mixed metal oxide catalysts on their structure, acidity/basicity, catalytic activity, selectivity and longevity towards the ketonisation of volatile fatty acids is investigated. Sulfated catalysts are more selective and more stable than pristine catalysts.

1:50 PM **Thu-MEBR-1350** Influence of Support Structure on the Cascade Reaction of Ethanol to Butadiene over Ag-Promoted TaOx or YOx Catalysts.  
**Konstantin Mamedov** and Robert J. Davis, *University of Virginia, USA*.

**Short Summary:**

Effective catalysts for the conversion of ethanol to butadiene via the Lebedev reaction are multifunctional, often composed of early transition metal oxides combined with late transition metal promoters. This work shows the superior activity of zeolite-supported Ta or Y compared to silica-supported analogues for the Ag-promoted system.

2:10 PM **Thu-MEBR-1410** Unraveling the Mechanism of Glycerol Oxidation to Dicarboxylic Acids over a Copper Oxide Catalyst.

**Prince Amaniampong**, *University of Poitiers, CNRS, France*.

**Short Summary:**

The catalytic performances of non-noble CuO prepared by a fast (5 min) and simple sonochemical approach is reported in the oxidation of glycerol to Oxalic and Tartronic acid. A significant advantage of this sonochemical synthesis technique is the incredibly fast synthesis time along with *in-situ* pseudo-calcinations of the catalyst.

2:30 PM **Thu-MEBR-1430** Lactic Acid Production from C6 Carbohydrates over Sn-Beta Catalyst Using Polar Aprotic Solvents.

**Isabel Hortal-Sánchez**<sup>1</sup> and Nelson Cardona-Martínez<sup>2</sup>, (1)*University of Puerto Rico at Mayagüez, USA*, (2)*University of Puerto Rico - Mayagüez, USA*.

**Short Summary:**

Polar aprotic solvents with low amounts of water are effective for the conversion of carbohydrates into alpha-hydroxy acids. Both gamma-valerolactone and acetone improve the TOF and reduce the yield towards undesired products compared to water. Acetone increases the production of lactic acid while decreasing production of acetic and formic acid.

2:50 PM **Thu-MEBR-1450** Perovskite-Based, Phase Transition Catalytic Sorbents for Sorption Enhanced-Steam Reforming of Glycerol.

**Runxia Cai**, Leo Brody, Alajia Thornton and Fanxing Li, *North Carolina State University, USA*.

**Short Summary:**

The perovskite-structured phase transition sorbents in this study overcame the deactivation issue for conventional CaO-based sorbents and exhibited excellent catalytic performance for sorption-enhanced steam reforming of glycerol. The novel sorbent design strategy we demonstrated significantly broadens the design space for effective catalytic sorbents to intensified catalytic processes.

## Biomass to Chemicals III: Process Innovation

**Session Chairs:** Sudhakar Jale, *W.R. Grace, USA* and Bin Liu, *Kansas State University, USA*.

3:30 PM **Thu-MEBR-1530** Bio-Olefins from Crude Industrial Waste Glycerol and Sugar Alcohols *Via* Ru-Catalyzed Hydrodeoxygenation in Ionic Liquids.

Kwinten Janssens and **Dirk De Vos**, *KU Leuven, Belgium*.

**Short Summary:**

A bifunctional homogeneous Ru/IL catalytic system selectively converts crude industrial glycerol waste streams and sugar alcohols directly into their respective bio-olefins *via* hydrodeoxygenation. The formation of the Ru-Carbonyl-Halide complex was crucial to achieve high tolerance for common impurities like water, salts and methanol. XAS experiments (EXAFS/XANES) were performed at ESRF.

3:50 PM **Thu-MEBR-1550** Production of Chemicals from Sugars Via Glycolaldehyde.

**Esbén Taarning**<sup>1</sup>, Christian B. Schandel<sup>1</sup>, Christian M. Osmundsen<sup>1</sup>, Martin Høj<sup>2</sup>, Anker D. Jensen<sup>2</sup>, Juan Martínez-Espín<sup>1</sup> and Søren Tolborg<sup>1</sup>, (1)*Haldor Topsøe A/S, Denmark*, (2)*Technical University of Denmark, Denmark*.

**Short Summary:**

Cracking of sugars to glycolaldehyde, combined with catalytic processing, is a new strategy to produce several useful chemicals from biomass. Recent developments within catalytic processing of glycolaldehyde to bio-monomers and upscaling of the sugar cracking process at Haldor Topsøe A/S will be presented.

4:10 PM **Thu-MEBR-1610** Solvent Effects in Glucose-to-Fructose Isomerization in Modulated MOF UiO-66.

**Roshan Patel**<sup>1</sup>, Matheus Dorneles de Mello<sup>1</sup>, Tyler R Josephson<sup>1</sup>, Michael Tsapatsis<sup>1,2</sup>, J. Ilja Siepmann<sup>1</sup> and Matthew Neurock<sup>1</sup>, (1)*University of Minnesota, Twin Cities, USA*, (2)*Johns Hopkins University, USA*.

**Short Summary:**

Alcohol solvents were used for UiO-66 MOF-catalyzed glucose-to-fructose isomerization, an important reaction in the production of the platform chemical, hydroxymethyl furfural. Our combined computational and experimental study shows that use of 1-propanol favors selective fructose formation, whereas the side reaction of etherification is favored in the 'more acidic' methanol solvent.

4:30 PM **Thu-MEBR-1630** Glycolaldehyde As Bio-Based C2 Platform Chemical: Catalytic Reductive Amination of Vicinal Hydroxyl Aldehydes.

**Sofie Van Praet** and Bert F. Sels, *KU Leuven, Belgium*.

**Short Summary:**

Given the reactivity of  $\alpha$ -carbonyls, the selectivity control in parallel and consecutive reactions during reductive amination is challenging. Through clever selection of the process parameters and catalysis design, the process selectivity to alkanolamines and diamines could be tuned, and the potential of glycolaldehyde as a renewable platform molecule was affirmed.

## Rendezvous Trianon

### THURSDAY MORNING

#### Homogeneous and Molecular Catalysis I

**Session Chairs:** Boris Sheludko, *Amogy, Inc., USA* and Karena Smoll, *Dow, USA*.

9:30 AM **KEYNOTE Thu-RZVS-0930 Integrating Organometallic and Electrochemical Catalysts for Sustainable Polyketone Synthesis.** Alexander Miller<sup>1</sup>, Henry Dodge<sup>1</sup>, Ben Natinsky<sup>2</sup>, Scott Chapp<sup>1</sup>, Haochuan Zhang<sup>3</sup>, Yu Mu<sup>3</sup>, Dunwei Wang<sup>3</sup> and Chong Liu<sup>2</sup>. (1)University of North Carolina at Chapel Hill, USA, (2)University of California, Los Angeles, USA, (3)Boston College, USA.

**Short Summary:**

An integrated catalysis approach to the synthesis of polyketone with up to 50% CO<sub>2</sub>-derived repeat units is presented. A dual catalysis approach is taken, pairing a heterogeneous electrocatalyst for CO<sub>2</sub> reduction to CO with a homogeneous organometallic catalyst for CO copolymerization with ethylene.

10:10 AM **Thu-RZVS-1010 Strategies for Tuning the Kinetic Relevance of Redox Half Cycles in Metal-Organic Framework Mediated Single Site Catalysis.**

Jacklyn N. Hall<sup>1</sup>, A. Jeremy Kropf<sup>2</sup> and Praveen Bollini<sup>1</sup>, (1)University of Houston, USA, (2)Argonne National Laboratory, USA.

**Short Summary:**

This work exploits metal-organic framework nodes as hosts for well-defined active sites replicating the coordination environment of single site structures hitherto explored predominantly using homogeneous complexes. A combination of kinetic and spectroscopic tools (including X-ray absorption based techniques) help establish clear relationships between metal-oxo coordination environment and kinetic properties.

10:30 AM **Thursday, May 26, 2022: 9:30 AM Mechanistic Insights into Organometallic Iridium Catalysts Immobilized within a Metal–Organic Framework.**

Zoha Syed<sup>1,2</sup>, Massimiliano Delferro<sup>1</sup> and Omar K. Farha<sup>2</sup>, (1)Argonne National Laboratory, USA, (2)Northwestern University, USA.

**Short Summary:**

Metal–organic frameworks (MOFs) are crystalline, porous nanomaterials that are attractive for many applications. MOFs have gained attention in the catalysis world, both as a reactive material and as a solid support for active sites. Herein, we explore structure–activity relationships using an organoiridium catalyst tethered onto a MOF support.

10:50 AM **Thu-RZVS-1050 Mechanism of Palladium(II)-Mediated O-Deallylation Uncaging Reaction: Effect of Chloride in the Local Environment.** Gean Dal Forno<sup>1</sup>, Eloah Latocheski<sup>1</sup>, Albert St John<sup>1</sup>, Steffany Luczynski<sup>1</sup>, Felipe Schneider<sup>1</sup>, Giovanni Caramori<sup>1</sup>, Frédéric Avenier<sup>2</sup> and Josiel Domingos<sup>1</sup>, (1)Federal University of Santa Catarina, Brazil, (2)Université Paris Saclay, France.

**Short Summary:**

Mechanistic insights of local chloride concentration effect on bioorthogonal uncaging reactions triggered by palladium, is disclosed in this work. The evaluation was performed in the rate and yield of the C-O bond cleavage of an O-allyl protected coumarin substrate, by means of kinetic, energetic, structural and theoretical analysis.

11:10 AM **Thu-RZVS-1110 Mechanism of Nitrile Hydrogenation with an Iron PNP Complex.**

Simon Velasquez Morales and Alan Allgeier, *The University of Kansas, USA*.

**Short Summary:**

Toward the development of continuous flow hydrogenation with earth-abundant metal catalysts, the mechanism of nitrile hydrogenation by Fe PNP complexes has been studied by a combination of kinetics and spectroscopy. The previously unknown intermediacy of oligomeric intermediates has been characterized by high-pressure NMR and single crystal XRD.

11:30 AM **Thu-RZVS-1130 Reduction of the Phillips Catalyst By Aldehydes.**

Juili Parab and Friederike C. Jentoft, *University of Massachusetts Amherst, USA*.

**Short Summary:**

The Phillips catalyst is generally reduced by the monomer ethylene or by CO to generate active polymerization sites. Systematic evaluation reveals that various aldehydes can serve as alternative reductants for Cr(VI)/SiO<sub>2</sub>, provided the redox products are thermally desorbed. Reduction by aldehydes enhances polymerization activity relative to reduction by ethylene.

### THURSDAY AFTERNOON

#### Homogeneous and Molecular Catalysis II

**Session Chairs:** Matthew Conley, *University of California, Riverside, USA* and Wes Sattler, *ExxonMobil, USA*.

1:10 PM **KEYNOTE Thu-RZVS-1310 Catalysis with Earth Abundant Transition Metals: Unlocking New Opportunities in Synthesis and Sustainability.** Paul Chirik, *Princeton University, USA*.

**Short Summary:**

Much is made about our “carbon footprint”. Why just focus on one element? For sustainable future, we must be mindful of our elemental footprint. My lecture will focus on catalysis using Earth abundant metals in catalysis and highlight the new opportunities presented in synthesis.

1:50 PM **Thu-RZVS-1350** Carbon Monoxide Acting As a Ligand for CO Oxidation on a Heterogeneous Single Atom Catalyst on Reducible Supports. Coogan Thompson<sup>1</sup>, Liping Liu<sup>1</sup>, Denis Leshchev<sup>2</sup>, Adam Hoffman<sup>3</sup>, Jiyun Hong<sup>3</sup>, Dimosthenis Sokaras<sup>3</sup>, Thomas Kroll<sup>3</sup>, Simon Bare<sup>3</sup>, Raymond R. Unocic<sup>4</sup>, Eli Stavitski<sup>2</sup>, Hongliang Xin<sup>1</sup> and **Ayman M. Karim<sup>1</sup>**, (1)Virginia Polytechnic Institute and State University, USA, (2)Brookhaven National Laboratory, USA, (3)SLAC National Accelerator Laboratory, USA, (4)Oak Ridge National Laboratory, USA.

**Short Summary:**

We demonstrate through microscopy, spectroscopy, and kinetics that iridium single atom catalysts on reducible supports employ a nonreacting, CO ligand into the active site for CO oxidation. This result explains how single atom catalysts are not poisoned by CO and provides a foothold into ligand chemistry for heterogeneous catalysis.

2:10 PM **Thu-RZVS-1410** Identify the Active Site Structure of a Supported Organovanadium Catalyst Using Integrated Mechanistic Study and XANES Simulations.

Cong Liu<sup>1</sup>, **Prajay Patel<sup>1</sup>**, Robert Wells<sup>2</sup>, Rex Skodje<sup>2</sup>, A. Jeremy Kropf<sup>1</sup>, David Kaphan<sup>1</sup> and Massimiliano Delferro<sup>1</sup>, (1)Argonne National Laboratory, USA, (2)University of Colorado Boulder, USA.

**Short Summary:**

An integrated mechanistic study and computational XANES simulations were carried out to investigate the active site structure of a silica supported organovanadium catalyst for styrene hydrogenation.

2:30 PM **Thu-RZVS-1430** Halide Abstraction By R<sub>3</sub>Si<sup>+</sup> Supported on Oxides: A Robust Methodology to Form Well-Defined Heterogeneous Catalysts.

**Matthew Conley**, University of California, Riverside, USA.

**Short Summary:**

This lecture will describe a new methodology to generate well-defined catalytic sites on oxides by abstracting M–X (X = halides) by R<sub>3</sub>Si<sup>+</sup> sites supported on weakly coordinating oxides.

2:50 PM **Thu-RZVS-1450** Developing Design Rules for Homogeneous Catalysts.

Zhenzhuo Lan and **Shaama Mallikarjun Sharada**, University of Southern California, USA.

**Short Summary:**

We propose a novel framework for developing linear free energy relationships to drive design of molecular transition metal complex catalysts for activation of strong CH bonds.

## Catalyst Manufacturing

**Session Chairs:** William Borghard, Rutgers, The State University of New Jersey, USA and Michael Ross, Evonik Corporation, .

3:30 PM **KEYNOTE Thu-RZVS-1530 Optimization and Scale-up of Catalyst Manufacturing Unit Operations.** Benjamin Glasser, Rutgers, The State University of New Jersey, USA.

**Short Summary:**

An ongoing challenge in catalyst manufacturing is the scale-up from the laboratory and pilot plant scales to the manufacturing scale. Our research seeks to provide a methodology for scale-up through understanding of the effects of material properties, operating conditions and system size on the unit operation.

4:10 PM **Thu-RZVS-1610** Revealing the Effect of Gas Atmosphere and Scale up of Template Removal Processes within Mesophase MCM-41.

**Santiago Palencia Ruiz<sup>1</sup>**, Alexander Sachse<sup>1</sup>, Canan Gucuyener<sup>2</sup>, Nicolas Bats<sup>2</sup>, Nuno rocha-Batalha<sup>1</sup> and Ludovic Pinard<sup>1</sup>, (1)Université de Poitiers, France, (2)Johnson Matthey Technology Centre, United Kingdom.

**Short Summary:**

Calcination of the as-synthesized MCM-41 has been performed at sample loadings at least 1000 times higher compared to open literature, which permitted the *in-situ* examination of the heat transfer phenomena and describe the template removal mechanism under (an)aerobic conditions employing advance analytical technics.

4:30 PM **Thu-RZVS-1630** Heat Transfer in a Rotary Drum with Baffles: Effect of Operating Conditions and Particle Properties.

**Elaheh Ardalani**, William Borghard, Benjamin Glasser and Alberto Cuitino, Rutgers, The State University of New Jersey, USA.

**Short Summary:**

Understanding the relationship between particle properties and rotary drum operating conditions on thermal time is critical and can enable us to predict processing time in real-world applications. In this study, we computationally investigated the heat transfer scale-up of granular flows in rotating drums equipped with baffles.

4:50 PM **Thu-RZVS-1650** Comparison of 3D Printed Substrate with Conventional Extruded Honeycomb Monolith for Catalytic Converter Applications.

**Callum Davidson** and Aidan Doyle, Manchester Metropolitan University, United Kingdom.

**Short Summary:**

Lab scale catalytic converter prototypes, prepared using 3D printing, showed improved catalytic activity in the oxidation of methane relative to conventional unidirectional substrates. This enhancement is attributed to the increased turbulence/mass transfer and surface area caused by the greater complexity of the 3D structures than that in straight channel arrangements.

5:10 PM **Thu-RZVS-1710** Highly Attrition Resistant & High Purity Microsphere Alumina Catalysts for CO Control in Fccu.

**Yun-feng Chang**, Sigma Innova LLC, USA; Sigma Innova (Tianjin) Co. Ltd., China.

**Short Summary:**

Highly attrition resistant alumina microspheres were developed as supports for noble metals and transition metals to meet demanding fluidized bed catalytic cracking applications and liquid phase hydrogenation or coupling applications where particle mechanical strength is critical.



## Sutton North

### THURSDAY MORNING

#### Alkane Dehydrogenation I

**Session Chairs:** David Barton, *The Dow Chemical Company, USA* and Jeffrey Camacho-Bunquin, *Exxon, USA*.

9:30 AM **Thu-SUNO-0930** The Role of Added Hydrogen on Pt-Alloy Catalysts for Dehydrogenation.

**Ryan Alcalá** and Abhaya Datye, *University of New Mexico, USA*.

**Short Summary:**

The stability of Pt based alloy catalysts in high temperature alkane dehydrogenation reactions limits the commercial feasibility of producing ethylene and propylene from natural gas in one catalytic step. Here we demonstrate a strategy to allow operation of the catalyst for long durations without the need for oxidative regeneration.

9:50 AM **Thu-SUNO-0950** First Principles Analysis of Trends in Propane Dehydrogenation on Bimetallic Alloys: Stability Descriptors and Catalyst Screening.

Ranga Rohit Seemakurthi<sup>1</sup>, Stephen Purdy<sup>2</sup>, David Dean<sup>1</sup>, Fabio H. Ribeiro<sup>1</sup>, Jeffrey T. Miller<sup>1</sup> and **Jeffrey Greeley**<sup>3</sup>, (1)*Purdue University, USA*, (2)*Oak Ridge National Laboratory, USA*, (3)*Davidson School of Chemical Engineering, Purdue University, USA*.

**Short Summary:**

First principles energetics, microkinetic modeling, and experiments are employed to elucidate the active site geometries, as well as rate- and selectivity-controlling steps, of propane dehydrogenation on a series of Pt- and Pd-based bimetallic alloys. The results are used as the basis to screen bimetallic alloys for enhanced PDH selectivity.

10:10 AM **Thu-SUNO-1010** Platinum Alloy Catalysts Exhibiting High Propane Dehydrogenation Performance in Zeolite Mesopores.

**Ryong Ryoo**<sup>1,2</sup>, Hanyoung Park<sup>2,3</sup> and Jeong-Chul Kim<sup>3</sup>, (1)*Kentech, Korea, Republic of (South)*, (2)*Korea Advanced Institute of Science and Technology (KAIST), Korea, Republic of (South)*, (3)*IBS, Korea, Republic of (South)*.

**Short Summary:**

The authors report on their exciting discovery indicating that propane-dehydrogenation catalytic lifetime increases dramatically when platinum is co-supported with zinc or yttrium on mesoporous zeolites, where surface-dangling silanol groups on the mesopore walls play a key role in the formation of alloy nanoparticles with specific stoichiometry and structure.

10:30 AM **Thu-SUNO-1030** An Efficient Route for Low Temperature Regeneration of Coked Pt Catalysts.

Siamak Nakhaie<sup>1</sup>, **Sabine Wrabetz**<sup>1</sup>, Jasmin Allan<sup>1</sup>, Hannah Nerl<sup>1</sup>, Maria Dimitrakopoulou<sup>1</sup>, Piyush Ingale<sup>2</sup>, Raoul Naumann d'Alnoncourt<sup>2</sup>, Frank Rosowski<sup>3,4</sup>, Stefan Kotrel<sup>4</sup>, Thomas Lunkenbein<sup>1</sup>, Katarzyna Skorupska<sup>1</sup> and Robert Schlögl<sup>1,5</sup>, (1)*Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany*, (2)*BasCat – UniCat BASF JointLab: Technische Universität Berlin, Germany*, (3)*Technische Universität Berlin, Germany*, (4)*BASF SE, Germany*, (5)*Max Planck Institute for Chemical Energy Conversion, Germany*.

**Short Summary:**

We demonstrate that an efficient regeneration of coked Pt catalysts is feasible at temperatures as low as 310°C using NO<sub>x</sub>, plus they show a better performance in PDH reaction than air-regenerated catalyst. The findings in this study can be of high importance for industry to develop more efficient regeneration processes.

10:50 AM **Thu-SUNO-1050** Propane and Butane Dehydrogenation Catalyzed By Isolated PtZn<sub>4</sub> Site Supported over Self-Pillared Zeolite Nanosheets.

Liang Qi<sup>1,2</sup>, Yanfei Zhang<sup>1,2</sup> and **Alexis T. Bell**<sup>1,2</sup>, (1)*University of California, Berkeley, USA*, (2)*Lawrence Berkeley National Laboratory, USA*.

**Short Summary:**

We report a method for dispersing Pt atoms onto ZnO<sub>x</sub> moieties created over self-pillared zeolite nanosheets. The catalyst exhibits exceptionally high activity and selectivity, and no deactivation for propane dehydrogenation. For butane dehydrogenation reaction, the selectivity to dehydrogenation butenes and butadiene reached 98.9%, and the selectivity to butadiene was 45%.

11:10 AM **KEYNOTE Thu-SUNO-1110 Bayesian Analysis for Identifying the Active Sites for Platinum-Catalyzed Propane Dehydrogenation.** Charles Fricke and **Andreas Heyden**, *University of South Carolina, USA*.

**Short Summary:**

Identifying the active sites and their role in a catalyst is essential for optimization of heterogeneous metal catalysts. Here, we identified the active sites for the propane dehydrogenation over Pt-based catalysts by coupling experimental data with computational models and Bayesian uncertainty analysis.

## THURSDAY AFTERNOON

### Hydrocarbon Reactions in Zeolites

**Session Chairs:** Victor J. Sussman, *The Dow Chemical Company, USA* and Yunwen Zhou, *Shell, USA*.

1:10 PM **Thu-SUNO-1310** Reaction, Diffusion, and Deactivation Rates of Aromatic Alkylation and Alcohol Etherification on Hierarchical Zeolites.

**Hayat Adawi** and Michele Sarazen, *Princeton University, USA*.

**Short Summary:**

Reactions of (poly)substituted aromatics on solid-acid zeolite catalysts suffer from severe diffusional barriers within narrow zeolite micropores. Reaction-diffusion-deactivation analysis of competitive aromatics alkylation and alcohol etherification on hierarchical zeolites containing larger, mesoporous voids provides fundamental insight into the potential for more atom-efficient conversions of aromatic species.

1:30 PM **Thu-SUNO-1330** Kinetic and Mechanistic Assessments of the Influence of Active Site Distribution in MFI Zeolites on Toluene Methylation Catalysis.

**Sopuruchukwu Ezenwa**<sup>1</sup>, Deng (DY) Jan<sup>2</sup> and Rajamani Gounder<sup>1</sup>, (1)*Purdue University, USA*, (2)*Honeywell UOP, USA*.

**Short Summary:**

Kinetic studies of low-temperature toluene methylation on MFI zeolites synthesized with different bulk and atomic properties reveal that xylenes formation rates (per H<sup>+</sup>) and isomer selectivity depend weakly on intracrystalline residence time and external acid site content, but strongly on the location and proximity of active sites within microporous voids.

1:50 PM **Thu-SUNO-1350** Effect of Water and Acid Site Proximity on Cumene Dealkylation over H-ZSM-5 Zeolites.

**Han Chau**, Abhishek Gumidyal, Tram Pham and Steven P. Crossley, *University of Oklahoma, USA*.

**Short Summary:**

In this study, the intriguing enhancement effect of acid site proximity and water on the reaction rate of cumene dealkylation over H-ZSM-5 zeolites was revealed, which is explained by the entropy gain of the reaction transition state. Water was also found to improve catalyst stability in this reaction.

2:10 PM **Thu-SUNO-1410** Butane Hydrocracking Mechanism on Pt/HZSM-5 Bifunctional Catalyst.

**Prasanna Dasari** and Robert Broekhuis, *SABIC, USA*.

**Short Summary:**

Hydrocracking efficiently converts butanes with a combined product selectivity to ethane and propane >90% at almost complete butane conversion. This work focuses on deconvolution of the complex reaction mechanism of butane hydrocracking on Pt/HZSM-5 bifunctional catalyst.

2:30 PM **Thu-SUNO-1430** Catalytic Consequences of Metal-Acid Site Proximity for Bifunctional Alkane Isomerization and  $\beta$ -Scission Reactions.

Gina Noh, **Wenshuo Hu** and Enrique Iglesia, *University of California, Berkeley, USA*.

**Short Summary:**

Rigorous reaction-diffusion treatments reveal that the significant enhancements in *n*-heptane isomerization rates resulting from nanoscale metal-acid site proximity reflect an enhanced diffusion of primary product alkenes because of decreased sizes of acid domains, which allows the scavenging of product alkenes to relieve local intracrystalline equilibration among reactant and product alkenes.

2:50 PM **Thu-SUNO-1450** Zeolite-Assisted Core-Shell Redox Catalyst for Redox Oxidative Cracking of Cyclohexane with High Olefin Yield.

Fang Hao<sup>1,2</sup>, Yunfei Gao<sup>1</sup>, Ryan Dudek<sup>1</sup>, **Luke Neal**<sup>1</sup>, Pingle Liu<sup>2</sup> and Fanxing Li<sup>1</sup>, (1)*North Carolina State University, USA*, (2)*Xiangtan University, China*.

**Short Summary:**

We present a highly effective redox catalyst platform for redox oxidative cracking of naphtha. It consists of doped ZSM-5 and perovskite core-shell redox catalysts that take advantage of the selective hydrogen combustion properties of a molten salt modified perovskite oxygen carrier and the tunability of the metal exchanged ZSM-5.

### Light Hydrocarbons to Liquids

**Session Chairs:** Eric Duskocil, *BP, USA* and Andrew Ingram, *Gevo, Inc., USA*.

3:30 PM **Thu-SUNO-1530** Rationalizing Olefin Oligomerization on Single Site Ga<sup>3+</sup> Catalysts on Amorphous Silica: A First Principles Study Combined with Experiments and Automated Reaction Network Explorations.

**Yinan Xu**<sup>1</sup>, Nicole A. LiBretto<sup>1</sup>, Qiyuan Zhao<sup>1</sup>, Brett Savoie<sup>1</sup>, Jeffrey T. Miller<sup>1</sup> and Jeffrey Greeley<sup>2</sup>, (1)*Purdue University, USA*, (2)*Davidson School of Chemical Engineering, Purdue University, USA*.

**Short Summary:**

The DFT analysis, combined with XAS insights, reveals delicate relationships between site heterogeneity of Ga<sup>3+</sup>/SiO<sub>2</sub> system and the dominant ethylene oligomerization cycles. We determine that the less-constrained Ga<sup>3+</sup> sites exhibit unique catalytic flexibility by enabling both an accessible transition state for ethylene insertion and an unreported facile  $\beta$ -hydride transfer step.

3:50 PM **Thu-SUNO-1550** Stable Nickel Olefin Oligomerization Metal Organic Framework Catalysts: Structure, Site Densities, Kinetics, and Mechanism.

**Benjamin Yeh**<sup>1</sup>, Stephen Vicchio<sup>2</sup>, Saamil Chheda<sup>1</sup>, Jian Zheng<sup>3</sup>, Julian Schmid<sup>3</sup>, Steven Prinslow<sup>1</sup>, Laura Löbbert<sup>4</sup>, Ricardo Bermejo de Val<sup>4</sup>, Oliver Y. Gutierrez<sup>3</sup>, Johannes A. Lercher<sup>3,4</sup>, Connie Lu<sup>1</sup>, Matthew Neurock<sup>1</sup>, Rachel Getman<sup>2</sup>, Laura Gagliardi<sup>5</sup> and Aditya Bhan<sup>1</sup>, (1)University of Minnesota, Twin Cities, USA, (2)Clemson University, USA, (3)Pacific Northwest National Laboratory, USA, (4)Technical University of Munich, Germany, (5) University of Chicago, USA.

**Short Summary:**

Nickel functionalized metal organic frameworks are stable for olefin oligomerization. We present spectroscopy, transient and steady state kinetics, and DFT calculations to elucidate the structure of the nickel situated on (Ni/Uio-66) and in (Ni-MIL-127) MOF nodes and the mechanism for olefin oligomerization on these materials.

4:10 PM **Thu-SUNO-1610** Ethylene Oligomerization Catalyzed By Isolated Ni<sup>2+</sup> Single Sites on Lacunary Wells Dawson Polyoxometalate.

**Yoonrae Cho**, Jessica A. Muhlenkamp, Allen Oliver and Jason C. Hicks, *University of Notre Dame, USA.*

**Short Summary:**

In this work, the application of lacunary defects on Wells Dawson polyoxometalate as stable and regenerable molecular level platforms to isolate nickel single sites for ethylene oligomerization.

4:30 PM **Thu-SUNO-1630** Oligomerization of Light Olefines on Ni-Uio-66 MOFs: Elucidation of the Active Site and Reaction Mechanism.

**Julian Schmid**<sup>1</sup>, Laura Löbbert<sup>2</sup>, Jian Zheng<sup>1</sup>, Saamil Chheda<sup>3</sup>, John Fulton<sup>1</sup>, Oliver Y. Gutierrez<sup>1</sup>, Matthew Neurock<sup>3</sup>, Laura Gagliardi<sup>3</sup> and Johannes A. Lercher<sup>1</sup>, (1)Pacific Northwest National Laboratory, USA, (2)Technical University of Munich, Germany, (3)University of Minnesota, Twin Cities, USA.

**Short Summary:**

Our study provides fundamental insight into synthesis of well-defined Ni active sites on MOFs and their application for the selective production of linear alpha olefins (raw materials for high performance polymers) by describing how to precisely control the structure of Ni sites and the reaction mechanisms that they promote.

4:50 PM **Thu-SUNO-1650** Catalysts Development and Characterization for Converting Shale Gas Condensate to Aromatics.

**Jun Wang**, Kaiwalya Sabnis, Dustin Farmer, Kevin Bazazzadeh, Alla Khanmamedova, Jianguo Fan, Travis Conant and Scott Stevenson, *SABIC, USA.*

**Short Summary:**

The Pt/NaGe-ZSM5 catalyst with both aromatization and isomerization functionalities was developed for shale gas condensate type of model feed. This catalyst demonstrated the best benzene yield. Through the combination of different characterization, theoretical calculation and kinetics, the reaction mechanism and different roles of the components of the catalyst were proposed.

5:10 PM **Thu-SUNO-1710** Plasma-Assisted Approaches for the Direct Production of Liquid Products from Shale Gas.

**Deanna Poirier**, Gerardo Rivera-Castro and Jason C. Hicks, *University of Notre Dame, USA.*

**Short Summary:**

We report a one-pot, plasma-assisted process involving various alkanes and molecular nitrogen for the production of hydrocarbons, ammonia, and nitrogen-containing liquids. Variations in feed composition, power input, and space velocity can affect the diverse product slate, and catalyst selection can enhance the selectivity to desired products.

## Sutton South

### THURSDAY MORNING

#### Reaction Modelling and Theory

**Session Chairs:** Fanglin Che, *University of Massachusetts Lowell, USA* and Jean-Sabin McEwen, *Washington State University, USA.*

9:30 AM **Thu-SUSO-0930** Elucidating Effects of Potential, Hydrogen Peroxide, and Interlayer Interactions on Site Structure, Stability, and Activity of Fe-N-C Catalysts for Electrochemical O<sub>2</sub> Reduction in Acidic Media.

**Ankita Morankar**<sup>1</sup>, Siddharth Deshpande<sup>2</sup>, Zhenhua Zeng<sup>2</sup>, Alyssa McNarney<sup>1</sup>, Plamen Atanasov<sup>3</sup> and Jeffrey Greeley<sup>1</sup>, (1)Davidson School of Chemical Engineering, Purdue University, USA, (2)Purdue University, USA, (3)University of California, Irvine, USA.

**Short Summary:**

The dependence of site environment (nature of ligating nitrogen, location, clustering) on the in-situ structure of FeN<sub>x</sub> moieties, is probed in the presence of water and hydrogen peroxide at different voltages. In-situ structural insights are then tied to each site's stability and activity towards electrochemical O<sub>2</sub> reduction in acidic media.

9:50 AM **Thu-SUSO-0950** The Importance of Activation Barriers in Designing Optimal Active Sites for the Oxygen Evolution Reaction.

**Craig Plaisance**<sup>1</sup>, Simeon Beinlich<sup>2</sup> and Karsten Reuter<sup>2</sup>, (1)Louisiana State University, USA, (2)Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany.

**Short Summary:**

We show that the widely used electrocatalyst design strategy based only on thermodynamics can be misguided when certain steps have significant activation barriers, as is the case in the oxygen evolution reaction. An alternative kinetics-based approach is presented.

10:10 AM **Thu-SUSO-1010** Constructing Orbital Coupling-Modulated Active Sites of Metal-Nitrogen-Doped Carbon Catalyst for Highly Active Electrochemical CO<sub>2</sub>.

**Byoung Joon Park** and Jeong Woo Han, *Pohang University of Science and Technology (POSTECH), Korea, Republic of (South)*.

**Short Summary:**

We established a computational screening route for highly active and selective metal-nitrogen-doped carbon (M-N-C) catalysts for CO<sub>2</sub>RR. Beyond single M-N-Cs, dual atomic M-N-C catalysts with Fe pair was proposed. Using density functional theory calculations, it was confirmed that the orbital coupling between Fe dual-sites improves the CO<sub>2</sub>RR-to-CO activity.

10:30 AM **Thu-SUSO-1030** Understanding and Controlling the Electrochemical Kinetics of Hydrocarbon Synthesis from CO<sub>2</sub>: A Unified Picture of Surface Intermediates and Their Interaction with Electrolyte Ions.

**Marcel Schreier**, *University of Wisconsin-Madison, USA; University of Wisconsin-Madison, USA*.

**Short Summary:**

Improving the electrocatalytic synthesis of hydrocarbon products such as ethylene and methane from CO<sub>2</sub> requires a fundamental understanding of the electrochemical processes governing CO<sub>2</sub> electrocatalysis. Using data from nonaqueous model systems and aqueous gas diffusion electrodes, I will shed light onto the catalytic networks which govern the electrosynthesis of hydrocarbons.

10:50 AM **Thu-SUSO-1050** Accelerated Mapping of Pure Metal and Ligand Compositions for Light-Driven Hydrogen Production.

**Maya Bhat**<sup>1</sup>, Eric Lopato<sup>1</sup>, Zoe Simon<sup>2</sup>, Jill Millstone<sup>2</sup>, Stefan Bernhard<sup>1</sup> and John R. Kitchin<sup>1</sup>, *(1)Carnegie Mellon University, USA, (2)University of Pittsburgh, USA*.

**Short Summary:**

We demonstrate an accelerated framework to survey a multi dimensional light-driven process with the use of high throughput experimentation and design of experiments methods. Through the use of both computational and experimental techniques, we are able to identify active pure metal and ligand compositions for enhanced hydrogen production.

11:10 AM **Thu-SUSO-1110** Describing Electrocatalytic Hydrogenation to Form Fuels and Chemicals through the Langmuir-Hinshelwood Mechanism.

**Nirala Singh** and Bryan Goldsmith, *University of Michigan-Ann Arbor, USA*.

**Short Summary:**

In this work we discuss how electrocatalytic hydrogenation of model bio-oil compounds to fuels and nitrate to ammonia both follow a Langmuir-Hinshelwood mechanism. Understanding the mechanism allows us to identify active facets, increase catalyst utilization, and design new catalysts with improved performance.

11:30 AM **Thu-SUSO-1130** Understanding Differences in the Requirements for CO and Methanol Electro-Oxidation with Ag<sub>x</sub>Pd<sub>1-x</sub> Alloys.

Adam Baz, Taylor Spivey, Lindsey Hamblin and **Adam Holewinski**, *University of Colorado Boulder, USA*.

**Short Summary:**

We explore the degree to which CO-tolerance is correlated to methanol electro-oxidation activity using a series of carbon-supported Ag<sub>x</sub>Pd<sub>1-x</sub> alloy electrocatalysts. Tradeoffs are revealed relating to both site ensemble requirements and intrinsic activity toward dehydrogenation and CO removal steps, which vary with electronic modification of the Pd sites by Ag.

## THURSDAY AFTERNOON

### Fuel Cell Catalysis

**Session Chairs:** G. T. Kasun Kalhara Gunasooriya, *Technical University of Denmark, Denmark* and Adam Holewinski, *University of Colorado Boulder, USA*.

1:10 PM **Thu-SUSO-1310** Chemical and Electrochemical O<sub>2</sub> Reduction on Heterogeneous Non-Precious Metal Catalysts and Relevance to Mediated Electrolysis.

**Jason Bates**<sup>1</sup>, Sourav Biswas<sup>2</sup>, Sung-Eun Suh<sup>1</sup>, Mathew Johnson<sup>1</sup>, Biswajit Mondal<sup>1</sup>, Thatcher Root<sup>1</sup> and Shannon Stahl<sup>1</sup>, *(1)University of Wisconsin-Madison, USA, (2)State University of New York Buffalo State, USA*.

**Short Summary:**

Hydroquinone-mediated O<sub>2</sub> reduction occurs on earth-abundant M-N-C catalysts by inner-sphere mechanisms distinct from those of electrocatalytic ORR, as revealed by kinetic analysis and linear free energy relationships with HQ potential. Inner-sphere mechanisms circumvent on-electrode Tafel relationships, and motivate developing new catalyst design criteria for aerobic oxidations on M-N-C.

1:30 PM **Thu-SUSO-1330** IrRu-Based Catalyst for Mitigating the Degradation of Automotive Proton Exchange Membrane Fuel Cell Under Transient Situations.

**Chanho Pak**<sup>1</sup>, Seung Woo Lee<sup>1</sup>, Chaekyung Baik<sup>1</sup>, Eunyoung You<sup>2</sup> and Myounggi Min<sup>3</sup>, *(1)Gwangju Institute of Science and Technology, Korea, Republic of (South), (2)Hyundai Mobis, Korea, Republic of (South), (3)Samsung SDI, Korea, Republic of (South)*.

**Short Summary:**

The IrRu catalyst with OER activity showed the ability to successfully mitigate the carbon corrosion in both anode and cathode for automotive PEMFC under transitory conditions such as fuel starvation and start-up and shut-down processes, which is very significant for suggesting the new approach for mitigating the fatal degradation.

1:50 PM **Thu-SUSO-1350** Oxygen Reduction By Non-Stoichiometric Mixed Metal Oxides: Avenues for Engineering Active and Stable Cationic Centers.

**Samji Samira**, Xiangkui Gu and Eranda Nikolla, *Wayne State University, USA*.

**Short Summary:**

The studies described here provide a framework where experimentally measurable properties are used to identify active and stable non-stoichiometric mixed metal oxides electrocatalysts for oxygen reduction – knowledge critical for the design of complex oxides for targeted electrochemical reactions.

2:10 PM **Thu-SUSO-1410** Probing the Effects of Acid Electrolyte Anions on Electrocatalyst Activity and Selectivity for the Oxygen Reduction Reactioncatalysts.

**Jose Zamora Zeledon**<sup>1,2</sup>, Gaurav Kamat<sup>1,2</sup>, G. T. Kasun Kalhara Gunasooriya<sup>3</sup>, Jens K. Nørskov<sup>3</sup>, Michaela Burke Stevens<sup>1,2</sup> and Thomas F. Jaramillo<sup>1,2</sup>, (1)*SLAC National Accelerator Laboratory, USA*, (2)*Stanford University, USA*, (3)*Technical University of Denmark, Denmark*.

**Short Summary:**

Microenvironment engineering presents a pathway to control electrocatalytic performance. Therefore, investigating the role of catalyst-electrolyte microenvironment components such as electrolyte anions helps guide the rational design of tuned electrochemical interfaces. This work demonstrates that oxygen reduction reaction selectivity can be controlled by acid electrolyte anion identity.

2:30 PM **Thu-SUSO-1430** Rational Synthesis of Polynitrogen N<sub>8</sub>- and Its ORR Mechanism.

**Xianqin Wang**, *New Jersey Institute of Technology, USA*.

**Short Summary:**

A highly active electrocatalyst, N<sub>8</sub><sup>-</sup>, was synthesized by accelerating the rate-limiting step with the UV irradiation. A four-electron process at N<sub>8</sub><sup>-</sup> is confirmed with the SHINERS experiments and DFT calculations. N<sub>8</sub><sup>-</sup> is found to be more stable and more active than the Pt/C commercial catalyst in DMFCs.

2:50 PM **Thu-SUSO-1450** Pulsed Laser in Liquids Synthesized Nanomaterials for Electrocatalysis.

**Astrid Müller**, *University of Rochester, USA*.

**Short Summary:**

We show how the catalysis community can capitalize on pulsed laser in liquids synthesis to advance catalyst development. We also solved the challenge of immobilizing nanoparticulate catalysts on inert, high surface area carbon substrates for electrocatalysis in aqueous electrolytes, by preparing structurally intact carbon fiber paper with long-lasting hydrophilicity.

## New Tools and Surface Science I

**Session Chairs:** Anatoly Frenkel<sup>1</sup>, Rebecca Fushimi<sup>2</sup> and Ashley Head<sup>3</sup>, (1)*Stony Brook University, USA*(2)*Idaho National Laboratory, USA*(3)*Brookhaven National Laboratory, USA*.

3:30 PM **Thu-SUSO-1530** Elucidating the Influence of Electric Fields on Fe Oxidation Via Multiscale Models and Atom Probe Tomography.

**Naseeha Cardwell**<sup>1</sup>, Sten Lambeets<sup>2</sup>, Isaac Onyango<sup>1</sup>, Yong Wang<sup>2</sup>, Thierry Visart de Bocarme<sup>3</sup>, Daniel Perea<sup>2</sup> and Jean-Sabin McEwen<sup>1</sup>, (1)*Washington State University, USA*, (2)*Pacific Northwest National Laboratory, USA*, (3)*Université Libre de Bruxelles, Belgium*.

**Short Summary:**

Catalytic Fe is highly selective for H<sub>2</sub>O, but prone to oxidative deactivation. Via density functional theory, we show that the application of an external electric field reduces surface oxidation, determining the equilibrium oxygen distribution on a multifaceted iron grain as the field strength varies, consistent with experimental work.

3:50 PM **Thu-SUSO-1550** *In Situ* ambient Pressure X-Ray Photoelectron Spectroscopy Investigations of Silicon Oxide Encapsulated Platinum Electrodes.

**Marissa Beatty**<sup>1</sup>, Ethan J. Crumlin<sup>2</sup> and Daniel Esposito<sup>1</sup>, (1)*Columbia University, USA*, (2)*Lawrence Berkeley National Laboratory, USA*.

**Short Summary:**

The following work demonstrates operando measurements of a confined electrocatalyst surface using Ambient Pressure X-ray Photoelectron Spectroscopy. The buried interface of a silicon oxide encapsulated Pt electrode was characterized via XPS across 0.0-1.4V to analyze hydrogen bonding and Pt oxidation behavior in various electrolytes.

4:10 PM **Thu-SUSO-1610** Characterizing Selectivity of Electrochemical Conversions Via Chemical Titration.

**Eric McShane**<sup>1</sup> and Bryan McCloskey<sup>2</sup>, (1)*University of California, Berkeley, USA*, (2)*Lawrence Berkeley National Laboratory, USA*.

**Short Summary:**

This work describes a novel mass spectrometry titration (MST) technique which can be used to quantify solid-electrolyte interphase species that deposit on electrodes in existing (e.g., lithium-ion battery) and emerging (e.g., electrochemical ammonia synthesis) electrochemical systems.

4:30 PM **Thu-SUSO-1630** Surface Sensitive Measurement Techniques Reveal Copper Hydride Phase Formation during Electrocatalysis.

**Brian Tackett**<sup>1</sup>, David Raciti<sup>2</sup>, Angela Hight-Walker<sup>2</sup> and Thomas Moffat<sup>2</sup>, (1)*Purdue University, USA*, (2)*National Institute of Standards and Technology, USA*.

**Short Summary:**

Electrochemical mass spectroscopy and Raman vibrational spectroscopy are combined to reveal the formation of a surface hydride phase on Cu(111) at potentials negative of 0 V vs RHE in acid electrolytes that decomposes at open circuit potential. The CuH phase could impact understanding of electrocatalytic CO<sub>2</sub> reduction reactions.



4:50 PM **Thu-SUSO-1650** Photocatalytic CO<sub>2</sub> Reduction on Semiconductors: Mechanistic Understanding and Evaluation of Future Potential.

Nikolaos Moustakas<sup>1</sup>, Felix Lorenz<sup>1</sup>, Abdo Hezam<sup>1</sup>, Minoo Tasbihi<sup>2</sup>, Tim Peppel<sup>1</sup>, Reinhard Schomäcker<sup>2</sup> and **Jennifer Strunk**<sup>3</sup>, (1)*Leibniz Institute for Catalysis, Germany*, (2)*Technische Universität Berlin, Germany*, (3)*Leibniz Institute for Catalysis / University of Rostock, Germany*.

**Short Summary:**

Photogenerated holes have a pivotal role in photocatalytic CO<sub>2</sub> reduction on TiO<sub>2</sub>. Splitting of oxidation and reduction reaction is not possible on pure TiO<sub>2</sub>. Our mechanistic insights lead to the conclusion that new Z-scheme and heterojunction composites are needed. Alternatively, photo-reforming of CH<sub>4</sub> with CO<sub>2</sub> is an interesting alternative.

5:10 PM **Thu-SUSO-1710** Electrochemistry with Oxygen: New Design Principles for Reactivity of Next Generation Electrocatalysts.

**Michal Bajdich**<sup>1</sup>, Benjamin Comer<sup>2</sup>, Md Delowar Hossain<sup>1</sup>, Jiang Li<sup>1</sup>, Kirsten T. Winther<sup>1</sup> and Frank Abild-Pedersen<sup>1</sup>, (1)*SLAC National Accelerator Laboratory, USA*, (2)*Stanford University, USA*.

**Short Summary:**

The oxygen electrochemistry necessarily evolves around metal-oxides, since they are the most stable catalysts. Design principles for electrocatalysis of metal-oxides across the periodic table and oxidation states are non-existent. This work provides a first uniform approach to their surface reactivity and is tested on experimental catalysts with a breakthrough performance.

## Trianon Ballroom

### THURSDAY MORNING

#### Fundamentals of Catalysis: Fundamental Mechanisms II

**Session Chairs:** Maura MacTaggart, *Bristol Myers Squibb, USA* and Alyssa Hensley, *Washington State University, USA*.

9:30 AM **Thu-TRBR-0930** Mechanisms of Programmable Catalyst Surfaces.

**Paul J. Dauenhauer**, *University of Minnesota, Twin Cities, USA*.

**Short Summary:**

Temporal perturbation of catalytic materials with charge manipulation allows for continuous modulation of catalytic properties to control rate, selectivity, and extent of conversion. Understanding the fundamental relationships between perturbation methods and programmable catalysis remains the key challenge for designing and optimizing transient catalyst devices and the focus of this paper.

9:50 AM **Thu-TRBR-0950** Structure Sensitivity on Cu(*hkl*) Surfaces Spanning Surface Orientation Space.

**Andrew J. Gellman** and Carlos Fernandez-Caban, *Carnegie Mellon University, USA*.

**Short Summary:**

Surface reaction kinetics have been measured experimentally on spherically curved Cu(*hkl*) samples that expose continuous distributions of surface orientations. In total >500 different Cu(*hkl*) surface orientations have been studied, providing rate constants for the decomposition of tartaric, meso-tartaric, and aspartic acid with unparalleled resolution of surface structure space.

10:10 AM **Thu-TRBR-1010** STM Studies of H<sub>2</sub> Interaction with Inverse ZnO<sub>x</sub>/CuO<sub>x</sub>-Cu(111) Catalysts.

**Vikram Mehar** and Jose A. Rodriguez, *Brookhaven National Laboratory, USA*.

**Short Summary:**

We investigated the reduction of CuO<sub>x</sub> and inverse ZnO/CuO<sub>x</sub>/Cu(111) system towards H<sub>2</sub>. Our results demonstrate that H<sub>2</sub> dissociation is facile on ZnO promoting faster reduction compared to pure CuO<sub>x</sub>. Microscopic studies can thus provide insights into the factors responsible for higher catalytic activity and the role played by the intermediates.

10:30 AM **Thu-TRBR-1030** Real-Time Surface Oxidation of a Fe Single Nanoparticle Observed By Field Ion Microscopy and Operando Atom Probe Tomography.

**Sten Lambeets**<sup>1</sup>, Naseeha Cardwell<sup>2</sup>, Isaac Onyango<sup>2</sup>, Thierry Visart de Bocarmé<sup>3</sup>, Jean-Sabin McEwen<sup>2</sup> and Daniel Perea<sup>1</sup>, (1)*Pacific Northwest National Laboratory, USA*, (2)*Washington State University, USA*, (3)*Université Libre de Bruxelles, Belgium*.

**Short Summary:**

We present the unique capability of the newly developed Operando Atom Probe to explore surface chemistry on complex surfaces mimicking single nanoparticles. OAP is capable to reconstruct a real-time movie of the oxidation map of one Fe nanoparticle and highlight dynamic variations along the different surface structures composing the nanoparticle

10:50 AM **Thu-TRBR-1050** Surface Science Contribution to the Design of Co-Mo-S Hydrotreating Catalysts : Surface-Dependent Activity..

Ricardo Garcia de Castro<sup>1,2</sup>, Elodie Devers<sup>2</sup>, Mathieu Digne<sup>2</sup>, Gerhard Pirngruber<sup>2</sup> and **Xavier Carrier**<sup>1</sup>, (1)*Sorbonne Université, France*, (2)*IFP Energies Nouvelles, France*.

**Short Summary:**

Aqueous-phase preparation of model alumina-supported CoMo catalysts on various  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> surface planes allows one to probe a surface-selective hydrotreating activity. This surface-dependence and a structural analogy between  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> model wafers and  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> industrial supports should help a rational design of new generation alumina supports.

11:10 AM **Thu-TRBR-1110** Kinetic Description of Site Ensembles on Catalytic Surfaces.

**Neil Kanth Razdan** and Aditya Bhan, *University of Minnesota, Twin Cities, USA*.

**Short Summary:**

We demonstrate that the ubiquitously-used Langmuir-Hinshelwood (LH) formalism is incomplete and inappropriate for both simple reactions such as  $A_{(g)} + A_{(g)} \rightarrow A_{2(g)}$  and industrially-relevant reactions such as ammonia synthesis. We derive a higher-order analytical framework that redresses spatial myopia of the LH method and accounts for lateral interactions.

11:30 AM **Thu-TRBR-1130** Dynamics of Brønsted Acidity of PtWOx Inverse Catalysts.

Jiayi Fu<sup>1</sup>, Shizhong Liu<sup>1</sup>, **Weiqing Zheng**<sup>1</sup>, Renjing Huang<sup>1,2</sup>, Cong Wang<sup>1</sup>, Raymond J. Gorte<sup>1,2</sup>, Stavros Caratzoulas<sup>1</sup> and Dionisios G. Vlachos<sup>1</sup>, (1)*University of Delaware, USA*, (2)*University of Pennsylvania, USA*.

**Short Summary:**

Metal-metal oxide (M-MO) catalysts are central to many industrially important reactions. The dynamics of these multifunctional catalysts remains elusive, hindering the rational catalyst design. In this work, we demonstrate a methodology for investigating, understanding, and controlling core-shell M-MO catalysts. A strategy for maintaining a high active site density is presented.

## THURSDAY AFTERNOON

### Imaging of Catalysts I

**Session Chairs:** Matteo Cargnello, *Stanford University, USA* and Thomas J. Schwartz, *University of Maine, USA*.

1:10 PM **Thu-TRBR-1310** Sinter-Resistance and Nanoparticle Accessibility in Raspberry-Colloid-Templated Catalysts Unraveled with Dual-Axis Electron Tomography.

**Jessi E.S. van der Hoeven**<sup>1,2</sup>, Stephan Kraemer<sup>2</sup>, Simone Dussi<sup>2</sup>, Tanya Shirman<sup>2</sup>, Kyoo-Chul Park<sup>3</sup>, Christopher Rycroft<sup>2</sup>, David Bell<sup>2</sup>, Cynthia Friend<sup>2</sup> and Joanna Aizenberg<sup>2</sup>, (1)*Utrecht University, Netherlands*, (2)*Harvard University, USA*, (3)*Northwestern University, USA*.

**Short Summary:**

In this study we employ dual-axis electron tomography and epitaxial overgrowth to unravel the origin of sinter-resistance and nanoparticle accessibility in raspberry colloid templated catalysts. Our quantitative characterization approach contributes to a better understanding of the interplay between metal-support interfaces and nanoparticle stability and activity in heterogeneous catalysis.

1:30 PM **Thu-TRBR-1330** The Limit of Low Dose Electron Microscopy: Measuring Pristine Catalyst Structure One Electron at a Time.

**David Yancey**<sup>1</sup>, Christian Kisielowski<sup>2</sup>, Petra Specht<sup>3</sup>, Alyssa Fielitz<sup>1</sup>, Tom Fielitz<sup>1</sup>, Steve Rozeveld<sup>1</sup>, Joo Kang<sup>1</sup> and David Barton<sup>1</sup>, (1)*The Dow Chemical Company, USA*, (2)*Lawrence Berkeley National Laboratory, USA*, (3)*University of California, Berkeley, USA*.

**Short Summary:**

This work demonstrates the ultimate limit of low-dose TEM where electron diffraction patterns are collected with single electron sensitivity. The methods developed provide a comprehensive framework for measuring pristine structure of beam-sensitive catalyst materials and a model that describes damage trajectories based on lattice heat flow and scattering cross sections.

1:50 PM **Thu-TRBR-1350** Environmental TEM Study of Ni-Mo Bimetallic Catalyst Formation Via Thermal Reduction of Nickel Molybdate Nanorods.

**Stephen House**, Rituja Patil, Aayush Mantri, Judith Yang and James McKone, *University of Pittsburgh, USA*.

**Short Summary:**

Ni-Mo electrocatalysts were examined using *in situ* Environmental TEM – alongside other *in situ* and *ex situ* characterization – to study the compositional and morphological evolution of NiMoO<sub>4</sub> nanorod precursors undergoing thermal reduction in hydrogen. The results provide insight into the formation, microstructural control, and optimization of active Ni-Mo catalysts.

2:10 PM **Thu-TRBR-1410** Challenges in Characterizing Supported Metal Atoms and Clusters.

**Jingyue Liu**, *Arizona State University, USA*.

**Short Summary:**

Characterization of supported metal atoms is critical to understanding the structure-performance relationship of single-atom and atomically dispersed metal catalysts. Challenges and opportunities are discussed.

2:30 PM **Thu-TRBR-1430** In Situ Environmental TEM Observation of Cu/Cu<sub>2</sub>O Interface Modulated Methanol Reaction Dynamics.

**Meng Li**, Judith Yang, Stephen House, Götz Vesper, Wissam Saidi and Matthew Curnan, *University of Pittsburgh, USA*.

**Short Summary:**

How the dynamically formed metal/metal oxide interfaces during redox reactions affect catalytic reactions is unclear. Here we use *in situ* environmental transmission electron microscopy (ETEM) to investigate how Cu<sub>2</sub>O/Cu interface structure impact the Methanol reduction reaction dynamics. We find Cu<sub>2</sub>O/Cu interface structure can modulate the active site of the reaction.

2:50 PM **Thu-TRBR-1450** Artificial Intelligence – Augmented Scanning Electron Microscopy for FCC Catalyst Research.

**Vasileios Komvokis**, Ke-Bin Low, Melissa Mastry, Jian Shi, Bilge Yilmaz, Chansoon Kang and Karl Kharas, *BASF Corporation, USA*.

**Short Summary:**

Application of Artificial Intelligence – Augmented Scanning Electron Microscopy for Fluid catalytic cracking catalyst to study the effect of Iron poisoning by Iron nodules formation on the catalyst and new insights on crystalline boehmite to passivate alumina on FCC catalysts. The AI-augmented SEM approach offers increasing analytical throughput and efficiency.

## Imaging of Catalysts II

**Session Chairs:** Melis Duyar, *University of Surrey, United Kingdom* and Jingyue Liu, *Arizona State University, USA*.

3:30 PM **Thu-TRBR-1530** Nano-Scale Visualization and Analysis of Elemental Relations inside Small, Medium and Large Pore Zeolite Materials Studied with Atom Probe Tomography.

**Sophie H. van Vreeswijk**<sup>1</sup>, Jonathan D. Poplawsky<sup>2</sup> and Bert M. Weckhuysen<sup>1</sup>, (1)*Utrecht University, Netherlands*, (2)*Oak Ridge National Laboratory, USA*.

**Short Summary:**

Small, medium and large pore zeolites are analyzed with atom probe tomography to reveal nano-scale relations between framework elements and coke deposits. The relations and distributions can be visualized and analyzed to contribute to the better understanding of these materials' activation and deactivation mechanisms in, for instance, the MTH process.

3:50 PM **Thu-TRBR-1550** 3D Atomic Structures and Catalytic Activities of Heterogeneous Catalysts By Liquid Phase EM.

Junyoung Heo, Sungin Kim and **Jungwon Park**, *Seoul National University, Korea, Republic of (South)*.

**Short Summary:**

We introduce a new single particle structure analysis method – one-particle Brownian reconstruction based on liquid phase EM – and apply it to analyze the 3D atomic structure of individual Pt nanoparticles, and the coordination numbers and the generalized coordination numbers assigned for individual surface atoms.

4:10 PM **Thu-TRBR-1610** Structure and Growth of Nano-Sized Palladium Species in Small-Pore Zeolite Investigated Via Cryogenic Electron Microscopy.

**Jongbaek Sung**<sup>1,2</sup>, Yongwoo Kim<sup>1</sup>, Sungsu Kang<sup>1,2</sup>, Jaeha Lee<sup>1</sup>, Min-Ho Kang<sup>1,2</sup>, Sungha Hwang<sup>1</sup>, Hayoung Park<sup>1,2</sup>, Joodeok Kim<sup>1,2</sup>, Younhwa Kim<sup>1,2</sup>, Eun Won Lee<sup>1</sup>, Do Heui Kim<sup>1</sup> and Jungwon Park<sup>1,2</sup>, (1)*Seoul National University, Korea, Republic of (South)*, (2)*Institute for Basic Science (IBS), Korea, Republic of (South)*.

**Short Summary:**

Cryogenic electronic microscopy coupled with ultramicrotomy is utilized to investigate the structure and growth mechanism of palladium species in electron-beam-sensitive SSZ-13 zeolite. Direct observation results elucidate that the controlled thermal treatment rationally generates highly dispersed PdO clusters in SSZ-13 with high phase uniformity, active toward CH<sub>4</sub> combustion reaction.

4:30 PM **Thu-TRBR-1630** Visualizing Surface Redox Dynamics in VO<sub>x</sub>/TiO<sub>2</sub> Catalysts.

Martin Ek<sup>1,2</sup>, Logi Arnarson<sup>2</sup>, Poul Georg Moses<sup>2</sup>, Magnus Skoglundh<sup>3</sup>, Eva Olsson<sup>3</sup>, Quentin Ramasse<sup>4</sup>, Søren Birk Rasmussen<sup>2</sup>, **Lars Pilsgaard Hansen**<sup>2</sup> and Stig Helveg<sup>5</sup>, (1)*Lund University, Sweden*, (2)*Haldor Topsøe A/S, Denmark*, (3)*Chalmers University of Technology, Sweden*, (4)*SuperSTEM Laboratory, United Kingdom*, (5)*Technical University of Denmark, Denmark*.

**Short Summary:**

*In situ* studies of VO<sub>x</sub>/TiO<sub>2</sub> catalysts by transmission electron microscopy and spectroscopy reveal facet-dependent surface structures and stoichiometry; {001} facets are superior in retaining V(V) states that offers higher activity in the SCR reaction. Thus, a new approach discloses surface redox dynamics of importance to the understanding of oxide catalysis.

## Gramercy

### FRIDAY MORNING

#### Bi- Inter- and Multi-Metallic Catalysts

**Session Chairs:** Partha Nandi, *Corporate Research, ExxonMobil Research and Engineering, USA* and David Yancey, *The Dow Chemical Company, USA*.

8:00 AM **Fri-GRAM-0800** Learnings about Silica-Supported Bimetallic Noble Metal Catalysts.

**Stuart Soled**, Sal Miseo, Michael Lanci and Chris Kliewer, *ExxonMobil Research and Engineering, USA*.

**Short Summary:**

Studies on supported noble metal catalysts on silica prepared with aqueous solutions with aminoalcohols or aminoacids have been extended to include the six bimetallic phases of Ru, Ir, Pt, and Rh. Details about particle sizes and mixing of the bimetallics are presented along with some hydrogenation results.

8:20 AM **Fri-GRAM-0820** Accelerating Catalytic Materials Discovery for Ammonia Electrooxidation Via Interpretable Deep Learning.

**Hemanth Somarajan Pillai**<sup>1</sup>, Yi Li<sup>2</sup>, Shih-Han Wang<sup>1</sup>, Qingmin Mu<sup>1</sup>, Luke E.K. Achenie<sup>1</sup>, Gang Wu<sup>3</sup> and Hongliang Xin<sup>1</sup>, (1)*Virginia Polytechnic Institute and State University, USA*, (2)*Jiangsu University, China*, (3)*University at Buffalo (SUNY), USA*.

**Short Summary:**

In this Talk, we present an analysis of the thermodynamics and kinetics for the NH<sub>3</sub> oxidation to N<sub>2</sub> on various transition metals from density functional theory (DFT) calculations. Then machine learning is used to screen and find improved electrocatalysts, finally experimental validation and machine learning driven insights are provided.

8:40 AM **Fri-GRAM-0840** Synergistic Effect of Co and Fe Catalysts for Ammonia Decomposition.

**Shilong Chen**<sup>1</sup>, Denise Rein<sup>1,2</sup>, Sharif Najafshirvari<sup>1</sup>, Franz Schmidt<sup>3</sup>, Frank Girgsdies<sup>3</sup>, Anna Rabe<sup>1</sup>, Klaus Friedel Ortega<sup>1</sup>, Thomas Lunkenbein<sup>3</sup> and Malte Behrens<sup>1</sup>, (1)*Christian-Albrechts-Universität zu Kiel, Germany*, (2)*Max Planck Institute for Chemical Energy Conversion, Germany*, (3)*Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany*.

**Short Summary:**

We have successfully fabricated a highly active CoFe-MgO catalyst for NH<sub>3</sub> decomposition by a spinel approach and made first progress in understanding this synergistic effect, which shows the potential of CoFe catalyst in the application for H<sub>2</sub> storage, resulting in a bridge for the use of renewable energies.

9:00 AM **Fri-GRAM-0900** High-Performance Electrocatalytic Nitrate Reduction on Ordered Intermetallic Alloys: Overcoming Linear Scaling Relationships.

**Qiang Gao**, *Virginia Polytechnic Institute and State University, USA*.

**Short Summary:**

Combining interpretable machine learning algorithms with precision synthesis, we successfully synthesized monodisperse ordered intermetallic CuPd nanocubes with a one-step solution-phase protocol, which demonstrated highly efficient nitrate reduction to ammonia performance.

## Hierarchically Engineered Catalysts

**Session Chairs:** Juliana Silva Alves Carneiro, *Georgia Institute of Technology*, and Rong Xing, *Clariant Corporation, USA*.

9:40 AM **Fri-GRAM-0940** Oxidative Dehydrogenation of Propane Via Tandem Catalysis.

Yan Huan, Peter C. Stair and **Justin Notestein**, *Northwestern University, USA*.

**Short Summary:**

A tandem catalyst for selective hydrogen combustion and propane dehydrogenation was designed using atomic layer deposition and showed outstanding performance.

10:00 AM **Fri-GRAM-1000** Designing Multifunctionality within Single Hierarchical Porous Structures for Catalytic Cascade Reactions.

**Christopher Parlett**, *University of Manchester, United Kingdom*.

**Short Summary:**

Cascade reactions are sequential chemical transformations in which the starting substrate undergoes a reaction whose product becomes the substrate for the next step. Here we report catalysts synthesis strategies that direct one-pot cascade processes, for oxidations and biofuel production, via active site location control and compartmentalisation within hierarchical porous architectures.

10:20 AM **Fri-GRAM-1020** Stable and Selective Catalyst/Membrane System for Propane Dehydrogenation at the Thermodynamic Limit and Beyond.

**Rawan Almallahi**<sup>1</sup>, Ali Hussain Motagamwala<sup>1</sup>, James Wortman<sup>1</sup>, Valentina Igenegbai<sup>1</sup> and Suljo Ljicic<sup>2</sup>, (1)*University of Michigan-Ann Arbor, USA*, (2)*University of Michigan, USA*.

**Short Summary:**

A stable and selective Pt<sub>1</sub>Sn<sub>1</sub>/SiO<sub>2</sub> catalyst is developed for propane dehydrogenation (PDH). In a conventional packed-bed reactor, this catalyst can operate at the thermodynamic limits. Coupling this catalyst with a SiO<sub>2</sub>/Al<sub>2</sub>O<sub>3</sub> hollow fiber membrane can yield performance beyond equilibrium limits.

10:40 AM **Fri-GRAM-1040** Hierarchically Multi-Voids Mesoporous Silica Spheres (MVmSiO<sub>2</sub>) As a Highly Efficient Maze-like Support for Thermocatalytic Gas-Phase Reactions.

Mohammadreza Kosari<sup>1,2</sup>, Abdul Majeed Seayad<sup>1</sup>, **Armando Borgna**<sup>1</sup> and Hua Chun Zeng<sup>2</sup>, (1)*Institute of Chemical and Engineering Sciences, A\*STAR, Singapore*, (2)*National University of Singapore, Singapore*.

**Short Summary:**

Through endowing core-shell porosity to Stöber SiO<sub>2</sub> spheres, a novel maze-like reactor systems, with complex hierarchical porosity, were developed. Such maze-like nanoreactors provide 1D channels in the shell and interconnected compartmented voids in core, boosting catalysis performance and improving utilization of metal active phase during CO<sub>2</sub> hydrogenation to methanol.

11:00 AM **Fri-GRAM-1100** Synthesis of Hierarchical Siliceous Zeolites By Post-Synthetic Surfactant Templating.

**Kaivalya Gawande**, William Curtis Conner and Wei Fan, *University of Massachusetts Amherst, USA*.

**Short Summary:**

Surfactant-templating lacks precise control over mesopore created while incorporating hierarchy in microporous zeolites. This study focuses on the fraction of defect-containing Si-atoms in the microporous zeolites and tuning it to control the extent of hierarchy. The phenomenon of healing of defects by post-synthetic templating is discussed as well.

11:20 AM **Fri-GRAM-1120** Hierarchical Zeolites: Effect of Synthetic Strategy on Mesopore Configuration and Aromatics Conversion.

Ke Zhang, **Michael Forte** and Essam Sayed, *Aramco Services Company, USA*.

**Short Summary:**

Microporous zeolites are utilized in numerous industrial catalytic conversions, but often face diffusion limitations which lead to deactivation and poor product yields. We will discuss different methods of generating hierarchical zeolites and highlight our approach to creating mesoporous beta zeolites for the upgrading of pyrolysis oil to BTEX aromatics.

11:40 AM **Fri-GRAM-1140** Tunable Brønsted Acidity in SiO<sub>2</sub> overcoated Oxides.

**Andrew Wolek**, Kenton Hicks and Justin Notestein, *Northwestern University, USA*.

**Short Summary:**

Catalytically active Brønsted acid sites were generated by depositing SiO<sub>2</sub> domains onto Lewis acidic metal oxides. The strength and density of the generated Brønsted sites was controlled synthetically by adjusting the SiO<sub>2</sub> loading and underlying metal oxide identity. The catalytic performance of materials was evaluated in liquid-phase hydroalkoxylation reactions.

## Mercury Ballroom

### New Tools and Surface Science II

**Session Chairs:** Fanglin Che, *University of Massachusetts Lowell, USA* and Jean-Sabin McEwen, *Washington State University, USA*.

8:00 AM **Fri-MEBR-0800** Influence of an Electrified Interface on the Entropy and Energy of Solvation of Methanol Oxidation Intermediates on Platinum(111) Under Explicit Solvation.

**Ali Estejab**, Ricardo García Cárcamo and Rachel Getman, *Clemson University, USA*.

**Short Summary:**

We computed the energies and entropies of solvation for CH<sub>3</sub>OH, COH, and CO in the pathway of methanol oxidation, with applied electric field. We found that both the energy and entropy of solvation depend on the strength and direction of the field, with the entropy of solvation being significantly impacted.

8:20 AM **Fri-MEBR-0820** In Situ (electron)-Spectroscopy/Microscopy Characterization of Solid-Liquid Electrified Interfaces during Electrocatalytic Reactions, One Example: The CO<sub>2</sub>RR on Copper Electrodes.

**Juan Velasco Vélez**, *Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany*.

**Short Summary:**

These results highlight the importance of the *in situ/operando* characterization to describe the active species during reaction conditions, which cannot be quenched by *ex situ* analysis. These results provide fundamental understanding of the CO<sub>2</sub>RR on copper electrodes by means of in situ photoelectron spectroscopy and electron microscopy.

8:40 AM **Fri-MEBR-0840** Energy-Efficient CO<sub>2</sub> Reduction with Organic Photoredox Catalysts.

**Kareesa Kron**, Jonathan Ryan Hunt, Jahan Dawlaty and Shaama Mallikarjun Sharada, *University of Southern California, USA*.

**Short Summary:**

Organic photoredox catalysts perform energy-efficient, single-electron reductions of CO<sub>2</sub> but are under-studied mechanistically. By exploring underlying electronic and structural properties of these catalysts, we identify partial and complete charge-transfer states along the catalytic reduction of CO<sub>2</sub>. These key electronic states will aid identification of design parameters for improved, organic catalysts.

9:00 AM **Fri-MEBR-0900** A Theoretical Prediction of High-Spin Based Single Atom Electrocatalysts.

**Md Delowar Hossain**<sup>1,2</sup>, David Koshy<sup>1,2</sup>, Frank Abild-Pedersen<sup>2</sup>, Thomas F. Jaramillo<sup>1,2</sup> and Michal Bajdich<sup>1,2</sup>, (1)*Stanford University, USA*, (2)*SLAC National Accelerator Laboratory, USA*.

**Short Summary:**

Our study shows high spin always highly stable in SACs due to the broken square planar symmetry of MN<sub>4</sub> plane either tetrahedral distortion (D<sub>2d</sub> symmetry), or square-pyramidal distortion (C<sub>4v</sub> symmetry). Finally, our calculated isotropic hyperfine coupling constants for tetrahedrally distorted NiN<sub>4</sub> shows similar results with experimentally measured value.

## Electrocatalytic Activation of Water and Oxygen

**Session Chairs:** Ashley Head, *Brookhaven National Laboratory, USA* and G. T. Kasun Kalhara Gunasooriya, *Technical University of Denmark, Denmark*.

9:40 AM **KEYNOTE Fri-MEBR-0940 Dynamic Surface Reconstruction Unifies the Electrocatalytic Oxygen Evolution Performance of Non-Stoichiometric Mixed Metal Oxides.** Samji Samira<sup>1</sup>, Jiyun Hong<sup>2</sup>, John Carl Camayang<sup>1</sup>, Simon Bare<sup>2</sup> and Eranda Nikolla<sup>1</sup>, (1)*Wayne State University, USA*, (2)*SLAC National Accelerator Laboratory, USA*.

**Short Summary:**

This work provides an understanding of the surface dynamics of mixed metal oxides under electrochemical conditions and paves the way for identification of effective design criteria for describing their OER performance. It also demonstrates the use of these oxides as effective platforms for *in-situ* generation of catalytically active/stable surfaces.

10:20 AM **Fri-MEBR-1020** Engineered Bimetallic CuNi Nanoalloys As Model Sites for the Electrocatalytic Oxygen Evolution Reaction.

**Esteban Gioria**<sup>1,2</sup>, Shuang Li<sup>2</sup>, Raoul Naumann d'Alnoncourt<sup>1</sup>, Frank Rosowski<sup>2,3</sup> and Arne Thomas<sup>2</sup>, (1)*BasCat – UniCat BASF JointLab: Technische Universität Berlin, Germany*, (2)*Technische Universität Berlin, Germany*, (3)*BASF SE, Germany*.

**Short Summary:**

Engineered CuNi alloy nanoparticles of well-defined size, shape and composition were employed as model catalysts for the Oxygen Evolution Reaction. Synergistic effects related to modifications in the geometrical and electronic properties enhance the formation of highly active NiOOH species. Cu<sub>50</sub>Ni<sub>50</sub>NP showed the lowest overpotential, lower Tafel slope and excellent stability.



10:40 AM **Fri-MEBR-1040** Leveraging Bipolar Membrane-Enabled Ion Transport Control Toward Undersea O<sub>2</sub> Production Via Water Electrolysis.  
**Adam Nielander**<sup>1</sup>, Daniela Marin<sup>2</sup>, Joseph Perryman<sup>2</sup>, McKenzie Hubert<sup>2</sup> and Thomas F. Jaramillo<sup>1</sup>, (1)SLAC National Accelerator Laboratory, USA, (2)Stanford University, USA.

**Short Summary:**

We evaluated the performance of BPM/PEM electrolyzers for water electrolysis performance with seawater and seawater-like catholytes. The BPM demonstrated significantly improved performance with respect to limiting Cl<sup>-</sup> crossover and inhibiting Cl<sup>-</sup> oxidation with respect to the PEM electrolyzer, suggesting a role for BPMs in seawater electrolysis for O<sub>2</sub> production.

11:00 AM **Fri-MEBR-1100** Phase Discovery and Photoactivity within Ni-Sb-O System for Oxygen Evolution Reaction Catalysis.

**Karun Rao**<sup>1,2</sup>, Lan Zhou<sup>3</sup>, Matthias Richter<sup>3</sup>, John Gregoire<sup>3</sup> and Michal Bajdich<sup>2</sup>, (1)Stanford University, USA, (2)SLAC National Accelerator Laboratory, USA, (3)California Institute of Technology, USA.

**Short Summary:**

We fully explore a new Ni-Sb-O phase space for photoactive oxygen evolution reaction catalysts by combining experimental characterization (XRD, TEM, XAS) and theoretical (density functional theory) calculations. We identify new phases and quantify the role of vacancies in the operational durability, catalytic activity, and light harvesting properties for these materials.

11:20 AM **Fri-MEBR-1120** Is There Anything Better Than Pt for HER?.

**Karl Toudahl** and Jakob Kibsgaard, *Technical University of Denmark, Denmark.*

**Short Summary:**

Novel hydrogen evolution reaction catalysts are frequently reported in the literature while not considering applied catalyst loading, intrinsic activities, or possible mass-transport limitations. This work studies the influence of mass transport on the intrinsic Pt HER activity in acid with RDE measurements and report benchmark values of the specific activities.

11:40 AM **Fri-MEBR-1140** Interplay between S, and Se in S-Doped FeSe<sub>2</sub> Nanospheres Improves Kinetics for Oxygen Evolution Reaction.

**Bezawit Desalegn** and Jeong Gil Seo, *Hanyang University, Korea, Republic of (South).*

**Short Summary:**

S-FeSe<sub>2</sub> nanospheres were synthesized via a one-pot solvothermal route and utilized as OER electrocatalyst with an overpotential of 212 mV at 10 mA cm<sup>-2</sup>, outperforming previously reported monometallic anion doped chalcogenides. The presence of task specific components with optimized catalyst-intermediate interaction is believed to be the origin of enhanced performance.

## Murray Hill

### Mechanistic Modelling to Control C1 Selectivity

**Session Chairs:** Hao Luo, *ADM*, and Lei Zhang, *ExxonMobil*, .

8:00 AM **Fri-MHL-0800** Selective Methane Oxidation to Methanol on ZnO/Cu<sub>2</sub>O/Cu(111) Catalysts: Multiple Site-Dependent Behaviors.

**Erwei Huang**<sup>1</sup>, Ivan Orozco<sup>1</sup>, Sanjaya Senanayake<sup>2</sup>, Jose A. Rodriguez<sup>2</sup> and Ping Liu<sup>2</sup>, (1)Stony Brook University, USA, (2)Brookhaven National Laboratory, USA.

**Short Summary:**

An efficient catalyst, ZnO/Cu<sub>2</sub>O/Cu(111) with coarse surface, has been reported for achieving a direct methane to methanol conversion through different sites, in which step-rich ZnO sites could transform methane and oxygen to methanol while O-rich ZnO sites dominated the transformation of methane, oxygen and water to methanol.

8:20 AM **Fri-MHL-0820** Effect of Adsorption Potentials in Methane Electro-Oxidation.

**Hsiang-Sheng Chen**, Christine Lucky and Marcel Schreier, *University of Wisconsin-Madison, USA.*

**Short Summary:**

Varying the potential for methane electrosorption serves as a handle to modify the nature of intermediates. This reflects in the change in the overpotential for methane electro-oxidation, which shifts up to 150 mV when modifying the adsorption potentials from 0.05 V to 0.5 V (RHE).

8:40 AM **Fri-MHL-0840** Catalysis on Crowded Surfaces: Formic Acid Decomposition Pathways on Transition Metals.

**Stephanie Kwon**<sup>1</sup>, Ting Lin<sup>2</sup>, Unai De La Torre Larrañaga<sup>3</sup> and Enrique Iglesia<sup>2</sup>, (1)Colorado School of Mines, USA, (2)University of California, Berkeley, USA, (3)University of the Basque Country, Spain.

**Short Summary:**

This work combines kinetic, isotopic, spectroscopic, and transient experiments with DFT calculations to show how HCOOH adsorbed at interstitial sites within the \*HCOO\* adlayer can facilitate the decomposition of vicinal \*HCOO\* by stabilizing the C-H activation TS more so that it stabilizes the \*HCOO\* precursor.

9:00 AM **Fri-MHL-0900** Mechanistic Details of Formic Acid Decomposition on Pt Nanoparticles.

**Unai De La Torre Larrañaga**<sup>1,2</sup>, Stephanie Kwon<sup>3</sup> and Enrique Iglesia<sup>1</sup>, (1)University of California, Berkeley, USA, (2)University of the Basque Country, Spain, (3)Colorado School of Mines, USA.

**Short Summary:**

This work combines experimental and theoretical results to show how HCOOH dehydrogenation can proceed on Pt surfaces nearly saturated with CO\* at all conditions, where competitive adsorption of HCOOH and CO becomes feasible, but only at high CO\* coverages as the CO\* adlayer repels CO more so than HCOOH.

## Methane Oxidation to Chemicals

**Session Chairs:** Zili Wu, *Oak Ridge National Laboratory, USA* and Lei Zhang, *ExxonMobil, .*

9:40 AM **Fri-MHL-0940** Favoring the Methane Oxychlorination Reaction over EuOCl By Synergistic Effects with Lanthanum.

**Bas Terlingen**<sup>1</sup>, Ramon Oord<sup>1</sup>, Mathieu Ahr<sup>2</sup>, Eline Hutter<sup>1</sup>, Coert van Lare<sup>2</sup> and Bert M. Weckhuysen<sup>1</sup>, (1)*Utrecht University, Netherlands*, (2)*Nobian, Netherlands*.

**Short Summary:**

The partial replacement of Eu<sup>3+</sup> by La<sup>3+</sup> in EuOCl resulted in a synergistic effect that enhanced the catalytic performance in the methane oxychlorination reaction. *Operando* luminescence spectroscopy revealed that transport of chlorides from the La<sup>3+</sup>-rich phase to the active EuOCl takes place, facilitating the difficult EuOCl chlorination step.

10:00 AM **Fri-MHL-1000** Pd-Au/CeO<sub>2</sub> Catalyzed Coupling of Methane and Ethylene to Produce C<sub>3</sub> Oxygenates and Alkene at Relatively Low Temperature.

**A.K.M. Kazi Aurnob**, Kunlun Ding and James J. Spivey, *Louisiana State University, USA*.

**Short Summary:**

Our work focuses on the conversion of CH<sub>4</sub>, CO<sub>2</sub>, C<sub>2</sub>H<sub>4</sub>, and O<sub>2</sub> to C<sub>3</sub> oxygenates/alkene at a relatively low temperature using Pd-Au/CeO<sub>2</sub> catalyst. Propene, acetone, acetaldehyde and methyl acetate were produced from the reactions. These were not observed in the blank or CeO<sub>2</sub>-only runs, except for trace amounts of acetaldehyde.

10:20 AM **Fri-MHL-1020** Unlocking Synthesis-Structure-Activity Relationships in Cu-Mordenite for the Selective Oxidation of Methane.

**Sebastian Proding**<sup>1</sup>, Karoline Kvande<sup>1</sup>, Elisa Borfecchia<sup>2</sup>, Bjørnar Arstad<sup>3</sup>, Pablo Beato<sup>4</sup> and Stian Svelle<sup>1</sup>, (1)*University of Oslo, Norway*, (2)*University of Turin, Italy*, (3)*SINTEF, Norway*, (4)*Haldor Topsøe A/S, Denmark*.

**Short Summary:**

This contribution adds to the quest of understanding and designing selective oxidation materials for the activation of CH<sub>4</sub> by highlighting the importance of the zeolite support structure. By altering the Al distribution in MOR, the MeOH productivity can be positively influenced.

10:40 AM **Fri-MHL-1040** Spectroscopic Identification of a Highly Reactive [Cu-O-Cu]<sub>2</sub><sup>+</sup> Site in Cu-CHA for Partial Oxidation of Methane to Methanol.

**Dieter Plessers**<sup>1</sup>, Hannah M. Rhoda<sup>2</sup>, Alexander J. Heyer<sup>2</sup>, Max L. Bols<sup>1</sup>, Robert A. Schoonheydt<sup>1</sup>, Edward I. Solomon<sup>2</sup> and Bert F. Sels<sup>1</sup>, (1)*KU Leuven, Belgium*, (2)*Stanford University, USA*.

**Short Summary:**

The active site for partial methane oxidation on Cu-CHA zeolites was identified as a [Cu-O-Cu]<sub>2</sub><sup>+</sup> species by combining an improved activation procedure and a rigorous spectroscopic analysis (DR-UV-Vis, resonance Raman, <sup>18</sup>O shifts, kinetics). DFT models relate its exceptionally high experimental reactivity to its geometric structure imposed by zeolite lattice constraints.

11:00 AM **Fri-MHL-1100** Cu-Exchanged SSZ-13 in the Conversion of Methane to Methanol.

**Florian Göttl**<sup>1</sup>, Saurabh Bhandari<sup>2</sup>, Edgard Lebron Rodriguez<sup>2</sup>, Jake I. Gold<sup>2</sup>, Stacey I. Zones<sup>3</sup>, Ive Hermans<sup>4</sup>, James Dumesic<sup>2</sup> and Manos Mavrikakis<sup>2</sup>, (1)*The University of Arizona, USA*, (2)*University of Wisconsin-Madison, USA*, (3)*Chevron Energy Technology Company, USA*, (4)*University of Wisconsin-Madison, USA*.

**Short Summary:**

In this contribution we study the conversion of methane to methanol over Cu-exchanged SSZ-13. We use theoretically calculated phase diagrams to identify most stable Cu sites in the material, confirm their presence after activation in O<sub>2</sub> using various spectroscopic techniques, and study methane to methanol conversion over different sites.

11:20 AM **Fri-MHL-1120** Catalytic Partial Methane Oxidation to Produce Methanol.

**Jiajie Huo**<sup>1</sup>, Salai Cheettu Ammal<sup>2</sup>, Geoffrey McCool<sup>3</sup>, Barr Zulevi<sup>3</sup>, Andreas Heyden<sup>2</sup> and J. Will Medlin<sup>4</sup>, (1)*University of Colorado Boulder, USA*, (2)*University of South Carolina, USA*, (3)*Pajarito Powder, USA*, (4)*University of Colorado at Boulder, USA*.

**Short Summary:**

Direct methane partial oxidation to methanol was achieved with good activity, selectivity and stability using a Rh-doped graphene supported on Ni catalyst guided by DFT calculations. This will help to better understand alkane activation and potentially lead to further industrial applications.

11:40 AM **Fri-MHL-1140** Novel Method for Electrochemically Initiated MSA Production.

**Joel Britschgi** and Ferdi Schüth, *Max-Planck-Institut für Kohlenforschung, Germany*.

**Short Summary:**

A method to produce methanesulfonic acid from methane and oleum in an electrochemical high-pressure autoclave was developed. This is possible by anodic formation of a species that initiates a catalytic cycle. Different parameters of the system were studied in detail. Under optimized conditions a concentration of almost 2M was obtained.

## Rhineland Gallery

### NO<sub>x</sub> Abatement

**Session Chairs:** Marco J. Castaldi, *City College of New York, CUNY, USA* and Do Heui Kim, *Seoul National University, Korea, Republic of (South)*.

8:00 AM **Fri-RHLG-0800** Activity of Municipal Solid Waste Incineration Ash for the Reduction and Adsorption of NO<sub>x</sub>.

**Kaitlyn Lawrence** and Marco J. Castaldi, *City College of New York, CUNY, USA*.

**Short Summary:**

Ash residual derived from incineration of municipal solid waste was investigated as a catalyst in NO<sub>x</sub> reduction. Ash of particle sizes ranging from 75-125 μm to 250 μm was exposed to simulated combustion flue gas at 250 °C - 550°C to determine the kinetics of NO and NO<sub>2</sub> reduction reactions.

8:20 AM **Fri-RHLG-0820** Low-Temperature Activation of O<sub>2</sub> over Ammonia-Solvated Copper in Zeolite-Based SCR Catalysts.

**Magnus Skoglundh**<sup>1</sup>, Xueting Wang<sup>1</sup>, Lin Chen<sup>1</sup>, Peter N.R. Vennestrøm<sup>2</sup>, Ton V.W. Janssens<sup>2</sup>, Jonas Jansson<sup>3</sup> and Henrik Grönbeck<sup>1</sup>, (1)*Chalmers University of Technology, Sweden*, (2)*Umicore Denmark ApS, Denmark*, (3)*Volvo Group Trucks Technology, Sweden*.

**Short Summary:**

The adsorption of O<sub>2</sub> over CHA with mobile Cu(NH<sub>3</sub>)<sub>2</sub><sup>+</sup> complexes or framework-bound Cu<sup>+</sup> is directly measured using microcalorimetry combined with mass spectrometry. At low temperatures, the O<sub>2</sub> adsorption is found to be more facile over Cu(NH<sub>3</sub>)<sub>2</sub><sup>+</sup> than on framework-bound Cu<sup>+</sup>, which contributes to the understanding on low-temperature active SCR catalysts.

8:40 AM **Fri-RHLG-0840** Topological Effect of Zeolites on the Formation of Cu Active Sites for NH<sub>3</sub>-SCR.

**Yusuke Ohata**, Takeshi Ohnishi and Masaru Ogura, *The University of Tokyo, Japan*.

**Short Summary:**

In this work, the "cation density in micropores" of zeolites was defined to compare the catalytic activities among Cu-zeolites with different topologies. It was revealed that \*BEA zeolites exhibited extremely high turnover frequencies at a low Cu density in micropores generated by high reoxidation rate of Cu ion.

9:00 AM **Fri-RHLG-0900** The Operating Cycle of NO Adsorption and Desorption in Pd-Chabazite for Passive NO<sub>x</sub> Adsorbers.

Marvi Kaushik<sup>1</sup>, Tuhin S. Khan<sup>2</sup>, **M. Ali Haider**<sup>1</sup> and Divesh Bhatia<sup>1</sup>, (1)*Indian Institute of Technology Delhi, India*, (2)*CSIR-Indian Institute of Petroleum, India*.

**Short Summary:**

DFT simulations are invoked to envisage a NO<sub>x</sub> adsorption-desorption cycle in Pd/CHA, which is facilitated by the availability of Pd<sup>1+</sup> as an excellent binding site for NO and its transformation into Pd<sup>0</sup> sites with reduced binding strength. Water obstructs the operating cycle by inhibiting the transformation of Pd<sup>1+</sup> to Pd<sup>0</sup>.

### Catalytic Oxidation III

**Session Chairs:** Sara Colussi, *University of Udine, Italy* and Olaf Deutschmann, *Karlsruhe Institute of Technology (KIT), Germany*.

9:40 AM **Fri-RHLG-0940** Methane Oxidation Enhancement in Water Presence: Stabilizing Role of Praseodymium in Ceria-Supported Palladium Nanocatalysts.

**Sabrina Ballauri**<sup>1</sup>, Enrico Sartoretti<sup>1</sup>, Min Hu<sup>2</sup>, Carmine D'Agostino<sup>2</sup>, Zijuan Ge<sup>3</sup>, Liang Wu<sup>3</sup>, Chiara Novara<sup>1</sup>, Fabrizio Giorgis<sup>1</sup>, Marco Piumetti<sup>1</sup>, Debora Fino<sup>1</sup>, Nunzio Russo<sup>1</sup> and Samir Bensaid<sup>1</sup>, (1)*Politecnico di Torino, Italy*, (2)*University of Manchester, United Kingdom*, (3)*University of Science and Technology of China, China*.

**Short Summary:**

This work provides a comprehensive characterization of novel Pd/Ce-Pr catalysts and the investigation of their performance in the methane oxidation reaction. It is based on the study of the palladium-support interactions as well as on the different affinity of these materials for water.

10:00 AM **Fri-RHLG-1000** Novel Copper-Cerium Oxides Catalysts Synthesized By Multi-Inlet Vortex Reactor for the CO and Ethene Oxidation Reactions.

**Melodj Dosa**, Miguel Marin Figueredo, Enrico Sartoretti, Chiara Novara, Fabrizio Giorgis, Samir Bensaid, Debora Fino, Marco Piumetti and Nunzio Russo, *Politecnico di Torino, Italy*.

**Short Summary:**

Copper-cerium mixed oxides with different compositions were synthesized in a multi-inlet vortex reactor and characterized by complementary techniques, in order to investigate their physico-chemical properties. These nano-catalysts exhibit high activity for the CO and ethene total oxidation reactions, thanks to synergistic interactions between CeO<sub>2</sub> and CuO phases.

10:20 AM **Fri-RHLG-1020** Improved Thermal Stability of La<sub>2</sub>O<sub>3</sub> Doped on Cu/CZ for Low Temperature CO Oxidation.

**Dongwon Lee**<sup>1</sup> and Iljeong Heo<sup>2</sup>, (1)*University of Science and Technology, Korea, Republic of (South)*, (2)*Korea Research Institute of Chemical Technology, Korea, Republic of (South)*.

**Short Summary:**

While Cu/CZ is known as a catalyst for low temperature CO oxidation, low thermal stability have been considered issues to be overcome. In order to enhance catalytic stability, La<sub>2</sub>O<sub>3</sub> was doped on Cu/CZ, which significantly improved the activity after aging.

10:40 AM **Fri-RHLG-1040** Experimental Study of Low-Temperature CO Oxidation over Rh/Al<sub>2</sub>O<sub>3</sub> in a Stagnation-Flow Reactor.

**Nawaf M. Alghamdi**<sup>1</sup>, Ribhu Gautam<sup>1</sup>, Jorge Gascon<sup>1</sup>, Dionisios G. Vlachos<sup>2</sup> and S. Mani Sarathy<sup>1</sup>, (1)King Abdullah University of Science and Technology (KAUST), Saudi Arabia, (2)University of Delaware, USA.

**Short Summary:**

We investigated CO oxidation on Rh/Al<sub>2</sub>O<sub>3</sub> at 175 - 275 °C with different inlet concentrations and flowrates and in the absence and presence of H<sub>2</sub>O. The reactor setup is a stagnation-flow reactor, which allows to simulate the system as a one-dimensional reacting flow.

11:00 AM **Fri-RHLG-1100** Catalytic Total Oxidation of Methane – Towards a Better Understanding of the Water Inhibition Effect and the Influence of the Support Material.

**Kevin Keller**, Patrick Lott, Olaf Deutschmann, Jan-Dierk Grunwaldt and Maria Casapu, Karlsruhe Institute of Technology (KIT), Germany.

**Short Summary:**

A detailed reaction mechanism for the inhibition effect of water for the catalytic CH<sub>4</sub>-oxidation over PdO/Al<sub>2</sub>O<sub>3</sub> by loss of active sites is presented. Variations of the catalyst formulation provided further insight into the fundamental noble-metal support interactions and the impact of the support material on the water inhibition effect.

11:20 AM **Fri-RHLG-1120** Engineering Catalyst Supports to Anchor Pt Clusters with High Thermal Stability for Hydrocarbon Oxidation.

**Weixin Huang**<sup>1</sup>, Yixiao Li<sup>1</sup> and Yong Wang<sup>2</sup>, (1)Washington State University, USA, (2)Pacific Northwest National Laboratory, USA.

**Short Summary:**

Modifying the catalyst support with a transition metal could help stabilize metal clusters/nanoparticles for high temperature catalytic applications. Here we report a strategy to anchor Pt clusters on ceria support by coupling Mn doping. The Pt/Mn@CeO<sub>2</sub> catalyst showed the enhanced catalytic activity as compared to Pt/CeO<sub>2</sub>.

## Rendezvous Trianon

### Alkane Dehydrogenation II

**Session Chairs:** Eric Stangland, *The Dow Chemical Company, USA* and Wynter E. G. Osminski, *Evonik, USA*.

8:00 AM **Fri-RZVS-0800** Nanostructured Carbon Anode with Highly Active Iron Catalysts for Ethylene and Electricity Co-Production in Protonic Ceramic Electrochemical Cells.

Min Wang<sup>1,2</sup>, **Lucun Wang**<sup>2</sup>, Wei Wu<sup>2</sup>, Yingchao Yang<sup>2</sup> and Dong Ding<sup>2</sup>, (1)University of Maine, USA, (2)Idaho National Laboratory, USA.

**Short Summary:**

We demonstrate the co-production of ethylene and electricity in an ethane fueled proton conducting electrochemical cell with a new class of non-perovskite anode materials, carbon nanotube forests containing highly dispersed iron carbide nanoparticle electrocatalyst. The novel PCEC shows superior catalytic and electrochemical performances to that using conventional perovskite-based anodes.

8:20 AM **Fri-RZVS-0820** Ethane Non-Oxidative Dehydrogenation over Co/SiO<sub>2</sub> —Effects of Pretreatment and Regeneration.

**Kewei Yu**, Sanjana Srinivas, Weiqi Chen, Cong Wang, Weiqing Zheng and Dionisios G. Vlachos, *University of Delaware, USA*.

**Short Summary:**

We synthesize Co/SiO<sub>2</sub> for ethane dehydrogenation reaction and a high temperature pretreatment method was found to increase the initial activity of the catalyst up to 4 times. Spectroscopic characterizations using FTIR, XAS, and XPS were conducted to investigate the structure-function correlations. Catalyst deactivation and regeneration methods are also investigated.

8:40 AM **Fri-RZVS-0840** Ga+-Chabazite Zeolite: A Highly Selective Catalyst for Non-Oxidative Propane Dehydrogenation.

**Yong Yuan** and Raul F. Lobo, *University of Delaware, USA*.

**Short Summary:**

Ga-CHA catalysts have been identified, for the first time, as an effective catalyst for propane dehydrogenation with high propylene selectivity (96%). The active site of Ga-CHA is determined to be isolated extra-framework Ga<sup>+</sup> cations. Rates decrease over time due to the formation of polycyclic aromatics in the zeolite pores.

9:00 AM **Fri-RZVS-0900** Cobalt Phosphide Nanoparticles As Highly Selective and Stable Ethane Dehydrogenation Catalysts.

**Jessica A. Muhlenkamp**, Yoonrae Cho and Jason C. Hicks, *University of Notre Dame, USA*.

**Short Summary:**

This contribution highlights our work investigating Co-P as noble metal free catalysts for ethane dehydrogenation. Co-P shows improved dehydrogenation performance over Co alone due to geometric and electronic effects of P incorporation. Additionally, Co-P shows remarkable high temperature stability, demonstrating the promise these materials have as high temperature dehydrogenation catalysts.

## Hydroprocessing

**Session Chairs:** Victor J. Sussman, *The Dow Chemical Company, USA* and Zhenwei Wu, *Shell, USA*.

9:40 AM **Fri-RZVS-0940** Nanoscale Control of the Nickel Promoting Interaction with WS<sub>2</sub>/Al<sub>2</sub>O<sub>3</sub> Using Designed Ni-Containing Keggin Polyoxotungstates – a Rationale Approach for Synthesizing HDS Catalysts.

Acela Lopez-Benitez<sup>1</sup>, Alfredo Guevara-Lara<sup>1</sup> and Gilles Berhault<sup>2</sup>, (1)*Universidad Autonoma del Estado de Hidalgo, Mexico*, (2)*Université de Lyon, CNRS, France*.

**Short Summary:**

A rationalized approach correlating localized configuration of nickel inside polyoxotungstate precursors and the final hydrodesulfurization properties of resulting NiW/Al<sub>2</sub>O<sub>3</sub> catalysts has herein been achieved offering new possibilities to use polyoxometalates for a variety of catalytic applications.

10:00 AM **Fri-RZVS-1000** A Systematic Analysis of the Promotion of Hydrodesulfurization By Aromatics, Nitrogen Heterocycles, and Olefins.

Edgar M. Morales-Valencia, Omar Vargas, Nicolás Vega, Cristian Ardila and Victor Baldovino Medrano, *Centro de Investigaciones en Catálisis (CICAT), Colombia*.

**Short Summary:**

The competitive adsorption of aromatics and nitrogen heterocycles on the active sites typically causes inhibitory effects during the hydrodesulfurization. Contrary to this typical behavior, we report herein that it is possible to promote the scission of the C-S bond of dibenzothiophene by co-feeding the above compounds during hydropurification over NiMoS<sub>2</sub>/Al<sub>2</sub>O<sub>3</sub>.

10:20 AM **Fri-RZVS-1020** Understanding the Effects of Organic Nitrogen Types on Hydrodearomatization Reactions over Commercial NiMo Catalysts: A Transient Study.

Jacob Venuti Bjorkman<sup>1,2</sup>, Sarah Hruby<sup>2</sup>, Efthymios Kantarelis<sup>1</sup> and Lars Pettersson<sup>1</sup>, (1)*KTH Royal Institute of Technology, Sweden*, (2)*Nynas AB, Sweden*.

**Short Summary:**

The inhibition by acridine and carbazole on the hydrogenation of phenanthrene over a commercial NiMo catalyst was studied in a trickle bed reactor using step changes. Acridine is a much more severe inhibitor compared to carbazole. From co-feeding experiments, acridine is the main inhibitor for PAH hydrogenation and adsorbs strongly.

10:40 AM **Fri-RZVS-1040** Detailed Mechanistic Studies of Hydroprocessing Catalysts on Real Feeds for Ultra Low Sulfur Diesel (ULSD) Production.

Yi Du<sup>1</sup>, Bradley Wooler<sup>2</sup> and David Lebron<sup>1</sup>, (1)*ExxonMobil Research and Engineering, USA*, (2)*ExxonMobil, USA*.

**Short Summary:**

We developed a detailed mechanistic model to decouple a few key kinetic components (rate/order with respect to organosulfur species and H<sub>2</sub> partial pressure) using real feed at high conversion (90%+) for ultra-low sulfur diesel (ULSD) production.

11:00 AM **Fri-RZVS-1100** Investigation of SAM Location and Ordering for Ligand-Modified Hydrodeoxygenation Catalysts.

Zachary Blanchette<sup>1</sup>, Daniel K. Schwartz<sup>1</sup> and J. Will Medlin<sup>2</sup>, (1)*University of Colorado, USA*, (2)*University of Colorado at Boulder, USA*.

**Short Summary:**

The location and ordering of thiol and phosphonic acid SAMs on Pd/Al<sub>2</sub>O<sub>3</sub> and Pt/Al<sub>2</sub>O<sub>3</sub> catalysts was systematically investigated. Pd/Al<sub>2</sub>O<sub>3</sub> catalysts synthesized using “SAM-first” deposition showed large increases in activity in terms of normalized rate of production for benzyl alcohol hydrodeoxygenation due to reduced site-blocking compared to “metal-first” catalysts.

11:20 AM **Fri-RZVS-1120** Mechanochemical Prepared Bimetallic Catalysts for Selective Hydrogenation of High Concentrated Acetylene.

Klara S. Kley, Ferdi Schüth and Jacopo De Bellis, *Max-Planck-Institut für Kohlenforschung, Germany*.

**Short Summary:**

Utilizing natural gas for ethylene production by conversion to acetylene in a plasma assisted pyrolysis reactor requires selective hydrogenation of high concentrated acetylene streams. This is achieved with mechanochemical prepared bimetallic catalysts supported on  $\alpha$ -Al<sub>2</sub>O<sub>3</sub>. The synthesis method proofed to yield catalysts with a high stability compared to impregnated materials.

11:40 AM **Fri-RZVS-1140** Surface Modified CaMnO<sub>3</sub> As Effective Redox Catalysts for Selective Hydrogen Combustion in the Context of Redox Catalytic Cracking.

Yuan Tian<sup>1</sup>, Fang Hao<sup>2</sup>, Yunfei Gao<sup>1</sup>, Ryan Dudek<sup>1</sup>, Phillip Westmoreland<sup>1</sup> and Fanxing Li<sup>1</sup>, (1)*North Carolina State University, USA*, (2)*Xiangtan University, China*.

**Short Summary:**

We reported multi-functional ZSM-5/CaMn<sub>0.75</sub>Fe<sub>0.25</sub>O<sub>3</sub>@Na<sub>2</sub>WO<sub>4</sub> core-shell redox catalysts for redox oxidative cracking of cyclohexane with enhanced olefin yield up to 71%, tunable propylene/ethylene ratio up to 1.8, and low CO<sub>x</sub> selectivity (~4%) between 500 and 650 °C. The kinetics parameters and models in the context of selective hydrogen combustion were developed.

## Sutton North

### Biomass to Chemicals IV: Technologies

**Session Chairs:** Hai-Ying Chen, *Oak Ridge National Laboratory, USA* and Udayshankar Singh, *W.R. Grace & Co.- Conn., USA*.

8:00 AM **Fri-SUNO-0800** Cellulose Upgrading Using ZnCl<sub>2</sub> Molten Salt and Solid Acid Oxides.

Elise Albuquerque<sup>1</sup>, Mateus Paiva<sup>1</sup>, Priscilla de Souza<sup>1</sup>, Robert Wojcieszak<sup>1</sup> and Fábio Noronha<sup>1,2</sup>, (1)*Université de Lille, CNRS, Centrale Lille, France*, (2)*National Institute of Technology, Brazil*.



### Short Summary:

The high crystallinity of cellulose structure is an issue for its upgrading and production of chemicals. Currently, cellulose hydrolysis is performed by using inorganic acids that has several disadvantages. In our work, cellulose solubilization and depolymerization was carried out with molten salt hydrate using different heterogeneous catalysts at low temperature.

8:20 AM **Fri-SUNO-0820** Poisoning of Pt/Al<sub>2</sub>O<sub>3</sub> Aqueous Phase Reforming Catalysts By Di/Ketones.

**Bryan Hare**<sup>1</sup>, Ricardo Garcia<sup>2</sup>, Rachel Getman<sup>2</sup> and Carsten Sievers<sup>1</sup>, (1)Georgia Institute of Technology, USA, (2)Clemson University, USA.

### Short Summary:

We have hypothesized that ketone and diketone side products are responsible for deactivating supported Pt catalysts during the aqueous phase reforming of large polyols. We have thus employed infrared spectroscopy and well-characterized Pt/Al<sub>2</sub>O<sub>3</sub> catalysts to demonstrate the decrease in APR activity when these poisoning species are adsorbed to the surface.

8:40 AM **Fri-SUNO-0840** Modified Aluminum Phosphates As Efficient and Selective Catalysts for Valorization of Biomass-Derived Furfural.

Wenting Fang and **Anders Riisager**, Technical University of Denmark, Denmark.

### Short Summary:

Modified aluminum phosphate (APO-5) catalysts are designed by simple and benign approaches as efficient, selective and durable solid catalysts for the valorization of furfural and other industrially relevant bio-derived aldehydes into renewable fuel additives and polymer precursors.

9:00 AM **Fri-SUNO-0900** Performance-Advantaged Polymers from Diels-Alder Reactions with 5-Hydroxymethyl Furfural (HMF).

**Hochan Chang**, George Huber and James Dumesic, University of Wisconsin-Madison, USA.

### Short Summary:

We have produced high-performance polymers from a biomass resource, 5-hydroxymethyl furfural (HMF). Base-catalyzed aldol condensation and selective hydrogenation of HMF can synthesize monomers for polyurethanes with tunable properties. Moreover, acid-catalyzed acetalization of HMF can produce a monomer for recyclable Diels-Alder polymer.

## Biomass to Chemicals V: Catalyst Engineering

**Session Chairs:** Jun Hee Jang, National Renewable Energy Laboratory, USA and Sourav K. Sengupta, DuPont, USA.

9:40 AM **Fri-SUNO-0940** Metal-Modified Molybdenum Nitride As Selective Catalytic Surfaces for Ethanol Reforming and Glycerol Hydrodeoxygenation.

**Zhexi Lin**<sup>1</sup>, Steven Denny<sup>1</sup>, Salai Cheettu Ammal<sup>2</sup>, Kyung-Eun You<sup>2</sup>, Nongnuch Artrith<sup>3</sup>, Andreas Heyden<sup>2</sup> and Jingguang Chen<sup>1</sup>, (1)Columbia University, USA, (2)University of South Carolina, USA, (3)Utrecht University, Netherlands.

### Short Summary:

Ethanol reforming and glycerol hydrodeoxygenation are important reactions for renewable fuel and chemical production. In this work, we identified metal-modified Mo<sub>2</sub>N surfaces as low-cost and selective catalytic materials for these reactions using machine learning, DFT calculations, and surface science experiments, providing an effective strategy for accelerating rational catalyst design.

10:00 AM **Fri-SUNO-1000** Effect of Metal Identity on the Direct Reduction of Esters to Ethers with H<sub>2</sub> over Metal Exchanged H-FAU Catalysts.

**Claudia Berdugo-Díaz**<sup>1</sup>, Yangsik Yun<sup>1</sup>, Jieun Lee<sup>1</sup>, Melissa Manetsch<sup>1</sup>, Darian Angel Alonzo<sup>1</sup>, Jing Luo<sup>2</sup>, David Barton<sup>2</sup>, Ida Chen<sup>2</sup> and David Flaherty<sup>1</sup>, (1)University of Illinois Urbana-Champaign, USA, (2)The Dow Chemical Company, USA.

### Short Summary:

We synthesize, characterize and kinetically examine catalyst comprised of metal nanoparticles supported on faujasite (M-FAU, where M = Cu, Rh, Pd, Pt, Ru, Ni, and Co) for the direct reduction of esters to ethers, which give considerably higher selectivities than previously reported materials.

10:20 AM **Fri-SUNO-1020** Single-Atom Ru on Zeolites for the Production of Terephthalates from Bio-Based Muconic Acid.

**Ibrahim Khalil** and Michiel Dusselier, KU Leuven, Belgium.

### Short Summary:

In this work, we study the conversion of biobased Muconic acid into terephthalates using atomically dispersed Ru on BEA zeolites. A process optimization study was performed in order to achieve high productivity (40 g/L.h) and selectivity (>90%).

10:40 AM **Fri-SUNO-1040** Catalytic Cooperativity between Glucose Oxidase and Gold Nanoparticles in the Sequential Oxidation of Glucose to Glucaric Acid.

Joseph Brindle, Patrick Nelson, Chinmay Verma and **Michael M. Nigra**, University of Utah, USA.

### Short Summary:

A reaction cascade utilizing gold nanoparticles and glucose oxidase is demonstrated for two different reaction systems: oxidation of glucose to glucaric acid and benzyl alcohol oxidation. Results demonstrate cooperativity between the glucose oxidase catalytic site and the gold nanoparticle surface. Selectivity can be adjusted by pH and gold nanoparticle concentration.

11:00 AM **Fri-SUNO-1100** Elucidating the Nature of the Optimal Active Site for 2,3-Butanediol Dehydration to 1,3-Butadiene.

**Beruk Alemu Bekele**, Jeroen Poissonnier and Joris Thybaut, Ghent University, Belgium.

### Short Summary:

The nature of the optimal active sites for the selective dehydration of 2,3-butanediol into 1,3-butadiene have been elucidated. A dominant side product of the reaction have been suppressed into a minor product via optimal active sites. The change in reaction mechanism and reaction intermediate allowed to achieve high 1,3-butadiene yield.

11:20 AM **Fri-SUNO-1120** Resolving Impacts of Acidity and Morphology on Decarboxylation of  $\gamma$ -Valerolactone over Solid Acid Catalysts.

**Xinlei Huang**<sup>1</sup>, Weixuan Huang<sup>2</sup>, Ran Zhu<sup>2</sup>, Bowei Liu<sup>2</sup>, Robson Schuarca<sup>2</sup>, Anargyros Chatzidimitriou<sup>2</sup> and Jesse Bond<sup>2</sup>, (1)Delaware University, USA, (2)Syracuse University, USA.

### Short Summary:

This work indicates that GVL decarboxylation to butene is primarily catalyzed over Brønsted acid site. The MFI framework has a significant higher activity compare to FAU, BEA, MOR and FER—all of which perform comparably to amorphous, mesoporous silica-aluminas. This indicates that MFI framework zeolite is unique for catalyzing GVL decarboxylation.

11:40 AM **Fri-SUNO-1140** Knitting Nitrogen Patterns into Carbocatalysts for Strong Bond Activation.

Bin Wang<sup>1</sup>, Wenyu Huang<sup>2</sup> and Long Qi<sup>3</sup>, (1)University of Oklahoma, USA, (2)Iowa State University, USA, (3)USDOE Ames Laboratory, USA.

### Short Summary:

Our results establish a new type of active sites (graphitic N assemblies) discovered in the metal-free carbocatalyst, which demonstrates versatile activities only observed among transition metals. The discovery can open broad opportunities for rational design of new metal-free catalysts to meet the challenges for a carbon-neutral future.

## Sutton South

### Elucidation of Active Sites and Reaction Mechanisms I

**Session Chairs:** David Hibbitts, *University of Florida, USA* and Robert Warburton, *Yale University, USA*.

8:00 AM **Fri-SUSO-0800** Microkinetic Modeling-Driven Density Functional Theory Exploration of Ethylene Epoxidation on Partially Oxidized Silver Catalyst Surfaces.

Adhika Setiawan, Tiancheng Pu, Israel E. Wachs and Srinivas Rangarajan, *Lehigh University, USA*.

### Short Summary:

In an effort to explore and elucidate the mechanism of ethylene epoxidation on silver catalyst surfaces, we present a comprehensive analysis based on mean field microkinetic modeling (MKM) trained on reaction kinetics data, density functional theory (DFT) calculations, and subsequent kinetic Monte Carlo (kMC) simulations.

8:20 AM **Fri-SUSO-0820** Enhanced Formic Acid Dehydrogenation Rates at Pd/TiB<sub>2</sub> Interfaces Caused By Strong Metal Support Interaction Phenomena.

Luan Q. Le<sup>1</sup>, Quang T. Trinh<sup>1</sup>, Lavie Rekhil<sup>1</sup>, Roong Jien Wong<sup>1</sup>, Hui Ling Tan<sup>1</sup>, Renhong Li<sup>2</sup>, Wen Liu<sup>1</sup> and Tej S. Choksi<sup>1</sup>, (1)*Nanyang Technological University, Singapore*, (2)*Zhejiang Sci-Tech University, China*.

### Short Summary:

Noble metals supported on TiB<sub>2</sub> exhibit a first-of-its-kind strong metal support interaction phenomena that enhances the rate of HCOOH dehydrogenation. Using a DFT-based reaction pathway analysis and microkinetic model, we unravel how the boron termination and charge transfer from TiB<sub>2</sub> to Pd in these dynamically formed interfaces promote HCOOH dehydrogenation.

8:40 AM **Fri-SUSO-0840** Kinetics of MgO-Catalyzed Ethanol Conversion to 1,3-Butadiene.

Astrid Boje<sup>1</sup>, William Taifan<sup>2</sup>, Henrik Ström<sup>1</sup>, Tomáš Bučko<sup>3,4</sup>, Jonas Baltrusaitis<sup>2</sup> and Anders Hellman<sup>1</sup>, (1)*Chalmers University of Technology, Sweden*, (2)*Lehigh University, USA*, (3)*Comenius University in Bratislava, Slovakia*, (4)*Slovak Academy of Sciences, Slovakia*.

### Short Summary:

We investigate kinetic behaviour of the catalytic conversion of ethanol to 1,3-butadiene on MgO using microkinetic modelling and energy span analysis. We discuss observations of activity and selectivity using both perspectives and consider the impact of uncertainty in the underlying calculations on the kinetic predictions using a correlated error model.

9:00 AM **Fri-SUSO-0900** Methanol Synthesis on PdIn Intermetallic Sites - a Computational Study.

Minttu Kauppinen and Henrik Grönbeck, *Chalmers University of Technology, Sweden*.

### Short Summary:

We have used density functional theory and microkinetic modelling to compare the performance of In<sub>2</sub>O<sub>3</sub>, Pd/In<sub>2</sub>O<sub>3</sub>, and Cu/ZnO/Al<sub>2</sub>O<sub>3</sub> catalysts towards methanol synthesis. Our results suggest that the presence of PdIn on Pd/In<sub>2</sub>O<sub>3</sub> could lead to an increased performance thanks to the higher activity of PdIn compared to In<sub>2</sub>O<sub>3</sub>.

### Elucidation of Active Sites and Reaction Mechanisms II

**Session Chairs:** M. Ali Haider, *Indian Institute of Technology Delhi*, and Srinivas Rangarajan, *Lehigh University, USA*.

9:40 AM **Fri-SUSO-0940** Mechanistic Insights into Olefin Dimerization on MOF-Supported Transition Metal Catalysts.

Saamil Chheda<sup>1</sup>, Jian Zheng<sup>2</sup>, Laura Löbber<sup>3</sup>, Navneet Khetrapal<sup>1</sup>, Julian Schmid<sup>2</sup>, Carlo A. Gaggioli<sup>1</sup>, Benjamin Yeh<sup>1</sup>, Oliver Y. Gutierrez<sup>2</sup>, Ricardo Bermejo de Val<sup>3</sup>, Radha K. Motkuri<sup>2</sup>, J. Ilja Siepmann<sup>1</sup>, Matthew Neurock<sup>1</sup>, Laura Gagliardi<sup>4</sup> and Johannes A. Lercher<sup>2,3</sup>, (1)*University of Minnesota, Twin Cities, USA*, (2)*Pacific Northwest National Laboratory, USA*, (3)*Technical University of Munich, Germany*, (4)*University of Chicago, USA*.

### Short Summary:

Metalated-UiO-66 catalysts with well-defined isolated catalytic sites were investigated for olefin oligomerization. Ni<sup>2+</sup>-UiO-66 catalyst was demonstrated to achieve higher activity and selectivity towards the desired linear octenes as compared to the other metalated-UiO-66 catalysts. Moreover, undercoordinated single-atom catalytic sites in metalated-UiO-66 catalysts have been unveiled using theory, experiments, and characterization.

10:00 AM **Fri-SUSO-1000** Nature and Identity of the Active Sites of WGS and R-WGS Via Structure-Dependent Microkinetic Modeling and Machine Learning.

Raffaele Cheula<sup>1,2</sup>, Mie Andersen<sup>1</sup> and Matteo Maestri<sup>2</sup>, (1)*Aarhus University, Denmark*, (2)*Politecnico di Milano, Italy*.

### Short Summary:

We present a structure-dependent microkinetic analysis of direct and reverse water-gas shift based on the concerted simulation of structure and activity of catalysts materials under reaction conditions. The methodology is applied to describe an Rh catalyst system and successively extended to other catalyst compositions by application of machine learning techniques.

10:20 AM **Fri-SUSO-1020** Bridging Apparent Kinetics to Microscopic Insights: A Kinetic Modelling Strategy for NO<sub>x</sub> Selective Catalytic Reduction on Cu-CHA Zeolites.

**Anshuman Goswami**<sup>1</sup>, Siddarth Krishna<sup>2</sup>, Casey Jones<sup>2</sup>, Rajamani Gounder<sup>2</sup> and William F. Schneider<sup>1</sup>, (1)University of Notre Dame, USA, (2) Purdue University, USA.

**Short Summary:**

This work presents a microkinetic modelling strategy for NO<sub>x</sub> selective catalytic reduction (SCR) on copper-exchanged Chabazite (Cu-CHA) zeolites. We find that apparent SCR kinetics is primarily governed by mobility of solvated copper species tethered to the zeolite framework. These findings elucidate the relationship between SCR kinetics and the zeolite composition.

10:40 AM **Fri-SUSO-1040** Entropic Control of HD Exchange Rates over Dilute Pd-in-Au Alloy Nanoparticle Catalysts.

Jessi E.S. van der Hoeven<sup>1</sup>, **Hio Tong Ngan**<sup>2</sup>, Austin Taylor<sup>3</sup>, Nathaniel Eagan<sup>4</sup>, Joanna Aizenberg<sup>3</sup>, Philippe Sautet<sup>2</sup>, Robert Madix<sup>3</sup> and Cynthia Friend<sup>3</sup>, (1)Utrecht University, Netherlands, (2)University of California, Los Angeles, USA, (3)Harvard University, USA, (4)Tufts University, USA.

**Short Summary:**

HD exchange reaction was performed on dilute Pd-in-Au alloys to study their intrinsic hydrogen dissociation activity. Results from experiment and theory demonstrate that Pd single atoms have smaller apparent activation energy and yet lower reactivity than larger Pd ensembles. This reactivity difference was synergistically found to be of entropic origin.

11:00 AM **Fri-SUSO-1100** Spin-Crossing in Heterogeneous Catalysis By Atomically Dispersed Transition Metals: Ethane Dehydrogenation By Co/SiO<sub>2</sub>

**Sanjana Srinivas**, Dionisios G. Vlachos and Stavros Caratzoulas, University of Delaware, USA.

**Short Summary:**

This work uses Density Functional Theory (DFT) and microkinetic modelling to study the theoretical efficiencies offered by earth abundant 3d metals with partially filled d orbitals dispersed on amorphous-SiO<sub>2</sub> for small alkane dehydrogenation and the impact of surface heterogeneity on the kinetics.

11:20 AM **Fri-SUSO-1120** Decoding Reactive Structures in Dilute Alloy Catalysts.

Anna Plonka and **Anatoly Frenkel**, Stony Brook University, USA.

**Short Summary:**

New approach developed to resolve the active site structure of a dilute bimetallic catalyst at the atomic level. Using catalytic activity measurements, machine-learning enabled XAFS analysis and first-principles kinetic modeling we demonstrate the effect of treatment on catalyst nanostructure, active site distribution, and reactivity toward the prototypical HD exchange reaction.

11:40 AM **Fri-SUSO-1140** A DFT Study on a Histidine-Modified Cu Electrocatalyst for CO<sub>2</sub> Reduction.

**Juan-Manuel Arce Ramos**, Albertus Denny Handoko, Chee Koon NG, Jia Zhang and Yee-Fun Lim, Agency for Science, Technology and Research, Singapore.

**Short Summary:**

We investigated the effects of a histidine modification to the copper electrocatalyst for CO<sub>2</sub> reduction through DFT computations. The organic ligand modification affects reaction intermediates' stability, potentially increasing catalytic activity and selectivity towards specific products.

## Trianon Ballroom

### Catalyst Characterization and Reaction Mechanism Elucidation with Vibrational Spectroscopy

**Session Chairs:** Madelyn R. Ball, University of Wisconsin Madison, USA and Juan Bravo Suárez, The University of Kansas, USA.

8:00 AM **Fri-TRBR-0800** In Situ Raman Analyses of the CO Oxidation Reaction over Nanostructured Ceria-Based Catalysts.

**Enrico Sartoretti**, Chiara Novara, Fabrizio Giorgis, Marco Piumetti, Samir Bensaïd, Nunzio Russo and Debora Fino, Politecnico di Torino, Italy.

**Short Summary:**

Four nanostructured ceria-based catalysts, obtained via hydrothermal synthesis, were extensively studied by in situ Raman spectroscopy. Different analyses were carried out to monitor the presence and the evolution of defect sites at high temperature and during the CO oxidation reaction, investigating the role of these defects in the catalysis.

8:20 AM **Fri-TRBR-0820** A Quantitative *in-Situ* FTIR Analysis of Ce<sup>3+</sup> Densities and the Role of Oxygen Vacancies in Catalysis over Ceria Surfaces.

**Sadia Afrin** and Praveen Bollini, University of Houston, USA.

**Short Summary:**

*In-situ* quantification of the <sup>2</sup>F<sub>5/2</sub> to <sup>2</sup>F<sub>7/2</sub> electronic transition of reduced cerium leads to unique and clear insights into the role of oxygen vacancies and surface oxygens in three distinct ceria-catalyzed reactions. This approach could potentially be applicable to other industrially relevant reactions occurring over reducible metal oxide catalysts.

8:40 AM **Fri-TRBR-0840** CO<sub>2</sub> Assisted Ethane Oxidative Dehydrogenation over MoO<sub>x</sub> Catalysts Supported on Reducible CeO<sub>2</sub>-TiO<sub>2</sub>.

**Thu Nguyen**, Fuat E. Celik and George Tsilomelekis, *Rutgers, The State University of New Jersey, USA*.

**Short Summary:**

In the absence of a reducing agent, CO<sub>2</sub> was able to recover both the terminal and bridging molybdenum-oxygen signals in Raman but the recovery of all oxygen species were at a much lesser extent during reaction conditions.

9:00 AM **Fri-TRBR-0900** Effects of Atmosphere and Temperature on Au/CeO<sub>2</sub> Catalyst By Combined Raman and UV-Vis *in Situ* Spectroscopy..

**Mara Cordero-Garcia**, Elizabeth Salinas-Barríos, Elizabeth Rojas-García and Sergio Gomez Torres, *Universidad Autónoma Metropolitana-Iztapalapa, Mexico*.

**Short Summary:**

We study the *in-situ* behavior of Au/CeO<sub>2</sub> and CeO<sub>2</sub> during different pretreatments in temperature and atmosphere by Raman and Diffuse reflectance UV-Vis. These techniques allow us to follow in real-time, surface changes of Au nanoparticles and CeO<sub>2</sub> and obtain quantitative data relevant to the catalytic activity during the WGS reaction.

## Multi-modal Approaches for Catalyst Characterization

**Session Chairs:** Griffin Canning, *The Pennsylvania State University, USA* and Akbar Mahdavi-Shakib, *The Pennsylvania State University, USA*.

9:40 AM **Fri-TRBR-0940** Dynamic Pt Coordination in Dilute Ag-Pt Alloy Catalysts Under Reactive Environments.

**Jordan Finzel** and Phillip Christopher, *University of California, Santa Barbara, USA*.

**Short Summary:**

Through a combined experiment and theory approach, we identify how Pt active site structures in AgPt dilute alloy nanoparticle catalysts evolve under varying environmental conditions. We provide evidence for surface segregation of Pt species, the ability to modify Pt ensembles, and discuss implications for catalysis.

10:00 AM **Fri-TRBR-1000** Understanding the Promoting and Deactivating Effects of Carbon Deposits during 1-Butene Isomerization.

**Karoline Hebisch** and Carsten Sievers, *Georgia Institute of Technology, USA*.

**Short Summary:**

Carbon deposits provide active environments but also lead to catalyst deactivation during 1-butene isomerization over FER. XRD revealed that coke prevented a relaxation of the crystal structure after cooling. These structural changes and micropore filling occurred hours before optimal performance, suggesting that the reaction location is outside the pore channels.

10:20 AM **Fri-TRBR-1020** Improving the Stability of Atomically Dispersed Pt Catalysts By Aliovalent Doping of CeO<sub>2</sub>.

**Haodong Wang**<sup>1</sup> and Anatoly Frenkel<sup>1,2</sup>, (1)*Stony Brook University, USA*, (2)*Brookhaven National Laboratory, USA*.

**Short Summary:**

Atomically dispersed supported catalysts hold considerable promise as catalytic materials. Herein using a Gd-doped ceria support for atomically dispersed surface Pt atoms, we establish how the combined effects of aliovalent doping and oxygen vacancy generation provide dynamic mechanisms that serve to enhance the stability of supported single atom configurations.

10:40 AM **Fri-TRBR-1040** Impact of Nanoparticle–Support Interactions in Co<sub>3</sub>O<sub>4</sub>/Al<sub>2</sub>O<sub>3</sub> Catalysts for the Preferential Oxidation of Carbon Monoxide.

**Thulani Nyathi**<sup>1</sup>, Nico Fischer<sup>1</sup>, Andrew York<sup>2</sup>, Emma Gibson<sup>3</sup>, Peter Wells<sup>4</sup>, C. Richard A. Catlow<sup>5</sup> and Michael Claeys<sup>1</sup>, (1)*Catalysis Institute and c\*change (DSI-NRF Centre of Excellence in Catalysis), University of Cape Town, South Africa*, (2)*Johnson Matthey Technology Centre, United Kingdom*, (3)*University of Glasgow, United Kingdom*, (4)*University of Southampton, United Kingdom*, (5)*University College London, United Kingdom*.

**Short Summary:**

Our *in situ* analyses and kinetic data suggest that significant stability (against bulk reduction) of the active Co<sub>3</sub>O<sub>4</sub> phase is desired during the preferential oxidation of CO. However, the catalyst (surface) needs to be reducible (and “re-oxidisable”) to allow for the oxidation of CO *via* the Mars–van Krevelen mechanism.

11:00 AM **Fri-TRBR-1100** Ni-Cu-Al LDH Synthesis, Activation and Application on R<sub>w</sub>gs Reaction.

Li He<sup>1</sup>, Liseth Duarte<sup>1</sup>, Matus Stredansky<sup>1</sup>, Piyush Ingale<sup>2</sup>, Michael Geske<sup>2</sup>, Frank Rosowski<sup>3,4</sup>, Maike Hashagen<sup>1</sup>, Frank Girgsdies<sup>1</sup>, Travis Jones<sup>1</sup>, Walid Hetaba<sup>1,5</sup>, Thomas Lunkenbein<sup>1</sup>, Robert Schlögl<sup>1,5</sup> and **Katarzyna Skorupska**<sup>1</sup>, (1)*Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany*, (2)*BasCat – UniCat BASF JointLab: Technische Universität Berlin, Germany*, (3)*Technische Universität Berlin, Germany*, (4)*BASF SE, Germany*, (5)*Max Planck Institute for Chemical Energy Conversion, Germany*.

**Short Summary:**

A series of LDH samples with different NiCu ratio were investigated. One of interesting findings is that the alloy formation of Ni<sub>(1-x)</sub>Cu<sub>x</sub> on activated LDH samples has been confirmed by XRD, NEXAFS and EDX. The results presented that a lower decomposition temperature and Cu addition could significantly promote Ni reducibility.

11:20 AM **Fri-TRBR-1120** Promotion of CeO<sub>2</sub> Surface Reducibility By Pt-Activated H-Spillover: Influence Pt Surface Density, Structure, and CeO<sub>2</sub> Grain Growth.

**Jaeha Lee**<sup>1</sup>, Seungdo Yang<sup>2</sup>, Hyungjoo Kim<sup>2</sup>, Do Heui Kim<sup>2</sup> and Phillip Christopher<sup>1</sup>, (1)*University of California, Santa Barbara, USA*, (2)*Seoul National University, Korea, Republic of (South)*.

**Short Summary:**

How Pt promotes the reduction of CeO<sub>2</sub> surface was studied. The H-spillover is the primary mechanism for Pt promoted CeO<sub>2</sub> surface reduction. The rate at which this occurs is dictated first by Pt surface density, second by Pt structure and inherent reducibility, and third by CeO<sub>2</sub> grain growth.

11:40 AM **Fri-TRBR-1140** Copper Speciation in Cu-Zn-Y/Beta during Ethanol Upgrading to Butene Rich C<sub>3</sub>+ Olefins.

**Stephen Purdy**<sup>1</sup>, Gregory Collinge<sup>2</sup>, Junyan Zhang<sup>1</sup>, Kinga A. Unocic<sup>1</sup>, Evan C. Wegener<sup>3</sup>, Roger Rousseau<sup>2</sup>, Malsoon Lee<sup>2</sup>, Vassiliki-Alexandra Glezakou<sup>2</sup>, Theodore Krause<sup>3</sup>, Katharine Page<sup>4</sup> and Zhenglong Li<sup>1</sup>, (1)*Oak Ridge National Laboratory, USA*, (2)*Pacific Northwest National Laboratory, USA*, (3)*Argonne National Laboratory, USA*, (4)*University of Tennessee, USA*.

**Short Summary:**

Both Cu<sup>1+</sup> and Cu<sup>0</sup> sites coexist in Cu-Zn-Y/Beta during the ethanol to olefins reaction. Using a combination of spectroscopy, kinetic measurements, and DFT/AIMD calculations, it was found that both species catalyze the dehydrogenation of ethanol to acetaldehyde, with metallic copper having a higher rate.





## NAM27 Poster Program



# Monday May 23, 2022 Poster Program

<b>Americas Halls 1 &amp; 2</b>	<b>Catalysis for C<sub>1</sub> and SynGas Chemistry Poster Session I</b>
<b>Mon-P-2</b>	<b>Effect of Bi-Metallic Heterogeneous Catalysts for Carbon Dioxide Hydrogenation to Light Olefins</b> <u>Nicole Forte</u> <sup>1</sup> , Christian Moon <sup>1</sup> , Jaycie Esteban <sup>1</sup> , Sanjaya Senanayake <sup>2</sup> and Cheng Zhang <sup>1</sup> , (1)Long Island University (Post), USA, (2)Brookhaven National Laboratory, USA. Short Summary: Direct hydrogenation of CO <sub>2</sub> to lower olefins is highly desirable due to the wide variety applications of light olefins in polymers. Therefore, we report a selective CO <sub>2</sub> conversion to lower olefins through CO <sub>2</sub> hydrogenation over a series of bi-metallic catalyst supported on Fe <sub>2</sub> O <sub>3</sub> to compare with the respective mono-metallic catalysts.
<b>Mon-P-3</b>	<b>Effect of Na<sup>+</sup> Promoter on the Catalytic Performance of Carbon Nanosphere Encapsulated Fe<sub>1</sub>Co<sub>2</sub> for CO<sub>2</sub> Conversion</b> <u>Christian Moon</u> <sup>1</sup> , Jaylin Sasson <sup>2</sup> and Cheng Zhang <sup>1</sup> , (1)Long Island University (Post), USA, (2)Brookhaven National Laboratory, USA. Short Summary: Direct hydrogenation of CO <sub>2</sub> to lower olefins continues to be researched in order to promote sustainable energy. Therefore, we report the influence of Na as a promoter on carbon nanosphere encapsulated Fe <sub>1</sub> Co <sub>2</sub> through CO <sub>2</sub> hydrogenation to compare with a controlled carbon nanosphere encapsulated Fe <sub>1</sub> Co <sub>2</sub> catalyst.
<b>Mon-P-4</b>	<b>Spillover and Deactivation Studies of Os Promoted Co Fischer-Tropsch Catalysts</b> <u>Neil Coville</u> , DST-NRF Centre of Excellence in Catalysis, South Africa; University of the Witwatersrand, South Africa. Short Summary: Numerous promoters have been used to enhance the activity of Co Fischer-Tropsch catalysts. Herein we describe the use of Os as a promoter, as the OsOx reduces at T < 250 °C. Studies on Co supported inside/outside hollow carbon spheres to evaluate spillover effects from Os to Co are reported.
<b>Mon-P-5</b>	<b>Identifying Higher Oxygenate Synthesis Sites in Cu Catalysts Promoted and Stabilized By Atomic Layer Deposited Fe<sub>2</sub>O<sub>3</sub></b> <u>Arun Asundi</u> <sup>1</sup> , Sindhu Nathan <sup>2</sup> , Jiyun Hong <sup>1</sup> , Adam Hoffman <sup>1</sup> , Makenna Pennel <sup>2</sup> , Simon Bare <sup>1</sup> and Stacey Bent <sup>2</sup> , (1)SLAC National Accelerator Laboratory, USA, (2)Stanford University, USA. Short Summary: We demonstrate improved activity, selectivity, and stability of Cu/SiO <sub>2</sub> catalysts modified by atomic layer deposited Fe <sub>2</sub> O <sub>3</sub> for syngas conversion to higher oxygenates. Using in situ characterization methods we determine the chemical properties and morphology of the catalyst during reaction and understand the Cu/Fe interface sites responsible for higher oxygenate formation.
<b>Mon-P-6</b>	<b>Support Effects on CO<sub>2</sub> Conversion to Light Olefins over Promoted and Unpromoted Fe-Co Bimetallic Catalysts</b> <u>Daniel Weber</u> and Cheng Zhang, Long Island University (Post), USA. Short Summary: In this study, we investigate the effects of a wide range of supports on CO <sub>2</sub> conversion to light olefins (C <sub>2</sub> =-C <sub>4</sub> =) over a Mn promoted and unpromoted Fe-Co bimetallic catalyst.
<b>Mon-P-7</b>	<b>Na-Fe<sub>3</sub>O<sub>4</sub>@HZSM-5 to Enhance Gasoline-like Product from CO<sub>2</sub></b> Elena Corrao <sup>1</sup> , Fabio Salomone <sup>1</sup> , Emanuele Giglio <sup>2</sup> , Micaela Castellino <sup>1</sup> , Raffaele Pirone <sup>1</sup> and <u>Samir Bensaid</u> <sup>1</sup> , (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.
<b>Mon-P-8</b>	<b>Cobalt Ferrite Nanoparticles to Form a Catalytic Co-Fe Alloy Carbide Phase for Selective CO<sub>2</sub> Hydrogenation to Light Olefins</b> <u>Hojeong Lee</u> and Kwangjin An, Ulsan National Institute of Science and Technology (UNIST), Korea, Republic of (South). Short Summary: CoFe <sub>2</sub> O <sub>4</sub> nanoparticles were synthesized as efficient catalyst precursors for CO <sub>2</sub> hydrogenation to produce C <sub>2</sub> -C <sub>4</sub> olefins. The resulting Na-CoFe <sub>2</sub> O <sub>4</sub> catalyst exhibits high CO <sub>2</sub> conversion (~34%) and light olefin selectivity (~39%). The excellent performance of the Na-CoFe <sub>2</sub> O <sub>4</sub> /CNT catalyst can be attributed to unique bimetallic alloy carbide (Fe <sub>1-x</sub> Co <sub>x</sub> ) <sub>5</sub> C <sub>2</sub> .
<b>Mon-P-9</b>	<b>Understanding the Impact of Hydrogen Activation By SrCe<sub>0.8</sub>Zr<sub>0.2</sub>O<sub>3-δ</sub> perovskite Membrane Material on Direct Non-Oxidative Methane</b> <u>Sichao Cheng</u> and Dongxia Liu, University of Maryland - College Park, USA. Short Summary: Direct nonoxidative methane conversion over Fe/SiO <sub>2</sub> and SCZO membrane materials implies potential reaction pathways to upgrade methane to value-added chemicals. The mechanistic understanding of SCZO-oxide-hydrogen-activation over Fe/SiO <sub>2</sub> catalyst has been explored to achieve stable and high methane conversion and low coke selectivity by elimination of gas-phase reaction via hydrogen co-feed.

<p><b>Mon-P-10</b></p>	<p><b>Comparative Study on the Properties of Ni-MgO-CeZrO<sub>2</sub> Catalysts for Carbon Dioxide Reforming of Methane</b>  <u>Kyung-Won Jeon</u><sup>1</sup>, Jee-Eun Kim<sup>1</sup>, Ji-Hyeon Gong<sup>1</sup>, Min-Ju Kim<sup>1</sup>, Ru-Ri Lee<sup>2</sup>, Jae-Oh Shim<sup>2</sup>, Hyun-Seog Roh<sup>3</sup> and Won-Jun Jang<sup>1</sup>, (1)Kyungnam University, Korea, Republic of (South), (2)Wonkwang University, Korea, Republic of (South), (3)Yonsei University, Korea, Republic of (South).  Short Summary:  This study clarified the effect of Ni particle size on the performance of Ni-MgO-CeZrO<sub>2</sub> in CDR, and the dependence of size on the nature of support. It confirmed that the Ni particle size and OSC are found to be the primary and secondary factor that influence the CDR performance, respectively.</p>
<p><b>Mon-P-11</b></p>	<p><b>Selective Production of Long-Chain Hydrocarbons By Fe-Based Bimetallic Oxide</b>  Muhammad Kashif Khan, <u>Wonjoong Yoon</u>, Sheraz Ahmed, Muhammad Irshad and Jaehoon Kim, <i>Sungkyunkwan University, Korea, Republic of (South)</i>.  Short Summary:  To reduce the global warming, selective conversion of CO<sub>2</sub> to liquid hydrocarbons has great significance. We synthesized Fe-based bimetallic oxide to convert CO<sub>2</sub> into liquid hydrocarbons with low CH<sub>4</sub> and CO selectivity. Furthermore, catalyst structure and activity relationship was also studied.</p>
<p><b>Mon-P-12</b></p>	<p><b>A Highly Stable Copper-Based Tandem Catalyst for C<sub>2+</sub> Higher Alcohols Synthesis Via Direct Hydrogenation of CO<sub>2</sub></b>  Muhammad Irshad, <u>Heuntae Jo</u>, Muhammad Kashif Khan and Jaehoon Kim, <i>Sungkyunkwan University, Korea, Republic of (South)</i>.  Short Summary:  For CO<sub>2</sub> hydrogenation to higher alcohols synthesis, a single copper based catalyst has shown excellent catalytic performance and stability (1000 h on time stream) reported till to date has a great potential.</p>
<p><b>Mon-P-13</b></p>	<p><b>Role of Alkali Metal in the Na-Promoted FeAlO<sub>x</sub> Catalyst for the Conversion of CO<sub>2</sub> to Liquid Fuels</b>  <u>Wonjoong Yoon</u>, Muhammad Kashif Khan and Jaehoon Kim, <i>Sungkyunkwan University, Korea, Republic of (South)</i>.  Short Summary:  On this study, we try to find the role of alkali metal for CO<sub>2</sub> conversion with series of Na-promoted FeAlO<sub>x</sub> catalyst.</p>
<p><b>Mon-P-14</b></p>	<p><b>Highly Selective Aerobic Oxidation of Methane Yielding Formaldehyde over Platinum</b>  Eric van Steen, Sinqobile Mahlaba, Nasseela Hytoolakhan Lal Mahomed, Gerard Leteba, Junfeng Guo and Pierre Cilliers, <i>University of Cape Town, South Africa</i>.  Short Summary:  The selective, aerobic oxidation of methane over Pt-based catalysts in a continuous operation yielded selectively formaldehyde (up to 90%) when performing the reaction in the presence of liquid water. Water is required to limit the direct interaction of methane with the metal surface and to enhance product desorption.</p>
<p><b>Americas Halls 1 &amp; 2</b></p>	<p><b>Catalysis for Environmental Applications Poster Session I</b></p>
<p><b>Mon-P-16</b></p>	<p><b>CO<sub>2</sub> Deoxygenation to CO By Vacancies of CeO<sub>2</sub>-Based Mixed Oxides</b>  Shawn Lin, <i>National Taiwan University of Science and Technology, Taiwan</i>.  Short Summary:  CO<sub>2</sub> deoxygenation to CO can be viable for resolving the climate changes caused by greenhouse gas. This study illustrates that Ce<sub>7</sub>Fe<sub>3</sub>O<sub>y</sub> is active at mid-temperature range and that a nearby GDC membrane can enhance the reactivity, indicating the importance of balancing the activity and the mobility of oxygen vacancies.</p>
<p><b>Mon-P-17</b></p>	<p><b>Structure - Activity Effects for Cu/SSZ-39 and Cu/SSZ-13 Catalysts during SCR-NO<sub>x</sub> with NH<sub>3</sub></b>  <u>Gabriela I. Hernandez-Salgado</u><sup>1</sup> and Gustavo A. Fuentes<sup>2</sup>, (1)Autonomous Metropolitan University-Iztapalapa, Mexico, (2) Universidad Autónoma Metropolitana-Iztapalapa, Mexico.  Short Summary:  We investigate Cu/SSZ-39 and Cu/SSZ-13 using UV-Vis in situ and catalytic tests to establish a structure-activity effect during SCR-NO<sub>x</sub> with NH<sub>3</sub>. Our findings show that Cu<sup>2+</sup> is the active specie in both catalysts. We observed a formation of Cu complex that apparently is not active for the reaction.</p>
<p><b>Mon-P-19</b></p>	<p><b>Enhancing the Activation Entropy Via CO Spillover to Promote the CO Oxidation on CeO<sub>2</sub> Surface in Pt/CeO<sub>2</sub></b>  <u>Eun Won Lee</u>, Jaeha Lee, Sungha Hwang and Do Heui Kim, <i>Seoul National University, Korea, Republic of (South)</i>.  Short Summary:  A CO oxidation mechanism over Pt/CeO<sub>2</sub> is proposed based on CO spillover from Pt nanoparticles to CeO<sub>2</sub>. The spillover of CO allows CeO<sub>2</sub> to act as an additional active site, leading to an enhancement in the CO oxidation activity in physically mixed catalysts (Pt/CeO<sub>2</sub>+CeO<sub>2</sub>) by enhancing the activation entropy.</p>
<p><b>Mon-P-21</b></p>	<p><b>A Cost-Effective Approach for Low-Temperature-Combustion-Condition DeNO<sub>x</sub></b>  <u>Han Zong</u> and Chao Wang, <i>Johns Hopkins University, USA</i>.  Short Summary:  Our developed PNA can reduce and even bridge the NO<sub>x</sub> absorption gap between the “cold-start” period and the NH<sub>3</sub>-SCR operating window. The cost-effective approach for low-temperature-combustion condition DeNO<sub>x</sub> demonstrates a great commercialization potential and provides another viable path towards green economy.</p>



<b>Mon-P-22</b>	<p><b>Evaluating the Effect of Pt-Rh Interactions on Activity and Stability of Pt-Rh/Al<sub>2</sub>O<sub>3</sub> Three-Way Catalysts</b>  <u>Silvia Marino</u><sup>1</sup>, Yuntao Gu<sup>2</sup>, Wei Li<sup>2</sup> and William Epling<sup>1</sup>, (1)University of Virginia, USA, (2)General Motors Global R&amp;D, USA.  Short Summary:  Pt-Rh catalysts supported on alumina are used as a potential strategy to minimize the deactivation modes on Pt-only and Rh-only. 1.5%Pt-0.3%Rh/Al<sub>2</sub>O<sub>3</sub> H<sub>2</sub>-treated at 750°C showed lower deactivation after lean-rich ageing compared to the monometallic samples. Several characterization techniques showed Pt-Rh interactions, which might lead to a more stable catalyst.</p>
<b>Mon-P-24</b>	<p><b>Selective Oxidation and Chemisorption of CO on Li<sub>2</sub>MnO<sub>3</sub>: A New Promising Material for H<sub>2</sub> Purification from Syngas Mixtures</b>  <u>Carlos Hernández-Fontes</u> and Heriberto Pfeiffer, <i>Universidad Nacional Autónoma de México (UNAM), Mexico</i>.  Short Summary:  In this work Li<sub>2</sub>MnO<sub>3</sub> is presented as the first lithium ceramic capable to selectively oxidize and capture CO to purify H<sub>2</sub> from syngas mixtures. Results showed a high CO consumption at high temperatures (over 500 °C) as the H<sub>2</sub> is barely consumed, also the CO capture efficiency was highly increased.</p>
<b>Mon-P-25</b>	<p><b>Engineering Hydrothermally Stable Pt/CeO<sub>2</sub>-Al<sub>2</sub>O<sub>3</sub> Nanosheet Catalysts for TWC Applications</b>  Junjie Chen<sup>1</sup>, Chih Han Liu<sup>1</sup>, <u>Todd J. Toops</u><sup>2</sup> and Eleni A. Kyriakidou<sup>1</sup>, (1)University at Buffalo (SUNY), USA, (2)Oak Ridge National Laboratory, USA.  Short Summary:  This work shows Pt-only TWCs with a rationally designed structure can achieve comparable activity and durability with the state-of-the-art Rh-based catalyst with a much lower cost.</p>
<b>Mon-P-26</b>	<p><b>Enhanced SO<sub>2</sub> Resistance of V<sub>2</sub>O<sub>5</sub>/WO<sub>3</sub>-TiO<sub>2</sub> Catalyst Physically Mixed with Alumina for the Selective Catalytic Reduction of NO<sub>x</sub> with NH<sub>3</sub></b>  <u>Se Won Jeon</u><sup>1</sup>, Inhak Song<sup>1</sup>, Hwangho Lee<sup>1</sup>, Joonwoo Kim<sup>2</sup>, Youngchul Byun<sup>2</sup>, Dong Jun Koh<sup>2</sup> and Do Heui Kim<sup>1</sup>, (1)Seoul National University, Korea, Republic of (South), (2)Research Institute of Industrial Science &amp; Technology, Korea, Republic of (South).  Short Summary:  V<sub>2</sub>O<sub>5</sub>/WO<sub>3</sub>-TiO<sub>2</sub> physically mixed with alumina (VWTi + Al) catalyst was introduced as a new strategy for deactivation of vanadia catalysts by ammonium bisulfate. Its superior sulfur tolerance compared to conventional vanadia catalysts was derived from migration of ABS formed on vanadia sites to alumina sites through physical contact.</p>
<b>Mon-P-27</b>	<p><b>Mesoporous Sulfur-Decorated Pt-Al<sub>2</sub>O<sub>3</sub> Catalyst: Selective Change of the Adsorption Strength in Dehydrogenation of Perhydro-Benzyltoluene</b>  <u>Yeongin Jo</u> and Young-Woong Suh, <i>Hanyang University, Korea, Republic of (South)</i>.  Short Summary:  The mesoporous sulfur-decorated Pt-Al<sub>2</sub>O<sub>3</sub> catalyst exhibits the better synergy than the conventional S-added Pt/Al<sub>2</sub>O<sub>3</sub> in H<sub>2</sub> release from perhydro-benzyltoluene, in which the electron density of Pt is reduced by such a sulfur addition and thereby the adsorption of the aromatic dehydrogenation products on Pt atoms is weakened.</p>
<b>Mon-P-28</b>	<p><b>Toward the Development of Pd/SSZ-13 Passive NO<sub>x</sub> Adsorbers for Eliminating NO<sub>x</sub> Emissions during the Cold-Start Period</b>  Jaeha Lee<sup>1</sup>, Yongwoo Kim<sup>1</sup>, Sungha Hwang<sup>1</sup>, Youngseok Ryou<sup>1</sup>, Jonghyun Kim<sup>1</sup>, Eun Won Lee<sup>1</sup>, Hyokyoung Lee<sup>2</sup>, Chang Hwan Kim<sup>2</sup> and <u>Do Heui Kim</u><sup>1</sup>, (1)Seoul National University, Korea, Republic of (South), (2)Hyundai Motor Company, Korea, Republic of (South).  Short Summary:  ‘Hydrophobic’ Pd/SSZ-13 with high Si/Al, which was obtained after hydrothermal treatment, would be the good candidate passive NO<sub>x</sub> adsorber material since it has high NO storage ability, which approaches the theoretical NO/Pd of 1 as well as superior hydrothermal resistance compared with other zeolite supported catalysts.</p>
<b>Mon-P-29</b>	<p><b>Effects of SO<sub>2</sub> Poisoning and Regeneration on Spinel-Containing CH<sub>4</sub> Oxidation Catalysts</b>  <u>Natalia Diaz Montenegro</u> and William Epling, <i>University of Virginia, USA</i>.  Short Summary:  This work examines CH<sub>4</sub> oxidation and oxygen storage capacity performance in the absence and presence of SO<sub>2</sub>, and the regeneration of a new CH<sub>4</sub> oxidation catalyst formulation that incorporates spinel-structured materials with precious metal-based catalysts for the abatement of pollutants in stoichiometric natural gas engines.</p>
<b>Mon-P-30</b>	<p><b>Designing Pd/CHA Zeolite Catalysts for Complete Methane Oxidation</b>  <u>Jingzhi Liu</u><sup>1</sup>, Tala Mon<sup>2</sup>, Eleni A. Kyriakidou<sup>2</sup> and Viktor Cybulskis<sup>1</sup>, (1)Syracuse University, USA, (2)University at Buffalo (SUNY), USA.  Short Summary:  High-silica (Si/Al molar ratios &gt; 15) Pd/CHA (i.e., SSZ-13) zeolites exhibit superior low-temperature performance and durability for complete CH<sub>4</sub> oxidation in presence of H<sub>2</sub>O compared to conventional Pd/Al<sub>2</sub>O<sub>3</sub> catalysts. More hydrophobic CHA supports decrease the effect product inhibition on CH<sub>4</sub> oxidation rates and reduces Pd mobility at elevated temperatures.</p>

<p><b>Mon-P-31</b></p>	<p><b>Spatiotemporal Evolution of CH<sub>4</sub> and NO<sub>x</sub> Conversion Profiles and Their Interrelationship in a Natural Gas Three-Way Catalyst</b>  <u>Dhruba J. Deka</u>, Calvin R. Thomas, Josh A. Pihl and William Partridge, <i>Oak Ridge National Laboratory, USA</i>.  Short Summary:  Spatiotemporal evolution of reactant and product concentrations within a natural gas three-way catalyst was measured using SpaciMS which elucidated the interrelations between CH<sub>4</sub> conversion, intra-catalyst H<sub>2</sub> and CO formation, and NO<sub>x</sub> conversion. The TWC consisted of an oxidation zone, a CH<sub>4</sub> steam reforming zone, followed by a NO<sub>x</sub> conversion zone.</p>
<p><b>Mon-P-32</b></p>	<p><b>Synergistic Effect on Bimetallic Ru-Cu Catalysts Supported on Titania for the Hydrodeoxygenation of Anisole</b>  <u>Diego Duran Sanchez</u>, Jose Antonio De los Reyes and Omar Valdés, <i>Universidad Autónoma Metropolitana-Iztapalapa, Mexico</i>.  Short Summary:  The catalytic properties of two series of catalysts, a monometallic series of Cu and a bimetallic series of ruthenium-copper catalysts, were evaluated. It was found that by combining copper and ruthenium there is a resulting synergistic effect on the catalytic activity.</p>
<p><b>Mon-P-33</b></p>	<p><b>Enhanced CH<sub>4</sub> Conversion Using Dual Layer Pt-Pd/Spinel Oxide Catalysts</b>  <u>Debtanu Maiti</u><sup>1</sup>, Pak Wing Chen<sup>1</sup>, Ru-Fen Liu<sup>2</sup>, Michael P. Harold<sup>1</sup> and Lars C. Grabow<sup>1</sup>, (1)<i>University of Houston, USA</i>, (2)<i>CDTi Advanced Materials, USA</i>.  Short Summary:  We developed dual layer Pt-Pd/spinel oxide catalysts with lower CH<sub>4</sub> light-off temperatures as compared to commercial three-way-catalysts (TWC). The increased reactivity of CH<sub>4</sub> at low temperatures is linked to the oxygen storage capacity of spinels. We rank-ordered spinels according to their reducibility and correlated their performance to simple material descriptors.</p>
<p><b>Mon-P-34</b></p>	<p><b>Promoting Effect of Re on the Improvement of Perhydro-Dibenzyltoluene Dehydrogenation Ability in Pt-ReO<sub>x</sub>/Al<sub>2</sub>O<sub>3</sub> Catalyst</b>  <u>Ji Soo Jang</u><sup>1</sup>, Chan Hun Kim<sup>1</sup> and Kwan-Young Lee<sup>1,2</sup>, (1)<i>Korea University, Korea, Republic of (South)</i>, (2)<i>KU-KIST Green school, Korea, Republic of (South)</i>.  Short Summary:  In this study, the goal is to improve dehydrogenation activity at low temperatures by incorporating rhenium into the Pt/Al<sub>2</sub>O<sub>3</sub> catalyst. The catalyst was synthesized using a sequential incipient wetness impregnation method. Electron donating effect occurred from rhenium to platinum, thereby improving dehydrogenation activity.</p>
<p><b>Americas Halls 1 &amp; 2</b></p>	<p><b>Catalyst Characterization Poster Session I</b></p>
<p><b>Mon-P-35</b></p>	<p><b>Nature of Active Sites in Cu-Exchanged Small Pore Zeolites during NH<sub>3</sub>-SCR: An <i>Operando</i> X-Ray Absorption Spectroscopy Study</b>  Rachit Khare, Mirjam Wenig, <u>Andreas Jentys</u> and Johannes A. Lercher, <i>Technical University of Munich, Germany</i>.  Short Summary:  Ammonia-assisted selective catalytic reduction using Cu-exchanged small-pore zeolites is currently the leading technology to mitigate NO<sub>x</sub> emissions from engine exhaust. We present here a comprehensive study elucidating the nature of active sites in Cu-exchanged zeolites during NH<sub>3</sub>-SCR, utilizing X-ray absorption spectroscopy complemented with kinetic measurements and density functional theory calculations.</p>
<p><b>Mon-P-36</b></p>	<p><b>Revealing the Dynamics of Sabatier Reaction By IR Thermography</b>  <u>Emanuele Moio</u>li, <i>Paul Scherrer Institut, Switzerland</i>.  Short Summary:  The dynamics of CO<sub>2</sub> methanation reaction are analysed by means of infrared thermography</p>
<p><b>Mon-P-37</b></p>	<p><b>Ethylene Dimerization to <i>n</i>-butene with Nickel Sulfate on Zirconia: Investigation of the Molecular Structure and Activity of Surface Nickel and Sulfate Species</b>  <u>Erin Sobchinsky</u>, Shiao-Chien Tsai and Israel E. Wachs, <i>Lehigh University, USA</i>.  Short Summary:  To address the decrease in production of <i>n</i>-butene due to shifts to processing lighter hydrocarbon feedstocks, ethylene dimerization to <i>n</i>-butene with a heterogenous nickel sulfate zirconia catalyst was investigated. The molecular structure and important structure activity relationships were determined by applying several spectroscopic techniques under <i>in-situ</i> and <i>operando</i> conditions.</p>



<p><b>Mon-P-38</b></p>	<p><b>Effect of Tandem Modification on the Chemical and Textural Properties of Mexican Clinoptilolite for Use in Catalytic Pyrolysis of Seaweed</b>  Francisco Javier Pérez<sup>1</sup>, <a href="#">Carolina Solis Maldonado</a><sup>1</sup>, María Rebeca Rojas Ronquillo<sup>1</sup>, Rodrigo Cuervo<sup>1</sup>, Ladislao Sandoval-Rangel<sup>2</sup>, Lucía Atehortua<sup>3</sup>, Gloria Dimas Rivera<sup>4</sup> and Javier Rivera de la Rosa<sup>4</sup>, (1)Universidad Veracruzana, Mexico, (2) Instituto Tecnológico de Estudios Superiores de Monterrey, Mexico, (3)Universidad de Antioquia, Colombia, (4)Universidad Autónoma de Nuevo León, Mexico.  Short Summary:  Acidic (HCl and HNO<sub>3</sub>), alkaline (NaOH and KOH) and ion exchange (NaCl and NH<sub>4</sub>Cl) modifications were performed to the natural zeolite clinoptilolite (CL). And additionally, two and three aforementioned modifications were combined (tandem). The aim was to analyse the alterations on the chemical and structural properties of natural CL.</p>
<p><b>Mon-P-39</b></p>	<p><b>Direct Conversion of Ethylene to Propylene through Simultaneous Ethylene Dimerization and Olefin Metathesis with 8%NiSO<sub>4</sub>/8%ReO<sub>4</sub>/γ-Al<sub>2</sub>O<sub>3</sub> Catalyst</b>  <a href="#">Eli Ream</a>, Erwang Li and Israel E. Wachs, <i>Lehigh University, USA</i>.  Short Summary:  A supported 8%NiSO<sub>4</sub>/8%ReO<sub>4</sub>/γ-Al<sub>2</sub>O<sub>3</sub> catalyst was synthesized to convert ethylene directly into propylene through simultaneous ethylene dimerization and olefin metathesis. This catalyst was extensively characterized with Raman spectroscopy, <i>in situ</i> IR spectroscopy, <i>in situ</i> UV-vis spectroscopy, C<sub>2</sub>=TPSR spectroscopy, <i>in situ</i> XAS, HS-LEIS, and ammonia adsorption to probe surface acid sites.</p>
<p><b>Mon-P-40</b></p>	<p><b>Gas-Phase Synthesis and Characterization of Size-Selected Copper Nanoparticles for the Electrochemical CO/CO<sub>2</sub> Reduction Reactions Using Temperature Programmed Desorption: Establishing Trends in Activity</b>  <a href="#">Julius Lucas Needham</a> and Ib Chorkendorff, <i>Technical University of Denmark, Denmark</i>.  Short Summary:  In this study, we use CO temperature-programmed desorption measurements on size-selected copper nanoparticles of precise coverage in conjunction with electrochemical CO reduction measurements. This is enabled by a magnetron gas aggregation cluster source with a time-of-flight mass filter. The goal is to establish trends in the CO/CO<sub>2</sub> reduction reactions.</p>
<p><b>Mon-P-41</b></p>	<p><b>Transformation of Atomically Dispersed Platinum in SAPO-37 into Clusters: Catalyst for Ethylene Hydrogenation</b>  <a href="#">Jorge Perez-Aguilar</a><sup>1</sup>, James Hughes<sup>2</sup>, Cong-Yan Chen<sup>3</sup> and Bruce Gates<sup>3</sup>, (1)SLAC National Accelerator Laboratory, USA, (2) dexam, USA, (3)University of California, Davis, USA.  Short Summary:  SAPO-37-supported isolated platinum complexes were synthesized. FTIR and XAS data show that our catalyst clusters under ethylene hydrogenation conditions.</p>
<p><b>Mon-P-42</b></p>	<p><b>Partial Oxidation of Isobutylene Using Ni TiO<sub>x</sub></b>  <a href="#">Seth March</a><sup>1</sup>, Steven Suib<sup>1</sup>, Luisa Posada<sup>1</sup>, Inosh Perera<sup>1</sup>, Tharindu Kankanam Kapuge<sup>1</sup>, Vera Grankina<sup>2</sup> and Partha Nandi<sup>2</sup>, (1)University of Connecticut, USA, (2)Corporate Research, ExxonMobil Research and Engineering, USA.  Short Summary:  Using molecular oxygen to partially oxidize hydrocarbons is vital as the products of said reactions are precursors to valuable products. Herein, multiple Ni TiO<sub>x</sub> catalysts were able to partially oxidize isobutylene to produce p-xylene and isoprene. The latter of which was made without the use of the traditional co-reactant formaldehyde.</p>
<p><b>Mon-P-43</b></p>	<p><b>Differentiating Supported Platinum Single Atoms, Clusters and Nanoparticles By Styrene Hydrogenation</b>  <a href="#">Yuan Zhang</a> and Dongxia Liu, <i>University of Maryland - College Park, USA</i>.  Short Summary:  We demonstrate a simple method to assess the distribution of metal active sites in heterogeneous sample by styrene hydrogenation reaction. The relationship between reactivity and geometric/electronic properties of Pt sites influenced by particle sizes was developed. This correlation can be used to pre-screen supported Pt catalysts synthesized by different approaches.</p>
<p><b>Mon-P-44</b></p>	<p><b>Ni-Based Catalysts for CO<sub>2</sub> Methanation Probed By X-Ray Spectroscopy Under <i>in-Situ</i> Conditions</b>  <a href="#">Sven Wendholt</a> and Matthias Bauer, <i>Paderborn University, Germany</i>.  Short Summary:  A key challenge for future sustainable energy supply is the long-term storage of energy from renewable resources. Catalysts formed by the decomposition of MOFs can be used as promising catalysts for CO<sub>2</sub> methanation. However, for a deeper understanding, we need to investigate pre-catalysts as and catalytic studies <i>in-situ</i>.</p>
<p><b>Mon-P-45</b></p>	<p><b>Synthesis of Supported Pd/Au Dilute Limit Alloy Nanoparticles</b>  Abolfazl Shakouri, Anhua Dong, <a href="#">Christopher T. Williams</a> and John R. Regalbuto, <i>University of South Carolina, USA</i>.  Short Summary:  Dilute limit alloy (DLA) catalysts offer unique reactivity, but a facile synthesis and characterization remain challenging. We present strong electrostatic adsorption (SEA) for synthesizing ultra-small, homogeneously alloyed DLA catalysts and <i>in situ</i> CO adsorption in the FTIR technique for confirming site isolation.</p>

<b>Mon-P-46</b>	<p><b>On the Active Surface of Cu/ZnO/Al<sub>2</sub>O<sub>3</sub> Catalysts for the Methanol Synthesis</b>  <u>Tabea Gros</u>, Tim Kratky, Sebastian Günther and Olaf Hinrichsen, <i>Technical University of Munich, Germany</i>.  Short Summary:  The Power-to-Methanol concept is of growing interest due to its ability to store and transport energy from renewable sources. In this study, Cu/ZnO/Al<sub>2</sub>O<sub>3</sub> catalysts are characterized using a combination of surface sensitive X-ray photoelectron spectroscopy and measurements in a standard reactor setup to shed light on the active surface.</p>
<b>Mon-P-47</b>	<p><b>CO-FTIR Diagnosis of Dilute Limit Alloy Bimetallic Catalysts</b>  <u>Leandro De Castro</u><sup>1,2</sup>, Dia Sahrah<sup>2</sup>, Andreas Heyden<sup>2</sup>, Christopher T. Williams<sup>2</sup> and John R. Regalbuto<sup>2</sup>, (1)<i>University of the Philippines Los Baños, Philippines</i>, (2)<i>University of South Carolina, USA</i>.  Short Summary:  Fitted Gaussian functions for the proposed single-atom sites indirectly give the degree of binding energy relative to different base metals where the isolated atom is located. The trends could provide insights when comparing the rates and reaction mechanisms involved in using single atom alloy catalysts.</p>
<b>Mon-P-48</b>	<p><b>Quantifying Catalytic Sites in Lewis Acid Zeolite Beta</b>  <u>Leah Ford</u>, Alexander Spanos and Nicholas Brunelli, <i>The Ohio State University, USA</i>.  Short Summary:  This work demonstrates the importance of quantifying the fraction of catalytic sites in heterogeneous catalytic materials such as Sn-Beta. Through using different poisons, we can discern important synthesis-structure-function relationships.</p>
<b>Mon-P-49</b>	<p><b>Synthesis and Characterization of CuFe<sub>2</sub>O<sub>4</sub> Catalyst Supported over β-SiC Foam for Hydrogen Production in the S-I Cycle</b>  Sachin Tomar<sup>1</sup>, <u>Anshuman Goswami</u><sup>2</sup> and Sreedevi Upadhyayula<sup>1</sup>, (1)<i>Indian Institute of Technology Delhi, India</i>, (2)<i>University of Notre Dame, USA</i>.  Short Summary:  CuFe<sub>2</sub>O<sub>4</sub> supported over β-SiC foam was synthesized using wet impregnation followed by high temperature solid state route and characterized using various techniques such as XRD, FT-IR, and BET. Issues such as low catalytic activity, hot spot formation, and pressure drop can be tackled with the synthesized catalyst.</p>
<b>Mon-P-50</b>	<p><b>Nanoparticle Reconfiguration at Aupd Catalysts Driven By Reaction Atmosphere</b>  Adriano Braga<sup>1,2</sup>, Raiza R. G. Rezende<sup>1</sup>, Lais Reis Borges<sup>1</sup>, Adam Hoffman<sup>3</sup>, Simon Bare<sup>3</sup> and Liane Rossi<sup>1</sup>, (1)<i>University of São Paulo, Brazil</i>, (2)<i>Texas Tech University, USA</i>, (3)<i>SLAC National Accelerator Laboratory, USA</i>.  Short Summary:  Bimetallic nanoparticles undergo reconfiguration upon thermal treatments and reaction atmosphere. Here, we evaluated Au-Pd alloy containing catalysts in the gas phase oxidation of ethanol and for selective CO oxidation in presence H<sub>2</sub>, correlating structure of the nanoparticles with catalytic activity and selectivity.</p>
<b>Mon-P-51</b>	<p><b>Synthesis and Characterization of Bimetallic Cu-Ni/Bentonite Catalysts for Hydrogenation of Levulinic Acid</b>  Gloria Dimas Rivera<sup>1</sup>, Javier Rivera de la Rosa<sup>1</sup>, <u>Carlos Lucio Ortiz</u><sup>1</sup>, Ladislao Sandoval-Rangel<sup>2</sup>, David De Haro Del Rio<sup>1</sup> and Carolina Solis Maldonado<sup>3</sup>, (1)<i>Universidad Autónoma de Nuevo León, Mexico</i>, (2)<i>Tecnológico de Monterrey, Mexico</i>, (3)<i>Universidad Veracruzana, Mexico</i>.  Short Summary:  Gamma-valerolactone (GVL) is a chemical product which has had a significant impact due to its applications as fuel additive or green solvent. GVL synthesis generates from levulinic acid (AL) via catalytic hydrogenation, using noble metal catalysts such as Pt, Ru, and Pd [1].</p>
<b>Mon-P-52</b>	<p><b>Micro Computed Tomography Analysis of Four-Way Conversion Catalysts Using Artificial Intelligence-Enabled Image Processing</b>  <u>Robert M. Palomino</u><sup>1</sup>, Chunxin Ji<sup>1</sup>, Ke-Bin Low<sup>1</sup>, Ivan Petrovic<sup>1</sup>, Florian Waltz<sup>2</sup> and Thomas Schmitz<sup>2</sup>, (1)<i>BASF Corporation, USA</i>, (2)<i>BASF Catalysts GmbH, Germany</i>.  Short Summary:  Artificial intelligence-driven computer vision is used for robust semantic segmentation on tomographic data to enhance 3D structural elucidation, which paves the way for quantitative analysis. This is successfully demonstrated to quantify 3D morphological features of Four-Way Conversion catalyst (FWC) that are correlated with increased back-pressure.</p>
<b>Mon-P-53</b>	<p><b>Iso-Potential Spectroscopy: A New Concept for Operando Studies of Solid Catalysts in Reactors from Laboratory to Industrial Size</b>  Sarah-Franziska Stahl<sup>1</sup>, Sebastian Sichert<sup>2</sup>, <u>Oliver Korup</u><sup>2</sup> and Raimund Horn<sup>2</sup>, (1)<i>Reacnostics GmbH, Germany</i>, (2)<i>Hamburg University of Technology, Germany</i>.  Short Summary:  Operando studies deliver impressive insights into the structure and function of solid catalysts under industrial reaction conditions. Unfortunately, dedicated operando cells are often optimized to the spectroscopic environment, only, and show bad reaction engineering characteristics. To overcome this problem the concept of iso-potential spectroscopy is introduced in this contribution.</p>

## Americas Halls 1 & 2

### Catalyst Design and Synthesis Poster Session I

Mon-P-54

**A Redox Stability and *in Situ* Drifts Investigation into Low-Temperature CO Oxidation for Perovskite-Supported Copper**  
Tu Nguyen, Kandis Leslie Abdul-Aziz and Krassimir Bozhilov, *University of California, Riverside, USA*.

Short Summary:

To understand how perovskites can be used to stabilize catalysts, LaMnO<sub>3</sub> and LaFeO<sub>3</sub> loaded with Cu are compared for low temperature, CO Oxidation after cycling between oxidation at 850°C and reduction at 550°C. Additionally, *in situ* DRIFTS is used to determine the stability of CO-derived species at elevated temperatures.

Mon-P-55

**Mechanochemical Synthesis of Hierarchical Zeolites and Performance to Reduce the Deactivation in the Dealkylation of 4-n-Propylphenol**

Laura Silva<sup>1</sup>, Michael Stellato<sup>2</sup>, Mariana Rodrigues<sup>1</sup>, Jeffrey Kenvin<sup>3</sup>, Andreas Bommarius<sup>2</sup>, Leandro Martins<sup>1</sup> and Carsten Sievers<sup>2</sup>, (1)*UNESP, Brazil*, (2)*Georgia Institute of Technology, USA*, (3)*Micromeritics Instrument Corporation, USA*.

Short Summary:

The delamination of MCM-22 using shear forces in a vibratory ball mill, rather than chemical surfactants and sonication, is illustrated. The resulting material has comparable or improved physical properties compared to chemically delaminated MCM-22 without a significant loss of acid sites.

Mon-P-56

**Heterolytic H<sub>2</sub> Adsorption of Ru/MgO Contributes to Enhanced Hydrogen Storage into LOHC Compounds**

Tae Wan Kim and Young-Woong Suh, *Hanyang University, Korea, Republic of (South)*.

Short Summary:

The Ru/MgO catalysts prepared by loading Ru<sub>3</sub>(CO)<sub>12</sub> on surface OH-intact Mg(OH)<sub>2</sub> achieved surface Ru enrichment and exhibited higher LOHC compounds hydrogenation activity, compared to other supported Ru catalysts. This is due to the enhanced H<sub>2</sub> adsorption capacity by the realization of heterolytic H<sub>2</sub> adsorption at the Ru–MgO interface.

Mon-P-57

**Synthetic Methods to Influence the Spatial Distribution of Framework Al Sites in in MFI Zeolite Crystallites**

Ricem Diaz Arroyo, Sopuruchukwu Ezenwa and Rajamani Gounder, *Purdue University, USA*.

Short Summary:

Complex reaction networks in acid zeolites are often influenced by intracrystalline diffusional constraints, which depend on the proton density, diffusion path length, and crystallite-scale Al distribution and zoning. The synthesis of core-shell MFI zeolites to influence Al zoning provides materials that allow probing the effects of diffusional constraints on catalysis.

Mon-P-58

**Highly Selective and Stable Core/Shell Au/Pt Catalysts for Oxidation of Glucose to Glucaric Acid**

Junrui Li<sup>1</sup>, Chaochao Dun<sup>2</sup>, Sichi Li<sup>3</sup>, Yixiao Li<sup>1</sup>, Kecheng Wei<sup>4</sup>, Shouheng Sun<sup>4</sup>, Jeffery Urban<sup>2</sup>, Junming Sun<sup>1</sup>, Austin Winkelman<sup>1</sup>, Anthony Savoy<sup>1</sup> and Yong Wang<sup>5</sup>, (1)*Washington State University, USA*, (2)*Lawrence Berkeley National Laboratory, USA*, (3)*Lawrence Livermore National Laboratory, USA*, (4)*Brown University, USA*, (5)*Pacific Northwest National Laboratory, USA*.

Short Summary:

This work reported a highly selective and stable core/shell Au/Pt catalyst for the oxidation of glucose to glucaric acid. Core/shell Au/Pt nanoparticles (NPs) with tunable Pt overlayer thickness and AuPt alloy were synthesized. The core/shell Au<sub>44</sub>/Pt<sub>56</sub> showed enhanced selectivity and stability than alloy and pure Pt by mitigating nanoparticles aggregation.

Mon-P-134

**Supporting Gold Nanoclusters on Commercial Zeolites By Post-Synthetic Internal Surface Modifications**

Changbum Jo and Eun Ji Eum, *Inha University, Korea, Republic of (South)*.

Short Summary:

We developed a facile strategy for supporting 1- 2 nm-sized gold nanoparticles on commercial beta, MFI, and FAU zeolites by post-synthetic internal surface modification with thiol groups. The resulting gold supported zeolites exhibited a high activity in CO oxidation and acetylene hydrogenation reactions.

Mon-P-59

**Designing Finned and Core-Shell Zeolite Catalysts with Enhanced Diffusion Properties**

Kumari Shilpa, Heng Dai, Sungmin Han, Thuy T. Le and Jeffrey D. Rimer, *University of Houston, USA*.

Short Summary:

This work focuses on two different zeolite configurations with improved mass transport properties: finned zeolite and eggshell zeolite (reverse core-shell configuration). Both these configurations are shown to have superior catalytic performance compared to their conventional analogues, in terms of enhancement of catalyst lifetime, increased turnover numbers and greater diffusivity.

Mon-P-60

**Synthesis and Characterization of Meapo-36 Materials (Me = Zn, Co, Mg) and Zn-Modified ZSM-5 Zeolites Used for the Catalytic Conversion of Methanol**

José Gabriel Flores Aguilar and Julia Aguilar Pliego, *Universidad Autonoma Metropolitana-Azcapotzalco, Mexico*.

Short Summary:

This work presents a study of the use of zeolites and zeotypes for the transformation reaction of methanol to hydrocarbons (MTH). Materials of the aluminophosphate type MeAPO-36 were prepared where Me is Zn, Mg and Co, synthesized by the hydrothermal method, also with two commercial ZSM-5 zeolites modified with zinc

<b>Mon-P-61</b>	<p><b>Deposition of Gold Nanoparticle Catalysts inside the Pores of Zeolites Using Reversible Ionic Liquids</b>  Zengran Sun and <u>Steven Saunders</u>, <i>Washington State University, USA</i>.  Short Summary:  Herein, we demonstrate an improved SBA-15 supported gold nanoparticle catalyst preparation—the RevIL-stabilized gold nanoparticles are deposited in the prepared SBA-15 zeolites via an incipient wetness (IW) technique, leveraging the switchable nature of RevILs. This technique can prepare highly active and thermally stable catalysts that require minimal processing.</p>
<b>Mon-P-62</b>	<p><b>High-Silica Pd/LTA Catalysts for Low Temperature CH<sub>4</sub> Oxidation</b>  <u>Tala Mon</u><sup>1</sup>, Jingzhi Liu<sup>2</sup>, Viktor Cybulskis<sup>2</sup> and Eleni A. Kyriakidou<sup>1</sup>, (1)<i>University at Buffalo (SUNY), USA</i>, (2)<i>Syracuse University, USA</i>.  Short Summary:  Small-pore LTA zeolites were synthesized with Si/Al molar ratios from 22 to 52, ion-exchanged with 1 wt.% Pd, and evaluated for CH<sub>4</sub> oxidation performance. Pd/H-LTA catalysts with Si/Al ≥ 39 can convert 90% CH<sub>4</sub> at temperatures lower than 400 °C and have stable performance in the presence of water.</p>
<b>Mon-P-63</b>	<p><b>Mesoporous NiCo/Mg-Aluminate Catalyst with High Activity and Coke Resistance for Methane Reforming</b>  <u>Dong-Hyun Kim</u>, Jae-Rang Youn, Min-Jae Kim and Kyubock Lee, <i>Chungnam National University, Korea, Republic of (South)</i>.  Short Summary:  The significant enhancement in the performance after adding Co is due to the synergistic effect between the two active metals, and admirable resistance for coke deposition. The insights obtained from this study may have broad applications in developing highly stable NiCo bimetallic catalysts for methane reforming reactions.</p>
<b>Mon-P-64</b>	<p><b>Importance of Precise Nickel Siting and Dispersion in Supported Nickel Dry Reforming Catalysts</b>  <u>Jonathan Lucas</u>, <i>LSU, USA</i>.  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. Lower coking rates and greatly increased operation times are seen.</p>
<b>Mon-P-65</b>	<p><b>Identifying Active Sites in Pd-Zeolites for Direct H<sub>2</sub>O<sub>2</sub> Synthesis</b>  <u>Tomas Ricciardulli</u> and David Flaherty, <i>University of Illinois Urbana-Champaign, USA</i>.  Short Summary:  Palladium supported on zeolites can show significantly higher H<sub>2</sub>O<sub>2</sub> formation rates and selectivities in comparison to SiO<sub>2</sub> and Al<sub>2</sub>O<sub>3</sub> supports. The possible states of Pd within Pd-zeolites are discussed and characterized to identify the catalytically active form of Pd for H<sub>2</sub>O<sub>2</sub> synthesis.</p>
<b>Mon-P-66</b>	<p><b>Thin-Shelled Nickel Silicate Spheres for Methane Dry Reforming: Hollow Structure and Functionality Relationship</b>  Mohammadreza Kosari<sup>1,2</sup>, Abdul Majeed Seayad<sup>1</sup>, <u>Armando Borgna</u><sup>1</sup> and Hua Chun Zeng<sup>2</sup>, (1)<i>Institute of Chemical and Engineering Sciences, A*STAR, Singapore</i>, (2)<i>National University of Singapore, Singapore</i>.  Short Summary:  Hollow nanocatalysts are emerging nanomaterials with specific architectural features and favorable catalytic functionality. Herein, nickel silicate hollow spheres with different shell thickness and interior cavity size were designed and synthesized. Optimal curvature conformation and thin shell could minimize sintering and coking while improving catalytic performance during dry reforming.</p>
<b>Americas Halls 1 &amp; 2</b>	<p><b>Conversion of Biomass Resources and Polymers Poster Session I</b></p>
<b>Mon-P-68</b>	<p><b>Chemical Upcycling of Cellulosic Biomass into Polyhydroxyalkanoates</b>  <u>Md. Anwar Hossain</u><sup>1</sup>, Sarttrawat Tulaphol<sup>2</sup>, Mohammad Shahinur Rahaman<sup>1</sup>, Jie Dong<sup>1</sup> and Noppadon Sathitsuksanoh<sup>1</sup>, (1)<i>University of Louisville, USA</i>, (2)<i>King Mongkut's University of Technology Thonburi, Thailand</i>.  Short Summary:  We developed a combined chemical and biological technology to convert lignocellulose-derived glucose from rice straw and hemp hurd into medium-chain-length polyhydroxyalkanoates (mcl-PHAs). We achieved a high sugar release (&gt; 88 wt.%) using alkaline treatment at ambient condition and obtained 50-61g mcl-PHAs/L.</p>
<b>Mon-P-70</b>	<p><b>Controlling Lignin Catalytic Depolymerization ?</b>  Lucile Olivier, Christophe Geantet and <u>Dorothee Laurenti</u>, <i>Université de Lyon, CNRS, France</i>.  Short Summary:  Lignin derivatives might be more interesting than lignin if they are well-defined and possess higher amount of OH groups that can be further functionalized. In order to get OH-enriched oligomers from technical lignin, we undertook here a study to develop heterogeneous catalysts able to cleave selectively ether bonds.</p>
<b>Mon-P-72</b>	<p><b>Catalytic Upgrade of Pyrolysis Vapors: C-C Coupling of Acetic Acid on TiO<sub>2</sub> for Biofuels Production</b>  <u>Veronica Piazza</u>, Luca Lietti and Alessandra Beretta, <i>Politecnico di Milano, Italy</i>.  Short Summary:  C-C coupling processes of C2-C4 oxygenates represent an interesting solution for the upgrade of pyrolysis vapors and biofuels production. In this work, acetic acid chain-growth reactions are studied on TiO<sub>2</sub> catalyst, proving relevant performances in promoting not only ketonization but also secondary growth reactions with the formation of C8+ species.</p>

<b>Mon-P-73</b>	<p><b>Liquid Phase Hydrodeoxygenation of Guaiacol Using Activated Carbons As Supports: The Effects of Solvents and Support Properties</b></p> <p>Lei Yu, Jeffrey Page, Robert Gottlieb, Matthew Stuber and <u>Ioulia Valla</u>, <i>University of Connecticut, USA</i>.</p> <p>Short Summary:</p> <p>This study investigated the effects of AC support properties and solvents on the catalytic performance of guaiacol HDO in liquid phase. The results of the study reveal the reaction mechanism and interactions between catalysts and solvents during the reaction, which might assist researchers understand the fundamentals of HDO of bio-oils.</p>
<b>Mon-P-74</b>	<p><b>A New Route for Manufacturing Aromatics By Diels-Alder Reaction Using Ethanol and Furfural As Reactants</b></p> <p><u>Juan Gancedo</u>, Laura Faba and Salvador Ordóñez, <i>University of Oviedo, Spain</i>.</p> <p>Short Summary:</p> <p>We propose a new route for preparing aromatics from primary bio-platform molecules (furfural and ethanol) improving the catalytic selectivity and stability in comparison to the well-established Diels-Alder process using secondary bio-derived compounds, as furan and ethylene.</p>
<b>Mon-P-75</b>	<p><b>Effect of Pd Promotion and Catalyst Support on the Ni-Catalyzed Deoxygenation of Tristearin to Fuel-like Hydrocarbons</b></p> <p>Fei Wang<sup>1</sup>, Robert Pace<sup>2</sup>, Yaying Ji<sup>2</sup>, <u>Eduardo Santillan-Jimenez</u><sup>2</sup> and Mark Crocker<sup>2</sup>, (1)<i>Chinese Academy of Forestry, China</i>, (2)<i>University of Kentucky, USA</i>.</p> <p>Short Summary:</p> <p>A bifunctional catalyst comprising Ni promoted with a small amount of Pd can quantitatively convert tristearin to diesel-like hydrocarbons in excellent yield. Structure-activity relationships explaining the effects of Pd promotion and acidic supports on the reaction were deduced. Notably, the hydrotreatment pathway followed can be directed via the support acidity.</p>
<b>Mon-P-76</b>	<p><b>Engineering Surface Magnesium Silicates By Modified Wet-Kneading for One-Step Ethanol-to-Butadiene Lebedev Process</b></p> <p>Sang-Ho Chung, Tuiana Shoinkhorova, Ildar Mukhambetov, Adrian Ramirez, Edy Abou-Hamad, Selvedin Telaovic, Jorge Gascon and <u>Javier Ruiz-Martinez</u>, <i>King Abdullah University of Science and Technology (KAUST), Saudi Arabia</i>.</p> <p>Short Summary:</p> <p>Over 70 years, the origin and the location of magnesium silicates formed during wet-kneading have been unclear. Here we show direct relations of beneficial/detrimental magnesium silicates on one-step ethanol-to-butadiene process, and expect this study opens a new possibility for the development of the next generation Lebedev catalysts.</p>
<b>Mon-P-77</b>	<p><b>High Purity Bio-Based Acrylic Acid from Two-Step Oxidation of Allyl Alcohol Derived from Crude Glycerol</b></p> <p><u>Jinsuo Xu</u>, <i>Dow Inc., USA</i>.</p> <p>Short Summary:</p> <p>Shifting feedstock from fossil-based propylene to bio-renewable feeds can lead to more sustainable processes for acrylic acid (AA). Here we report the two-step oxidation of allyl alcohol over the same catalysts used for propylene. Combined with allyl alcohol production from crude glycerol, this route may advance large-scale bio-based AA production.</p>
<b>Mon-P-78</b>	<p><b>Novel ZSM-5/MCM-41 Composites for One-Step Hydropyrolysis and Hydrotreating Reactions of Biomass</b></p> <p><u>Jeffrey Page</u><sup>1</sup>, Lei Yu<sup>1</sup>, Azeem Farinmade<sup>2</sup>, Oluwole Ajumobi<sup>2</sup>, Vijay John<sup>2</sup> and Ioulia Valla<sup>1</sup>, (1)<i>University of Connecticut, USA</i>, (2)<i>Tulane University, USA</i>.</p> <p>Short Summary:</p> <p>This study reports on the hydropyrolysis of miscanthus × giganteus using composite ZSM-5/MCM-41 catalysts. The composite catalysts are shown to promote alkane production and produce comparable hydrocarbon yields to a two stage hydropyrolysis and hydrotreatment system.</p>
<b>Mon-P-79</b>	<p><b>Effect of Support on Anisole Hydrodeoxygenation over Ni-Based Catalysts</b></p> <p><u>Reyna Rios</u><sup>1</sup>, José Escobar<sup>2</sup> and Jose Antonio De los Reyes<sup>1</sup>, (1)<i>Universidad Autónoma Metropolitana-Iztapalapa, Mexico</i>, (2)<i>Instituto Mexicano del Petróleo, Mexico</i>.</p> <p>Short Summary:</p> <p>Anisole HDO over Ni catalysts was carried out to understand the support effect of catalysts with the aim to obtain desired activity and selectivity for potential bio-oil upgrading. High surface TiO<sub>2</sub>-ZrO<sub>2</sub> improved the selectivity to benzene and activity of TiO<sub>2</sub> and ZrO<sub>2</sub> single oxide supports in Ni catalysts for HDO.</p>
<b>Mon-P-80</b>	<p><b>Catalytic Role of Metals Supported on SBA-16 in Cyclohexene Epoxidation and Hydrodeoxygenation of Chemical Compounds Derived from Biomass Processing</b></p> <p>Agnieszka Feliczak-Guzik<sup>1</sup>, Paulina Szczyglewska<sup>1</sup>, Mietek Jaroniec<sup>2</sup> and <u>Izabela Nowak</u><sup>1</sup>, (1)<i>Adam Mickiewicz University, Poznan, Poland</i>, (2)<i>Kent State University, USA</i>.</p> <p>Short Summary:</p> <ul style="list-style-type: none"> <li>- use of mesoporous SBA-16 type silica materials modified with Ir, Ru, Pd, Pt atoms in hydrodeoxygenation of model chemicals (guaiacol, syringol, creosol) under mild experimental conditions (90 to 130; 25 to 60 bar H<sub>2</sub>);</li> <li>- high selectivity towards chemical compounds with lower O/C and higher H/C ratios.</li> </ul>



<b>Mon-P-81</b>	<p><b>Fixed Bed Hydrogenation of Proprietary Oleochemical Derivative</b>  Kelsey Abner, Miranda Jackson, Keith Johnson and <u>Robert Gulotty</u>, <i>Applied Ceramics, USA</i>.  Short Summary:  A sucrose ester, derived from sugar and vegetable oil is hydrogenated for use in paints, coatings, composites, adhesive and lubricants. A fixed bed continuous hydrogenation pilot reactor produces the hydrogenated sucrose ester with 97-99% conversion in a single reactor pass using an activated carbon monolith catalyst containing Palladium.</p>
<b>Mon-P-82</b>	<p><b>Selective Catalytic Hydrogenation of Biomass Derived Furans to Secondary Alcohols Under Mild Reaction Conditions</b>  <u>Jakob Albert</u> and Magdy Sherbi, <i>Hamburg University, Germany</i>.  Short Summary:  Promising bifunctional catalyst systems composed of platinum and polyoxometalates (POMs) were successfully applied for the selective catalytic hydrogenation of 2,5-dimethylfuran (DMF) to 2-hexanol at 80 °C and 10 bar H<sub>2</sub> pressure using decane as a carrier liquid. Hereby, an exceptionally high yield of 2-hexanol (72.5%) was achieved.</p>
<b>Mon-P-83</b>	<p><b>Enhanced Hydrogenation of Levulinic Acid over Ordered Mesoporous Alumina-Supported Ni-Cu Bimetallic Catalysts</b>  Reibelle Raguindin and Jeong Gil Seo, <i>Hanyang University, Korea, Republic of (South)</i>.  Short Summary:  <b>This work has provided significant advancements on the yield of GVL (100.0%) and 2-MTHF (73.0%) that can be obtained from LA under a solvent-free reaction environment, and on the performance and recoverability of alumina-supported catalysts.</b></p>
<b>Americas Halls 1 &amp; 2</b>	<p><b>Electrocatalysis and Photocatalysis Poster Session I</b></p>
<b>Mon-P-84</b>	<p><b>Dielectrics for Light-Matter Interaction: Application in Photocatalysis</b>  Ravi Teja Addanki Tirumala, <u>Sundaram Bhardwaj Ramakrishnan</u> and Marimuthu Andiappan, <i>Oklahoma State University, USA</i>.  Short Summary:  Dielectric refractive-indexed materials have the ability to enhance both electric and magnetic field from the incoming light. This ability arises from Mie resonance exhibited by these materials. These resonances can be tuned by controlling shape and size, which will give us the ability to harvest wider spectrum of solar-light.</p>
<b>Mon-P-85</b>	<p><b>Effect of Brookite on the Photocatalytic Activity Under Sunlight of Undoped TiO<sub>2</sub> Mixed Phases</b>  <u>Nicola Blangetti</u><sup>1</sup>, Francesca Freyria<sup>1</sup>, Maela Manzoli<sup>2</sup>, Serena Esposito<sup>1</sup> and Barbara Bonelli<sup>1</sup>, (1)<i>Politecnico di Torino, Italy</i>, (2)<i>University of Turin, Italy</i>.  Short Summary:  The photocatalytic activity under UV and sunlight is reported of undoped TiO<sub>2</sub> mixed phases: brookite-related heterojunctions enhanced the nanomaterials activity as they were able to efficiently exploit the small UV fraction in of solar radiation. The most active photocatalyst was the one obtained by a green synthetic route.</p>
<b>Mon-P-87</b>	<p><b>Oxidative Functionalization of Carbon Supports for Ni-Based Electrolyzer Catalysts</b>  <u>Manjodh Kaur</u>, Rituja Patil and James McKone, <i>University of Pittsburgh, USA</i>.  Short Summary:  Our laboratory is developing Ni-Mo and Ni-Fe alloys for alkaline hydrogen and oxygen evolution, respectively. This study highlights the impact of several treatments, involving pre-oxidation of the carbon support, catalyst composition, morphology, dispersion and practical performance of these catalysts in the laboratory and in alkaline anion exchange membrane (AEM) electrolyzers.</p>
<b>Mon-P-88</b>	<p><b>The Local Mass Transport of Ketene and Acetate Selectivity in Electrochemical CO Reduction</b>  <u>Haeun Shin</u><sup>1</sup>, Hendrik H. Heenen<sup>2</sup> and Feng Jiao<sup>1</sup>, (1)<i>University of Delaware, USA</i>, (2)<i>Technical University of Denmark, Denmark</i>.  Short Summary:  Electrochemical CO reduction to acetate is one of the promising CCUS technologies to convert CO<sub>2</sub> to high-value chemicals. We present a new comprehensive reaction mechanism of acetate formation in electrochemical CO reduction providing a rational catalyst design to improve selectivity.</p>
<b>Mon-P-89</b>	<p><b>Effects of SO<sub>2</sub> Trace Impurities in CO<sub>2</sub> Feed on Copper and Tin Based Catalysts during CO<sub>2</sub>RR</b>  <u>Subhajyoti Samanta</u><sup>1</sup>, Marcello Ferrara<sup>1,2</sup>, Manuela Bevilacqua<sup>3</sup>, Michele Melchionna<sup>4</sup>, Paolo Fornasiero<sup>4</sup> and Jonas Baltrusaitis<sup>1</sup>, (1)<i>Lehigh University, USA</i>, (2)<i>Università di Trieste, Italy</i>, (3)<i>ICCOM-CNR, Italy</i>, (4)<i>University of Trieste, Italy</i>.  Short Summary:  CO<sub>2</sub>RR has been a topic of research for decades, promising a green way to reuse our CO<sub>2</sub> output. However, few studies have been performed to understand the influence of gaseous impurities in CO<sub>2</sub> electroreduction. Herein, we studied the selectivity changes in Copper/Tin oxides with low concentrations of SO<sub>2</sub> (&lt;1%)</p>

Mon-P-90	<p><b>Sustainable Photocatalytic Water Remediation Via Strongly Coupled AgBiO<sub>3</sub> on PVDF/Pbsa Membranes</b>  <u>Bhanupriya Boruah</u><sup>1,2</sup> and Jayant M Modak<sup>2</sup>, (1)<i>The University of Kansas, USA</i>, (2)<i>Indian Institute of Science, India</i>.  Short Summary:  Photocatalyst AgBiO<sub>3</sub> nanoparticles are synthesized and characterized to study the optical and physical properties. Further, they are immobilized on PVDF/PBSA membranes and these could effectively decontaminate water from pathogens and dissolved organic compounds. In addition, incorporation of these nanoparticles enhanced the flux and antifouling properties of the pristine PVDF/PBSA membrane</p>
Mon-P-91	<p><b>Atomically Flat, Polycrystalline Surfaces for Metal/Metal-Oxide Interfacial Electrocatalysis</b>  James McKone, <u>Samantha Roenigk</u> and Rituja Patil, <i>University of Pittsburgh, USA</i>.  Short Summary:  Ultra-thin, flat, polycrystalline, metal surfaces are created by template stripping to observe metal/metal oxide interfaces that enhance the activity of the catalyst. The template stripped surface will be exposed to a metal salt creating a metal/metal-oxide film that will have bifunctional reactivity.</p>
Mon-P-93	<p><b>Insights into Proton Recombination in Ceramic Proton Conducting Electrodes</b>  <u>Jian Chang</u><sup>1</sup>, Colin Lehman<sup>1</sup>, John M. Vohs<sup>1</sup>, Raymond J. Gorte<sup>1</sup>, Aleksandra Vojvodic<sup>1</sup>, Kunli Yang<sup>2</sup> and Steven McIntosh<sup>2</sup>, (1)<i>University of Pennsylvania, USA</i>, (2)<i>Lehigh University, USA</i>.  Short Summary:  The effect of catalyst addition on H<sub>2</sub> evolution from composite electrodes of La<sub>0.7</sub>Sr<sub>0.3</sub>TiO<sub>3</sub> (LST) and BaZr<sub>0.1</sub>Ce<sub>0.7</sub>Y<sub>0.1</sub>Yb<sub>0.1</sub>O<sub>3-6</sub> (BZCYYb) was studied. The implications for potential application to electrochemical synthesis of ammonia are discussed.</p>
Mon-P-94	<p><b>Evaluation of Fe<sub>x</sub>/TiO<sub>2</sub> Catalysts in the Photocatalytic Degradation of Phenol Under Visible and Dark Light Region.</b>  <u>Felipe Sanchez</u>, Diego Alvarez, Carlos Santolalla and Victor Santes, <i>National Polytechnique Institute, Mexico</i>.  Short Summary:  FeS-X/TiO<sub>2</sub> catalyst were prepared to evaluate the photocatalytic degradation of phenol under visible and dark light region. Main results shows that the presence of FeCl<sup>+</sup> in solution, previously to impregnation, promotes the active sulphide species maintaining the band gap and improves the degradation of phenol.</p>
Mon-P-95	<p><b>Oxygen Vacancies and Hydroxyl Groups Drive Reduction of CO<sub>2</sub> on Cu<sub>2</sub>O Via Photocatalytic Hydrogenation</b>  Tien Le and <u>Bin Wang</u>, <i>University of Oklahoma, USA</i>.  Short Summary:  We found that the oxygen vacancies can be generated on Cu<sub>2</sub>O surfaces with relatively low energy. Hydroxyl groups could reduce the migration pathway of surface hydrogens. The oxygen vacancies can lower the intrinsic activation energy of CO<sub>2</sub> dissociation and localize non-equilibrium electrons to reduce it further.</p>
Mon-P-97	<p><b>First Principles Insights into the Electrocatalytic Reduction for Electrochemical Synthesis</b>  <u>Matthew Neurock</u><sup>1</sup>, Sahithi Gorthy<sup>1</sup>, Sagar Udyavara<sup>1</sup>, Ashwin Chemburkar<sup>1</sup> and Stuart Winikoff<sup>2</sup>, (1)<i>University of Minnesota, Twin Cities, USA</i>, (2)<i>Truman State University, USA</i>.  Short Summary:  We examine in detail and compare the interesting similarities in the reduction of CO<sub>2</sub> in ionic-liquid electrolytes over Bi and the reduction of phenyl ethanol in LiBr with protonating agents in aprotic solvents over Zn electrodes. We show how such systems can be tuned to increase their activities and selectivities.</p>
Mon-P-98	<p><b>Plasma-Catalytic Ammonia Synthesis in a Dielectric Barrier Discharge Reactor: A Combined Experimental Study and Kinetic Modelling</b>  <u>Jakob Afzali Andersen</u><sup>1</sup>, Jakob M. Christensen<sup>1</sup>, Martin Østberg<sup>2</sup>, Annemie Bogaerts<sup>3</sup> and Anker D. Jensen<sup>1</sup>, (1)<i>Technical University of Denmark, Denmark</i>, (2)<i>Haldor Topsøe A/S, Denmark</i>, (3)<i>University of Antwerp, Belgium</i>.  Short Summary:  Plasma-catalytic ammonia synthesis via dielectric barrier discharge has emerged as a possible route for electrification of nitrogen fixation. Here, we present a combination of experiments and a plasma kinetic model to investigate NH<sub>3</sub> synthesis from N<sub>2</sub> and H<sub>2</sub> both with and without a (potentially catalytic) packing material in the plasma.</p>
Americas Halls 1 & 2	<p><b>Fundamentals of Catalysis Poster Session I</b></p>
Mon-P-133	<p><b>Effects of Aqueous-Organic Solvent Mixtures on Alkene Epoxidations in Ti-BEA Zeolites</b>  <u>David Potts</u>, Ohsung Kwon and David Flaherty, <i>University of Illinois Urbana-Champaign, USA</i>.  Short Summary:  The majority of epoxidation reactions take place in environmentally impactful organic solvents. Here, we examine the effect of using large mole fractions of water (0 - 0.9) within organic solvents. We demonstrate that epoxidation rates increase with water fraction, leading to a more efficient and environmentally friendly process.</p>
Mon-P-99	<p><b>Nature and Enhanced Catalytic Performance of Brønsted Acid Sites Induced By Non-Framework Aluminum Species in H-ZSM5 Zeolite: A Theoretical Perspective</b>  <u>Vy T. Nguyen</u>, Tram Pham, Taha Salavati Fard, Steven P. Crossley and Bin Wang, <i>University of Oklahoma, USA</i>.  Short Summary:  The enhanced catalytic performance of propane cracking at Brønsted acid/non-framework aluminum synergistic sites can be attributed to the reduced activation energy, which depends on the structures of the non-framework aluminum species in the local environment.</p>

<p><b>Mon-P-100</b></p>	<p><b>Heterogeneous Versus Homogeneous Catalytic Pathways in Cuprous Oxide Nanoparticles-Catalyzed C-C Coupling Reactions</b>  <u>Ravi Teja Addanki Tirumala</u>, Andishaeh P. Dadgar and Marimuthu Andiappan, <i>Oklahoma State University, USA</i>.  Short Summary:  Heterogeneously catalyzed coupling reactions have numerous advantages as they can be used as a platform to develop energy-efficient flow process and further to exploit the optical properties of these Cu<sub>2</sub>O nanostructures and perform photocatalytic C-C coupling reactions using visible light, thus developing sustainable solutions for applications in pharmaceutical, chemical, fine chemical industries.</p>
<p><b>Mon-P-101</b></p>	<p><b>Density Functional Theory and Microkinetic Analysis for Electrooxidation of Ammonia on Transition Metal Catalysts</b>  <u>Hoyeon Jang</u> and Seoin Back, <i>Sogang University, Korea, Republic of (South)</i>.  Short Summary:  I'll discuss systematic computational results for NH<sub>3</sub> electrooxidation on 26 d-block transition metals. We considered all possible path, thermo-coupling, electrochemical and combined ones, resulting in total 9 pathways. By performing a microkinetic analysis, we determined the most favorable pathway, and we propose catalyst design strategy by constructing kinetic volcano plot.</p>
<p><b>Mon-P-102</b></p>	<p><b>In Situ STEM to Study the Promoting Effect of Pt on the Reduction of Co<sub>3</sub>O<sub>4</sub>-SiO<sub>2</sub> Catalysts</b>  <u>Min Tang</u>, Petra E. de Jongh and Krijn P. de Jong, <i>Utrecht University, Netherlands</i>.  Short Summary:  For the first time in situ and ex situ atomic resolution STEM was used to study the reduction of Co<sub>3</sub>O<sub>4</sub>/SiO<sub>2</sub> with and without Pt from which a detailed description of the Pt-catalyzed reduction was obtained.</p>
<p><b>Mon-P-103</b></p>	<p><b>The Role of Oxygen-Containing Functional Groups of Carbon Surfaces</b>  <u>Jiahua Zhou</u>, Weiqing Zheng and Dionisios G. Vlachos, <i>University of Delaware, USA</i>.  Short Summary:  The structure-function relationships, i.e., the identification, quantification as well as the corresponding reactivity of each oxygen-containing functional groups on carbon surfaces remain elusive. In this work, we successfully make a fundamental understanding of the oxygenated functionalities on carbon surfaces via combining XPS (including AP-XPS), probe reaction and machine learning.</p>
<p><b>Mon-P-104</b></p>	<p><b>Influence of Spin State and Electron Configuration on the Active Site and Mechanism for Catalytic Hydrogenation on Metal Cation Catalysts Supported on Nu-1000: Insights from Experiments and Microkinetic Modeling†</b>  <u>Hafeera Shabbir</u><sup>1</sup>, Steven Pellizzeri<sup>2</sup>, Magali Ferrandon<sup>3</sup>, In Soo Kim<sup>4</sup>, Nicholas Vermeulen<sup>5</sup>, Omar K. Farha<sup>6</sup>, Massimiliano Delferro<sup>3</sup>, Alex Martinson<sup>3</sup> and Rachel Getman<sup>1</sup>, (1)<i>Clemson University, USA</i>, (2)<i>Eastern Illinois University, USA</i>, (3)<i>Argonne National Laboratory, USA</i>, (4)<i>Korea Institute of Science and Technology (KIST), Korea, Republic of (South)</i>, (5)<i>NuMat Technologies, USA</i>, (6)<i>Northwestern University, USA</i>.  Short Summary:  The mechanism of ethene hydrogenation on six dicationic 3d transition metal catalysts is investigated. A combination of density functional theory (DFT), microkinetic modeling, and high throughput reactor experiments is used to interrogate the active sites and mechanisms for metals supported on the MOF NU-1000.</p>
<p><b>Mon-P-106</b></p>	<p><b>Generalized Linear Scaling Relationship for Transition Metal Adsorbates and Ultrathin Films: A Case Study for Strong Metal Support Interaction</b>  <u>Kaustubh Sawant</u><sup>1</sup>, Zhenhua Zeng<sup>1</sup> and Jeffrey Greeley<sup>2</sup>, (1)<i>Purdue University, USA</i>, (2)<i>Davidson School of Chemical Engineering, Purdue University, USA</i>.  Short Summary:  Scaling relationships use bond order conservation (BOC) principle to elucidate bonding of p block adsorbates on metal surfaces. However, BOC theory fails to explain bonding in transition metal films, which play important role in strong metal support interactions. We propose a generalized bonding model to explain deviations from BOC principle.</p>
<p><b>Mon-P-107</b></p>	<p><b>Reaction Mechanisms and Process Considerations for Plasma-Catalytic Ammonia Synthesis</b>  Kevin Rouwenhorst<sup>1</sup> and <u>Leon Lefferts</u><sup>2</sup>, (1)<i>University of Twente, Netherlands</i>, (2)<i>MESA + Institute for Nanotechnology, Netherlands</i>.  Short Summary:  Plasma-catalysis has recently gained traction to electrify ammonia synthesis. This research focuses on enhancing the synergy between the plasma and the catalyst, and improving the understanding of the reaction mechanisms involved. Ammonia synthesis has a strong academic literature on thermal catalysis and no byproducts.</p>
<p><b>Mon-P-69</b></p>	<p><b>Impregnation of Potassium on PdAu/SiO<sub>2</sub> catalysts Causes Structure Modification and Pd Leaching</b>  <u>Hunter Jacobs</u>, Welman Curi Elias, Kimberly Heck and Michael S. Wong, <i>Rice University, USA</i>.  Short Summary:  Potassium acetate (KOAc) promoter is often added to PdAu/SiO<sub>2</sub> catalysts to enhance activity and prevent catalyst deactivation during VAM synthesis. Utilizing ATR-FTIR, XRD, and ICP-OES techniques, we show that catalyst restructuring and Pd leaching occurs simply during the wet impregnation of KOAc promoter on PdAu/SiO<sub>2</sub> catalysts.</p>

<p><b>Mon-P-109</b></p>	<p><b>Roles of Bridge Carbon and Heteroatom during the Dehydrogenation Reaction of H<sub>12</sub>-2[n-Methylbenzyl]Pyridine on Pd and Pt Catalysts for LOHC System</b>  <u>Hyunwoo Yook</u><sup>1</sup>, Jeong Kwanyong<sup>2</sup>, Hwang Jinwoo<sup>1</sup>, Ji Hoon Park<sup>2</sup> and Jeong Woo Han<sup>1</sup>, (1)<i>Pohang University of Science and Technology (POSTECH), Korea, Republic of (South)</i>, (2)<i>Korea Research Institute of Chemical Technology, Korea, Republic of (South)</i>.  Short Summary:  This work shed light on the dehydrogenation mechanisms for hetero-cyclic compounds as well as the H<sub>12</sub>-MBP. The adsorption phenomenon on the catalytic surface can be changed due to the nitrogen atom, leading to change the catalytic reactivity.</p>
<p><b>Mon-P-110</b></p>	<p><b>Experimentally Simulating Dehydrogenation Catalysis in H<sub>2</sub>-Removal Membrane Reactors, without Using Membrane Reactors</b>  <u>Aaron Sattler</u>, Michele Paccagnini, Elaine Gomez, Randall Meyer and Sara Jacob, <i>ExxonMobil Research and Engineering, USA</i>.  Short Summary:  Catalytic dehydrogenation of ethane to ethylene in a membrane reactor can potentially compete with steam cracking, due to higher predicted thermodynamic conversions and yields. This work simulates what a catalyst experiences in a membrane reactor, and demonstrates the effect high olefin and low H<sub>2</sub> conditions have on catalytic materials.</p>
<p><b>Mon-P-111</b></p>	<p><b>Effects of Surface Hydrophobicity on Catalytic Transfer Hydrogenation of Styrene with Formic Acid in a Biphasic Mixture</b>  <u>Ezra Baghdady</u><sup>1</sup>, Daniel K. Schwartz<sup>2</sup> and J. Will Medlin<sup>2</sup>, (1)<i>University of Colorado, USA</i>, (2)<i>University of Colorado at Boulder, USA</i>.  Short Summary:  Amphiphilic modification of Pd/silica with alkyl silanes causes increase in transfer hydrogenation activity. Hydrophilic and hydrophobic functionality causes lower activity. The results are discussed in terms of catalyst interfacial activity. An observed change in apparent reaction order suggests changing surface wettability results in a switch from transport to kinetic-limitation.</p>
<p><b>Mon-P-112</b></p>	<p><b>Hydrogenation Catalysis By Site-Isolated Intermetallic Catalysts</b>  <u>Griffin Canning</u><sup>1</sup>, Haoran He<sup>2</sup>, Anish Dasgupta<sup>3</sup>, Angela Nguyen<sup>1</sup>, Michael Janik<sup>1</sup> and Robert Rioux<sup>1</sup>, (1)<i>The Pennsylvania State University, USA</i>, (2)<i>BASF Corporation, USA</i>, (3)<i>Intel Corporation, USA</i>.  Short Summary:  Catalytic sites active for ethylene hydrogenation are first isolated in an intermetallic structure and then site composition is tuned across a series of stoichiometries. Reaction kinetics are measured and then compared with DFT and microkinetics predictions to elucidate detailed reaction mechanism and structure-function relationships.</p>
<p><b>Mon-P-113</b></p>	<p><b>H<sub>2</sub> from Biomass and Bio-Ethanol: A Combined Kinetic and Spectroscopic Analysis in Annular Microreactor with Insight on Surface C-Formation</b>  Veronica Piazza<sup>1</sup>, Abdelrahman Mostafa<sup>1</sup>, Vittoria Troisi<sup>1</sup>, Roberto Batista da Silva Junior<sup>1</sup>, Delia Gazzoli<sup>2</sup>, Gianpiero Groppi<sup>1</sup> and <u>Alessandra Beretta</u><sup>1</sup>, (1)<i>Politecnico di Milano, Italy</i>, (2)<i>Sapienza Università di Roma, Italy</i>.  Short Summary:  Bio-streams are rich in oxygenates with strong coking tendency, affecting surface chemistry in catalytic reactions and opening new challenges for fundamental investigation. In this work, ethanol-to-H<sub>2</sub> reactions on Rh/Al<sub>2</sub>O<sub>3</sub> are studied in annular reactor with a novel methodological approach, combining gas-phase kinetic study and surface spectroscopic analysis.</p>
<p><b>Mon-P-114</b></p>	<p><b>Influence of Channel Sizes in Octahedral Molecular Sieves on Selective Oxidation of Ethane and Methanol</b>  <u>Adam Twombly</u><sup>1</sup>, Harshul Khanna<sup>2</sup>, Steven Suib<sup>2</sup> and Prashant Deshlahra<sup>1</sup>, (1)<i>Tufts University, USA</i>, (2)<i>University of Connecticut, USA</i>.  Short Summary:  Microporous channels in MnO<sub>6</sub> octahedral molecular sieves (OMS) play an important role in the selective oxidation of ethane and methanol. Molecule size dependent rate ratios vary significantly with diverse pore structure and size among OMS frameworks. Selectivity increases with tighter pores.</p>

## Americas Halls 1 & 2

## Modelling, Simulation, and Machine Learning in Catalysis Poster Session I

Mon-P-115

### Methane Oxidation on SSZ-13 Bridged Pd<sub>x</sub>O<sub>x</sub> Sites

Kevin Giewont, Jesse Canavan, [Eleni A. Kyriakidou](#) and Eric Walker, *University at Buffalo (SUNY), USA*.

Short Summary:

In such exhaust catalysts for natural gas vehicles, it is necessary that methane can be completely oxidized at relatively low-temperatures (~300-500 °C). Extensive DFT calculations combined with microkinetic modeling have shown for the first time that water-formation is most likely the rate-limiting step, instead of methane activation.

Mon-P-116

### Thermodynamic Analysis of Fischer-Tropsch Polymerization Using Equation of State and Modeling of Phases Approach, for Predicting Production of Biofuels.

[Délío Barroso de Souza](#) and Ricardo R. Soares, *Federal University of Uberlândia, Brazil*.

Short Summary:

Combining equations of state and phi-phi modeling, we build up minimization Gibbs Energy problem to find out an appropriate range of thermodynamics conditions would make feasible production of interested hydrocarbons (C8 – C12 for gasoline and kerosene of aviation, C13 – C17 for diesel, C18+ for waxes) by Fischer-Tropsch Synthesis.

Mon-P-117

### Single Atom Catalysts for Olefin Functionalization: Hydroformylation and Tandem-Hydrosilylation

[Jonas Amsler](#)<sup>1</sup>, Bidyut Sarma<sup>1</sup>, Jonglack Kim<sup>2</sup>, Claudia Weidenthaler<sup>2</sup>, Giovanni Agostini<sup>3</sup>, Norbert Pfaender<sup>4</sup>, Raul Arenal<sup>5</sup>, Gonzalo Prieto<sup>6</sup>, Philipp N. Plessow<sup>1</sup> and Felix Studt<sup>1</sup>, (1)*Karlsruhe Institute of Technology (KIT), Germany*, (2)*Max-Planck-Institut für Kohlenforschung, Germany*, (3)*ALBA Synchrotron Light Source, Spain*, (4)*Max Planck Institute for Chemical Energy Conversion, Germany*, (5)*ARAID Foundation, Spain*, (6)*ITQ Instituto de Tecnología Química (UPV-CSIC), Spain*.

Short Summary:

Metal-oxide supported Single Atom Catalysts (SACs) can potentially bridge the gap between the fields of homogeneous and heterogeneous catalysis. We identify key parameters for the application of Rh and Ru SACs supported on a variety of metal-oxide surfaces for the heterogeneously catalyzed hydroformylation and for a tandem catalyzed isomerization-hydrosilylation reaction.

Mon-P-118

### Kinetic Modeling of the Methanol Synthesis from CO<sub>2</sub> and H<sub>2</sub> over a CuO/CeO<sub>2</sub>/ZrO<sub>2</sub> Catalyst: The Role of CO<sub>2</sub> and CO Hydrogenation

[Serena Poto](#), Fausto Gallucci and Maria Fernanda Neira Dangelo, *Eindhoven University of Technology, Netherlands*.

Short Summary:

Herein, we investigate the kinetic of methanol synthesis from CO<sub>2</sub> over a CuO/CeO<sub>2</sub>/ZrO<sub>2</sub> catalyst. The selected model allow us to elucidate the reaction mechanism and to understand the role of the active sites. We focus also on the relative contribution of CO<sub>2</sub> and CO hydrogenation to the formation of methanol.

Mon-P-119

### Structure Sensitivity of Catalytic Transfer Hydrogenation of Furfural over Single-Atom Catalysts: A Computational Study

[Piaoping Yang](#)<sup>1</sup>, Stavros Caratzoulas<sup>1</sup>, Jiang Li<sup>2</sup> and Dionisios G. Vlachos<sup>1</sup>, (1)*University of Delaware, USA*, (2)*China University of Petroleum (Beijing), China*.

Short Summary:

We unraveled the structure-activity relationship of metal-N-C catalysts for the CTH reaction using ab initio calculations. We find that the geometry of metal-N<sub>x</sub> site has a great impact on reaction mechanisms and activity. This work provides important insights into the design of highly active metal-N-C catalysts for the CTH reaction.

Mon-P-120

### Unraveling the Structures of Key Molecular Intermediates for Dehydration in Zeolites By XAS and TD-DFT

[Sungmin Kim](#)<sup>1</sup>, Malsoon Lee<sup>1</sup>, John Fulton<sup>1</sup>, Oliver Y. Gutierrez<sup>1</sup>, Donald M. Camaioni<sup>1</sup>, Roger Rousseau<sup>1</sup>, Niri Govind<sup>1</sup>, Thomas Huthwelker<sup>2</sup> and Johannes A. Lercher<sup>1</sup>, (1)*Pacific Northwest National Laboratory, USA*, (2)*Paul Scherrer Institut, Switzerland*.

Short Summary:

We combined in situ Al K-edge XAS, TD-DFT, adsorption measurement and dehydration kinetics to resolve the Al T-site structures of HMFI with 1-propanol species. The quantitative analysis of the nature of adsorbed 1-propanol species allows us to understand and predict the confinement effects that impact catalytic rates within zeolite pores.

Mon-P-121

### Oxidative Decomposition of DMMP on Rutile TiO<sub>2</sub>(110):the Role of Oxygen Vacancies

[Celine Tesvara](#)<sup>1</sup>, Constantin Walenta<sup>2</sup> and Philippe Sautet<sup>1</sup>, (1)*University of California, Los Angeles, USA*, (2)*Harvard University, USA*.

Short Summary:

The decomposition of DMMP on TiO<sub>2</sub>(110) was studied with TPD and DFT. TPD shows DMMP desorbing until 600 K. Methanol and formaldehyde are seen at 650K. O vacancies seems to be the active sites as it lowers the barrier for P-O bond cleavage to produce active surface bound methoxy.

Mon-P-122

### Beyond Conventional Transition State Theory in Catalysis: Applications of Matrix Completion Methods

Stephen Jon Quiton, [Selin Bac](#), Kareesa Kron, Jeongmin Chae, Urbashi Mitra and Shaama Mallikarjun Sharada, *University of Southern California, USA*.

Short Summary:

We present the development of a novel matrix completion algorithm to render sophisticated rate theories more tractable for routine catalysis studies



<p><b>Mon-P-123</b></p>	<p><b>Kinetic Modeling of Oxidative Coupling of Methane: Effects of Promoters on the Catalytic Reaction Path</b>  <u>Yesol Woo</u><sup>1</sup>, Sangseo Gu<sup>2</sup>, Jeong-Myeong Ha<sup>2</sup> and Myung-June Park<sup>1</sup>, (1)<i>Ajou University, Korea, Republic of (South)</i>, (2)<i>Korea Institute of Science and Technology (KIST), Korea, Republic of (South)</i>.  Short Summary:  To kinetically evaluate the effects of different promoters (Zn, Co, Ce, Cu, Cr, Ni) on the reaction pathways and catalytic activity of the oxidative coupling of methane, kinetic models were developed by fitting experimental data.</p>
<p><b>Mon-P-124</b></p>	<p><b>Theoretical Investigation of the Catalysis of n-Butane Isomerization in H-SSZ-13</b>  <u>Lucas Spiske</u><sup>1</sup>, Philipp N. Plessow<sup>1</sup>, Kamila Kazmierczak<sup>2</sup>, Bart D. Vandegehuchte<sup>2</sup> and Felix Studt<sup>1</sup>, (1)<i>Karlsruhe Institute of Technology (KIT), Germany</i>, (2)<i>TotalEnergies, Belgium</i>.  Short Summary:  Different isomerization mechanisms for the n-butane to isobutane isomerization have been calculated using the cluster model and hybrid functional DFT level of theory. New mechanisms also propose different pathways that explain prominent side products. Free energies of the pathways are calculated and compared for H-SSZ-13 zeolite.</p>
<p><b>Mon-P-125</b></p>	<p><b>Atomic Structure-Free Representation of Active Motifs for Expedited Catalyst Discovery</b>  <u>Dong Hyeon Mok</u> and Seoin Back, <i>Sogang University, Korea, Republic of (South)</i>.  Short Summary:  We report an atomic structure-free representation of active motifs to predict binding energies. Our method enabled a quicker training compared to the previous models, and predicted binding energies with reasonable accuracy. Our method is capable of creating possible active motifs without DFT calculations and predicting their binding energies</p>
<p><b>Mon-P-126</b></p>	<p><b>Techno Economic Analysis of Gtl Applications To different Methane Containing Waste Gases</b>  <u>Federico Galli</u><sup>1</sup>, Jacopo De Tommaso<sup>2</sup>, Jun-Jie Lai<sup>3</sup> and Gregory S. Patience<sup>2</sup>, (1)<i>Université de Sherbrooke, Canada</i>, (2)<i>Polytechnique Montréal, Canada</i>, (3)<i>Taiwan University, Taiwan</i>.  Short Summary:  ASPEN simulated a GtL unit based on catalytic partial oxidation (Gibbs reactor) and Fischer-Tropsch reaction (detailed micro kinetic model) to assess the techno economics of a mobile modular unit to convert shale gas into hydrocarbon. A Python framework carried out a Monte-Carlo simulation to study the influence all the parameters.</p>
<p><b>Mon-P-127</b></p>	<p><b>Exploring the Relationship between Organic Structure Directing Agents and Al Distribution in CHA</b>  <u>Craig Waitt</u><sup>1</sup>, Xiaoyu Wang<sup>1</sup>, Yujia Wang<sup>1</sup>, Xuyao Gao<sup>1</sup>, Subramanian Prasad<sup>2</sup>, Anthony Debellis<sup>2</sup>, Ahmad Moini<sup>2</sup>, Edward Maginn<sup>1</sup> and William F. Schneider<sup>1</sup>, (1)<i>University of Notre Dame, USA</i>, (2)<i>BASF Corporation, USA</i>.  Short Summary:  In this work, we explore the orientational landscape of various OSDAs in CHA and their effect on Al distribution in the framework. We find unique Al-Al pair motifs under different configurations of OSDA orientation. These results point the way towards intentional control of Al location through selection of OSDAs.</p>
<p><b>Mon-P-128</b></p>	<p><b>Enhanced Efficiency and Accuracy of the CO<sub>2</sub> reduction Reaction Mechanism Screened on Transition State Metals</b>  <u>Simran Kumari</u>, <i>University of California, Los Angeles, USA</i>.  Short Summary:  The tools and workflows present in Schrodinger's material science suite provide us with efficient and accurate ways to run large-scale reaction mechanisms for various catalytic reactions on heterogeneous surfaces. This plays a significant role in automating the discovery of new catalysts while maintaining accuracy.</p>

<p><b>Mon-P-129</b></p>	<p><b>An Ab Initio Investigation of Confinement Driven [4+2] Diels-Alder Reactions between Ethene and Isoprene in H-ZSM5</b>  <u>Christopher Rzepa</u> and Srinivas Rangarajan, <i>Lehigh University, USA</i>.  Short Summary:  We computationally show that H-ZSM5 can catalyze Diels-Alder reactions of relatively unexplored classes of dienes derived from biomass. Implementing a microkinetic model, we found that favorable dispersive effects can enhance the reaction rate by stabilizing the transition states but overstabilization can render product desorption to be rate-controlling.</p>
<p><b>Mon-P-130</b></p>	<p><b>Integration of Immobilized Enzyme Reactors Under Activity Decay in Commercial Process Simulation Tools</b>  <u>Matthias Feige</u> and Olaf Hinrichsen, <i>Technical University of Munich, Germany</i>.  Short Summary:  In the presented study a methodology is depicted which allows the integration of process strategies tackling (enzymatic) deactivation processes in commercial process simulation environments. It could be shown that after a start-up time a quasi steady-state is reached. The model is applied to an epoxidation reaction catalyzed by immobilized enzymes.</p>
<p><b>Mon-P-131</b></p>	<p><b>Modelling of Single Pellet String Reactors By CFD Simulations Coupled with Detailed Heterogeneous Chemistry</b>  <u>Christian Bauer</u>, Hanh My Bui, Tabea Gros and Olaf Hinrichsen, <i>Technical University of Munich, Germany</i>.  Short Summary:  Single pellet string reactors are in both cases, experimentally and computationally, resource-saving alternatives to conventional fixed bed reactors for kinetic investigations. Since first results in literature suggest that this type of reactor is suitable for catalytic testing, we contribute to the investigations by CFD simulations coupled with detailed heterogeneous chemistry.</p>
<p><b>Mon-P-132</b></p>	<p><b>Predicting Relative Energies of Exchanged Divalent Cations in Zeolites</b>  <u>Asanka Wijerathne</u> and Christopher Paolucci, <i>University of Virginia, USA</i>.  Short Summary:  To predict the relative exchange energies (<math>\Delta E</math>) of divalent cations in zeolites, we develop a model which combines a forcefield for geometry optimizations with a Gaussian process regression for energy evaluations. The combined model captures the <math>\Delta E</math> trend (<math>R^2_{\text{test}}=0.92</math>, MAE=21 kJ/mol) without the need for DFT calculations, enabling faster screening.</p>

# Tuesday May 24, 2022 Poster Program

## Americas Halls 1 & 2

### Catalysis for C<sub>1</sub> and SynGas Chemistry Poster Session II

Tue-P-1

#### Evaluation of Metal Alloy and Metal Oxide Catalysts for CO<sub>2</sub> Hydrogenation to Methanol

Laura Proaño, Dhruvil Shah, Gabriel S Gusmão, Andrew J. Medford and Christopher Jones, *Georgia Institute of Technology, USA*.

Short Summary:

Ni<sub>5</sub>Ga<sub>3</sub>/SiO<sub>2</sub> and ZnZrOx were evaluated as catalysts during CO<sub>2</sub> hydrogenation to MeOH at high pressure and temperatures. It was observed that bimetallic NiGa provided active sites for H<sub>2</sub> dissociation which resulted in higher CO<sub>2</sub> conversion, while oxygen vacancies in the ZnZrOx metal oxide catalyst contribute to enhanced selectivity to MeOH.

Tue-P-2

#### Active Sites and Effects of Co-Adsorbed H<sub>2</sub>O on Methanol Dehydrogenation Using Pt/ $\gamma$ -Al<sub>2</sub>O<sub>3</sub> Catalysts

Bryan Hare<sup>1</sup>, Ricardo Garcia<sup>2</sup>, Tianjun Xie<sup>2</sup>, Paul Meza-Morales<sup>2</sup>, Rachel Getman<sup>2</sup> and Carsten Sievers<sup>1</sup>, (1)*Georgia Institute of Technology, USA*, (2)*Clemson University, USA*.

Short Summary:

Methanol was used as a chemical reagent to isolate and better understand the dehydrogenation reaction commonly seen in aqueous phase reforming. The reaction was probed by infrared spectroscopy while using various Pt/Al<sub>2</sub>O<sub>3</sub> catalysts to ascertain its sensitivity to different metal particle sizes and the presence of co-adsorbed H<sub>2</sub>O.

Tue-P-3

#### CeO<sub>2</sub> Addition on DMS Catalyst for Methanation of Carbon Dioxide

Ju Hyeong Lee and Jae Sung Lee, *Ulsan National Institute of Science and Technology (UNIST), Korea, Republic of (South)*.

Short Summary:

In CO<sub>2</sub> methanation, it is advantageous to use catalyst having high activity at low temperature. CeO<sub>2</sub> addition on dendritic mesoporous silica showed good performance compare with CeO<sub>2</sub> or DMS. Numerous layers on the surface of the catalyst allows Ni nanoparticles to maintain a small size without sintering during the reaction.

Tue-P-4

#### Assessment of Catalysts for Oxidative Coupling of Methane and Ethylene

Jordy Ramos-Yataco and Justin Notestein, *Northwestern University, USA*.

Short Summary:

Oxidative coupling of methane (OCM) catalysts were systematically evaluated under high conversion conditions for the role of alkali cation and La co-doping in the A<sub>2</sub>WO<sub>4</sub>-MnO<sub>x</sub>/SiO<sub>2</sub> system. Cofeeding of ethylene was also evaluated to promote cross-coupling for higher molecular weight hydrocarbon formation.

Tue-P-5

#### Highly Stable and Coke-Free Ni@CeO<sub>2</sub> Catalyst for Dry Methane Reforming

Seung Bo Kim, Min-Jae Kim, Dong-Hyun Kim, Ahmed Al-Shahat Eissa and Kyubock Lee, *Chungnam National University, Korea, Republic of (South)*.

Short Summary:

Incorporating Ni during the CeO<sub>2</sub> crystallization resulted in a more stable structure and smaller nanoparticles size with robust interaction with the support than post incorporation

Tue-P-6

#### Impact of Catalyst Formulation and Operating Conditions on Oxidative Coupling of Methane over Platinum-Based Catalysts

Sven Schardt<sup>1</sup>, Ahmet Celik<sup>1</sup>, Simon Bastian<sup>1</sup>, Jaspreet Chawla<sup>1</sup>, Stephan Andreas Schunk<sup>2</sup>, Patrick Lott<sup>1</sup> and Olaf Deutschmann<sup>1</sup>, (1)*Karlsruhe Institute of Technology (KIT), Germany*, (2)*hte GmbH, Germany*.

Short Summary:

The influence of reaction parameters and catalyst formulation on the formation of C<sub>2</sub>-species via OCM was investigated. We found an optimum for the Pt/Al<sub>2</sub>O<sub>3</sub> system and determined the effect of different promotor metals and supports. Our best case so far with Pt/ZrO<sub>2</sub> lead to 7.1% C<sub>2</sub>-species with 84% acetylene share.

Tue-P-7

#### Effect of Perovskite Structure and Mixed Oxide Support on Ni-CeO<sub>2</sub>-Based Catalyst for Biogas Steam Reforming

Min-Ju Park, Yu-Seung Heo and Dae-Woon Jeong, *Changwon National University, Korea, Republic of (South)*.

Short Summary:

The perovskite structure and mixed oxides affected the physicochemical properties of the Ni-CeO<sub>2</sub> catalyst. Especially, the Ni dispersion and the formation of complex NiO species was improved related to the performance and stability of the catalyst.

Tue-P-8

#### Highly Selective Water Gas Shift Reaction over Co-Fe Clusters Supported on N-Doped Graphitic Carbon

Ana Primo<sup>1</sup>, Lu Peng<sup>1</sup>, Bogdan Jurca<sup>2</sup>, Vasile Parvulescu<sup>2</sup> and Hermenegildo Garcia<sup>1</sup>, (1)*Universitat Politècnica de València, Spain*, (2)*University of Bucharest, Romania*.

Short Summary:

The present study has shown the remarkable performance of Co-Fe clusters of (sub)nanometer-size supported on defective [(N)G] compared to analogous metal NPs of size ranging from 1 to 5 nm. A small amount of highly dispersed Co-Fe clusters is sufficient to achieve a remarkable RWGS selectivity and high catalytic stability.

Tue-P-9	<p><b>Effects of Structure and Composition on the Hydrogenation of Surface Carbon to Methane on Ni, Co and NiCo Surfaces.</b>  <u>Sebastián Godoy</u><sup>1</sup>, Prashant Deshlahra<sup>2</sup>, Alejandro Karelavic<sup>1</sup> and Romel Jiménez<sup>1</sup>, (1)Universidad de Concepción, Chile, (2) Tufts University, USA.  Short Summary:  The effect of local geometry and composition on the hydrogenation of surface C to methane on Ni, Co and NiCo was studied by DFT means. Alloying NiCo stabilizes Co interactions with C-H bonds but lowers the otherwise higher activity of Ni atoms, specially on the less coordinated surfaces.</p>
Tue-P-10	<p><b>CO<sub>2</sub> Conversion to Platform Chemical over Mo<sub>2</sub>C-Based Catalysts</b>  <u>Wijnand Marquart</u>, Michael Claeys and Nico Fischer, <i>Catalysis Institute and c*change (DSI-NRF Centre of Excellence in Catalysis), University of Cape Town, South Africa.</i>  Short Summary:  In this study we are looking at utilizing Mo<sub>2</sub>C based catalysts for the CO<sub>2</sub> assisted oxidative dehydrogenation of ethane to ethylene, one of the world's largest chemical building blocks for the chemical industry. Currently, ethylene is mainly produced by means of steam cracking, known to emit significant amounts of CO<sub>2</sub>.</p>
Tue-P-11	<p><b>Conductive Packed Foam for the Kinetic Investigation of Methane Steam Reforming on Rh/Al<sub>2</sub>O<sub>3</sub></b>  Matteo Ambrosetti, Danilo Bonincontro, Alessandra Beretta, <u>Gianpiero Groppi</u> and Enrico Tronconi, <i>Politecnico di Milano, Italy.</i>  Short Summary:  Conductive packed foams are proposed as a solution for kinetic investigation in concentrated conditions of high thermally-demanding applications. In view of the growing interest towards small scale methane steam reforming, kinetics of Rh-Al<sub>2</sub>O<sub>3</sub> pellets was considered. New lumped kinetic rates were derived on the basis of experimental data.</p>
Tue-P-12	<p><b>Catalytic CO<sub>2</sub> Conversion to Value-Added Chemicals over Carbon Nanosphere Encapsulated Fe-Co Carbonized at a High Temperature</b>  <u>Daniel Weber</u>, Nicole Forte and Cheng Zhang, <i>Long Island University (Post), USA.</i>  Short Summary:  In an earlier study, we found the carbon nanosphere encapsulated Fe-Co carbonized at 1050° C performed better for converting CO<sub>2</sub> into light olefins (C<sub>2</sub>-C<sub>4</sub>). In this study, we attempted to investigate the stability of this catalyst under the optimized testing conditions.</p>
Tue-P-13	<p><b>Investigate the Promoters (K<sup>+</sup>, Na<sup>+</sup>, Guanidine, Mn<sup>2+</sup>) on the Catalytic Performance of Carbon Nanosphere Encapsulated Fe<sub>1</sub>Co<sub>2</sub> for CO<sub>2</sub> conversion</b>  <u>Christian Moon</u><sup>1</sup>, Jaylin Sasson<sup>2</sup> and Cheng Zhang<sup>1</sup>, (1)Long Island University (Post), USA, (2)Brookhaven National Laboratory, USA.  Short Summary:  Direct hydrogenation of CO<sub>2</sub> to lower olefins is still highly desirable as it produces polymers that promote sustainable energy. Therefore, we report the selectivity of light olefins through CO<sub>2</sub> hydrogenation over different promoters on carbon nanosphere encapsulated Fe<sub>1</sub>Co<sub>2</sub> core-shell catalyst.</p>
Tue-P-14	<p><b>Catalytic CO<sub>2</sub> Hydrogenation to Light Olefins over Carbon Nanosphere Encapsulated Fe-Co Species with Varying Fe to Co Mole Ratios</b>  <u>Nicole Forte</u><sup>1</sup>, Elizabeth Nestler<sup>1</sup>, Dimitriy Vovchok<sup>2</sup>, Sanjaya Senanayake<sup>2</sup> and Cheng Zhang<sup>1</sup>, (1)Long Island University (Post), USA, (2)Brookhaven National Laboratory, USA.  Short Summary:  Direct hydrogenation of CO<sub>2</sub> to lower olefins is highly desirable due to the wide variety applications of light olefins in polymers. Therefore, we report a selective CO<sub>2</sub> conversion to lower olefins through CO<sub>2</sub> hydrogenation over a series of carbon nanosphere encapsulated Fe-Co species with varying Fe to Co mole ratios.</p>
Americas Halls 1 & 2	<p><b>Catalysis for Environmental Applications Poster Session II</b></p>
Tue-P-15	<p><b>Catalytic CO<sub>2</sub> Hydrogenation to Light Olefins over Fe-Co Catalysts Supported on CeO<sub>2</sub> with Different Morphology</b>  <u>Tina He</u><sup>1</sup>, Matthew Wong<sup>2</sup>, Juan Jimenez<sup>3</sup>, Sanjaya Senanayake<sup>3</sup> and Cheng Zhang<sup>4</sup>, (1)University of Texas at Austin, USA, (2) Cornell University, USA, (3)Brookhaven National Laboratory, USA, (4)Long Island University (Post), USA.  Short Summary:  CO<sub>2</sub> hydrogenation into light olefins is attracting attention as a method for alleviating concerns caused by greenhouse gases. Comparisons between monometallic Fe, Co, and bimetallic Fe-Co catalysts supported on CeO<sub>2</sub> nanopowder versus CeO<sub>2</sub> nanorod have shown that Co-CeO<sub>2</sub> nanorod is the optimal catalyst for CO<sub>2</sub> conversion and C<sub>2</sub>-C<sub>3</sub> olefin selectivity/yield.</p>
Tue-P-16	<p><b>Unusual Enhancement of Passive NO Adsorption By Water over Pd Ion Exchanged Ferrierite-Type Zeolite</b>  Inhak Song, Konstantin Khivantsev, Yong Wang and <u>Janos Szanyi</u>, <i>Pacific Northwest National Laboratory, USA.</i>  Short Summary:  High temperature-induced relocation of Pd ions to more stable cationic sites located near the 6-membered ring of the ferrierite cage is responsible for an unusual enhancement of NOx adsorption by water.</p>

<p><b>Tue-P-17</b></p>	<p><b>An Experimental Study of Dual-Layer AdSCR Systems for NO<sub>x</sub> Abatement during Cold-Start Transients</b>          Maria Elena Azzoni, Federico Sascha Franchi, Nicola Usberti, Nicole Daniela Nasello, Federica Gramigni, Isabella Nova, Lidia Castoldi and <u>Enrico Tronconi</u>, <i>Politecnico di Milano, Italy</i>.          Short Summary:          A honeycomb monolith AdSCR system has been prepared in a Cu-zeolite+Ba/Al<sub>2</sub>O<sub>3</sub> dual-layer configuration. This configuration is a novelty in the scientific literature; this single device should provide both the SCR activity of a conventional Cu-based catalyst as well as the low-T NO<sub>x</sub> storage capacity of the BaO material.</p>
<p><b>Tue-P-18</b></p>	<p><b>Improved Nitrate Reduction Kinetics over Indium-Decorated PdAu Nanoparticle Catalysts</b>          Sujin Guo<sup>1,2</sup>, Hao Li<sup>3</sup>, <u>Kimberly Heck</u><sup>1,2</sup>, Xinying Luan<sup>2</sup>, Wenhua Guo<sup>2</sup>, Graeme Henkelman<sup>3</sup> and Michael S. Wong<sup>2</sup>, (1) <i>Nanotechnology Enabled Water Treatment (NEWT) Center, USA</i>, (2) <i>Rice University, USA</i>, (3) <i>University of Texas at Austin, USA</i>.          Short Summary:          Bimetal-promoted PdNP catalysts have shown promise for reduction of aqueous nitrate pollutant. We synthesized In-decorated PdAuNPs with varying Pd:Au. In-on-PdAuNPs showed higher activity than In-on-PdNPs for NO<sub>3</sub><sup>-</sup>. Higher NO<sub>2</sub><sup>-</sup> activity and N<sub>2</sub> selectivity was also observed. DFT results suggest possible origins for the enhancement of nitrite/nitrate reduction over In-on-PdAuNPs.</p>
<p><b>Tue-P-19</b></p>	<p><b>NH<sub>3</sub> Abatement Under Passive SCR Conditions on Dual-Layer ASC Commercial Catalyst: An Experimental and Modelling Study</b>          Nicola Usberti<sup>1</sup>, Nicole Daniela Nasello<sup>1</sup>, Sara Ciria<sup>1</sup>, Federico Bicego<sup>1</sup>, Andrea Meattelli<sup>1</sup>, Stefano Golini<sup>2</sup>, Edoardo Merlone Borla<sup>2</sup>, Gabriella Mancino<sup>2</sup>, Isabella Nova<sup>1</sup> and Enrico Tronconi<sup>1</sup>, (1) <i>Politecnico di Milano, Italy</i>, (2) <i>FPT Industrial S.p.A., Italy</i>.          Short Summary:          Passive-SCR converters represent a promising solution to avoid NH<sub>3</sub> emissions from natural gas fueled heavy-duty vehicles. The transient experimental campaign and the modelling study performed highlighted the relevance of implementing redox kinetic mechanisms to understand the performance and the ageing effect of commercial ASC catalysts under Passive SCR operating conditions.</p>
<p><b>Tue-P-20</b></p>	<p><b>Catalytic Oxidation of Toluene By Ce-Containing-LaMnO<sub>3</sub> Solid Solution</b>          Eddy Moreno-Román<sup>1</sup>, Arquimedes Cruz-Lopez<sup>1</sup>, Sonia Gil<sup>2</sup> and <u>Santiago-Iván Suárez-Vázquez</u><sup>1</sup>, (1) <i>Civil Engineering Faculty, Environmental Engineering Department, Mexico</i>, (2) <i>Université de Lyon, CNRS, France</i>.          Short Summary:          Different Ce species (doped, impregnated and segregated) were loaded on LaMnO<sub>3</sub> by hydrothermal synthesis. Results revealed that segregation produces CeO<sub>x</sub>-La<sub>1-x</sub>Ce<sub>x</sub>MnO<sub>3</sub> with Ce<sup>3+</sup> predominant on surface. The redox cycle between these species with Mn<sup>4+</sup> enhanced the catalytic oxidation of toluene. DRIFT study is also carried out to evaluate the mechanism reaction.</p>
<p><b>Tue-P-21</b></p>	<p><b>Glycerol Transesterification with Dimethylcarbonate over MgO-FeO<sub>x</sub> Catalysts</b>  <u>Lindelani Qwabe</u>, <i>Mangosuthu University of Technology, South Africa</i>.          Short Summary:          Glycerol carbonate was produced via transesterification of glycerol with dimethylcarbonate. The yield depends on basicity of the catalyst, reaction temperature and time taken for the reaction. Glycidol is a minor product and becomes increasingly prominent with increase in reaction time.</p>
<p><b>Tue-P-22</b></p>	<p><b>Reversible Hydrogenation and Dehydrogenation over Pd Catalyst Supported on Porous TiO<sub>2</sub> Nanosheets</b>  <u>Jihyeon Lee</u> and Kwangjin An, <i>Ulsan National Institute of Science and Technology (UNIST), Korea, Republic of (South)</i>.          Short Summary:          Liquid organic hydrogen carrier (LOHC) system is an attractive solution for hydrogen storage because hydrogen can be stored at ambient conditions for a long period. In this work, Pd catalyst with porous TiO<sub>2</sub> nanosheets successfully conduct reversible cycles for hydrogen storage in N-methylindole-based LOHC system.</p>
<p><b>Tue-P-23</b></p>	<p><b>CO Oxidation to Probe Cu Dimers in Cu-CHA Catalysts: The Impact of NH<sub>3</sub> Loading</b>          Roberta Villamaina<sup>1</sup>, <u>Umberto Iacobone</u><sup>2</sup>, Isabella Nova<sup>2</sup>, Enrico Tronconi<sup>2</sup>, Maria Pia Ruggeri<sup>1</sup>, Jillian Collier<sup>1</sup> and David Thompsett<sup>1</sup>, (1) <i>Johnson Matthey Technology Centre, United Kingdom</i>, (2) <i>Politecnico di Milano, Italy</i>.          Short Summary:          CO oxidation is an effective probe reaction for Cu<sup>II</sup> dimers in NH<sub>3</sub>-SCR Cu-CHA catalysts. The NH<sub>3</sub> coverage is a key factor to control Cu<sup>II</sup> dimers: NH<sub>3</sub> mobilizing Cu<sup>II</sup>OH species, promotes the dimer formation. Consequently, higher NH<sub>3</sub> loading determines greater Cu-dimers concentration which can catalyse the CO oxidation reaction to CO<sub>2</sub>.</p>
<p><b>Tue-P-24</b></p>	<p><b>Introduction of Ag/MnO<sub>x</sub>-CeO<sub>2</sub> Mixed Oxides for NO<sub>x</sub>-Assisted Soot Oxidation at Low Temperature</b>  <u>Eun Jun Lee</u> and Kwan-Young Lee, <i>Korea University, Korea, Republic of (South)</i>.          Short Summary:          The Ag/MnO<sub>x</sub>-CeO<sub>2</sub> catalyst was introduced to enhance NO<sub>x</sub>-assisted soot oxidation activity. In addition, main active factors in NO<sub>x</sub>-assisted soot oxidation activity were proposed through catalytic analysis. As a result, Ag/2MnO<sub>x</sub>-1CeO<sub>2</sub> catalyst was proposed as optimal catalysts.</p>



<p><b>Tue-P-25</b></p>	<p><b>Selective Production of Light Olefins from CO<sub>2</sub> Hydrogenation over Tailored SSZ-13 Zeolites and In<sub>2</sub>O<sub>3</sub> Catalysts</b>  Wei Di<sup>1</sup>, Sreetama Ghosh<sup>1</sup>, Oleg Pajalic<sup>2</sup>, Lars Josefsson<sup>3</sup>, <u>Louise Olsson</u><sup>4</sup> and Derek Creaser<sup>4</sup>, (1)Competence Centre for Catalysis and Chemical Engineering, Chalmers University of Technology, Sweden, (2)Perstorp Specialty Chemicals AB, Sweden, (3)Josefsson Sustainable Chemistry AB, Sweden, (4)Chalmers University of Technology, Sweden.  Short Summary:  SSZ-13 zeolites with isolated Al distribution were synthesized, modified well to couple with In<sub>2</sub>O<sub>3</sub> and gain the stable olefins production, with 70% of light olefin selectivity and 18% of CO<sub>2</sub> conversion during the CO<sub>2</sub> hydrogenation to olefins.</p>
<p><b>Tue-P-26</b></p>	<p><b>Photodegradation of Diuron Herbicide Using TiO<sub>2</sub> P25 Impregnated with Eu<sup>+3</sup> under UV, Visible and Solar Light Irradiation</b>  Maribel Enríquez Reséndiz<sup>1</sup>, <u>Carolina Solis Maldonado</u><sup>1</sup>, Raúl Luna<sup>1</sup>, Alfredo Cristóbal Salas<sup>1</sup>, Ladislao Sandoval-Rangel<sup>2</sup>, Gloria Dimas Rivera<sup>3</sup>, Daniela Xulú Martínez Vargas<sup>4</sup>, Norma Alicia Ramos Delgado<sup>5</sup> and Nayely Pineda Aguilar<sup>6</sup>, (1) Universidad Veracruzana, Mexico, (2)Instituto Tecnológico de Estudios Superiores de Monterrey, Mexico, (3)Universidad Autónoma de Nuevo León, Mexico, (4)Desarrollo Ambiental Máximo, Mexico, (5)Instituto Tecnológico de Nuevo León, Mexico, (6)Centro de Investigación en Materiales Avanzados S.C., Mexico.  Short Summary:  In the present work, the efficiency in the degradation of diuron, an herbicide whose inclusion in the aquatic environment causes adverse effects on the environment, it was measured using TiO<sub>2</sub> catalysts impregnated with 0.1% and 0.5% europium by weight, which allow better use of sunlight in water decontamination treatments.</p>
<p><b>Tue-P-27</b></p>	<p><b>Impact of Pd/Pt Ratio and Reaction Environment for Catalytic CH<sub>4</sub> Oxidation</b>  <u>Jiseok Park</u> and Sung Bong Kang, <i>Gwangju Institute of Science and Technology, Korea, Republic of (South)</i>.  Short Summary:  The effectiveness of bimetal Pd-Pt catalysts in oxidizing methane has been examined concerning the Pd:Pt ratio and oxygen concentrations in the feed. Density Functional Theory (DFT) calculations were also used to further understand and quantify the influence of Pt dopant on PdO in the C-H cleavage on catalyst surfaces.</p>
<p><b>Tue-P-28</b></p>	<p><b>Effects of Pd Nanoparticle Size and Water Pressure on the Formation of Mononuclear Pd(II) Cations in CHA Zeolites during High-Temperature Air Treatment</b>  Trevor M. Lardinois<sup>1</sup>, <u>Brandon K. Bolton</u><sup>1</sup>, Keka Mandal<sup>2</sup>, Vamakshi Yadav<sup>1</sup>, Asanka Wijerathne<sup>2</sup>, Christina Li<sup>1</sup>, Christopher Paolucci<sup>2</sup> and Rajamani Gounder<sup>1</sup>, (1)Purdue University, USA, (2)University of Virginia, USA.  Short Summary:  Pd-CHA zeolites were synthesized to contain monodisperse Pd particles of different size at their extracrystalline surfaces. The structural conversion of Pd particles into mononuclear Pd(II) cations, which are desired sites for passive NO<sub>x</sub> adsorbers, was found to depend on Pd particle size, air treatment temperature and time, and water pressure.</p>
<p><b>Tue-P-29</b></p>	<p><b>In Situ Drifts Analysis of Sb Promoted Vanadia-Titania Catalysts</b>  <u>Alexander Nellesen</u> and Per-Anders Carlsson, <i>Chalmers University of Technology, Sweden</i>.  Short Summary:  Antimony promoted vanadia-titania catalysts for NO<sub>x</sub> abatement in mobile sources were studied via in situ DRIFT spectroscopy. The aim is to understand how the promoter infer in vanadium and the support. Fundamental studies on NH<sub>3</sub>-SCR catalysts are essential for catalyst design and development for exhaust gas aftertreatment.</p>
<p><b>Tue-P-30</b></p>	<p><b>Effect of the Nb Content on the Performance of Nb-Promoted Cu/Zn Catalysts for Methanol Synthesis from CO<sub>2</sub> Hydrogenation</b>  Cássia Santana<sup>1</sup>, Luiza Shine<sup>1</sup>, Ricardo Passini<sup>1</sup>, Ernesto Urquieta-González<sup>1</sup>, Elisabete M. Assaf<sup>2</sup>, Jose M. Assaf<sup>1</sup> and <u>Janaina F. Gomes</u><sup>1</sup>, (1)Federal University of São Carlos, Brazil, (2)University of São Paulo, Brazil.  Short Summary:  We evaluated the effect of Nb content (0, 2.5, 5.0 and 10 wt.%) on Nb-promoted Cu/Zn catalysts in the CO<sub>2</sub> hydrogenation to methanol. The production of methanol was enhanced on the Cu/Zn/Nb catalysts and the best activity and selectivity to methanol (~50% at 200 °C) was reached for Cu<sub>50</sub>/Zn<sub>45</sub>/Nb<sub>5</sub>.</p>
<p><b>Tue-P-31</b></p>	<p><b>Coke-Promoted Ni/CaO As Multifunctional Materials for an Integrated CO<sub>2</sub> Capture and Utilization</b>  <u>Seongbin Jo</u> and Kandis Leslie Abdul-Aziz, <i>University of California, Riverside, USA</i>.  Short Summary:  Highly efficient CO and syngas production in a cyclic system was proposed using coke-promoted Ni/CaO (C-Ni/CaO) multifunctional materials. C-Ni/CaO exhibited high CO production in CO<sub>2</sub> conversion and syngas production in CH<sub>4</sub> conversion step, respectively.</p>
<p><b>Tue-P-32</b></p>	<p><b>What Is the Best Sampling Rate for Fast Spaci-MS in Catalytic Monoliths?</b>  Petr Koci<sup>1</sup>, Tomas Hlavaty<sup>1</sup>, Martin Isoz<sup>1</sup>, Dhruva J. DeKa<sup>2</sup> and William Partridge<sup>2</sup>, (1)University of Chemistry and Technology, Czech Republic, (2)Oak Ridge National Laboratory, USA.  Short Summary:  This study combines computational and experimental methods to identify and set up proper sampling rate in SpaciMS with the capillary inserted in a monolith channel. Such conditions guarantee that the measured component concentration in the channel is not affected by the capillary itself.</p>

Tue-P-33

**Catalytic Hydrogenation of Nitrate: Research Insights of the Past, Present, and Future**

Juliana Levi and Paul Westerhoff, *Arizona State University, USA*.

Short Summary:

To give catalytic hydrogenation of nitrate the best chance of being scaled up and utilized in the water treatment field, a critical review of previous research in the field as well as recommended next steps will be outlined.

Americas Halls  
1 & 2

**Catalyst Characterization Poster Session II**

Tue-P-34

**Oxidative Dehydrogenation of n-Octane over Vox/MgO Powders Prepared Using Solution Combustion Synthesis**

Pinkie Ntola, *Durban University of Technology, South Africa*.

Short Summary:

We report findings of a structural characterization of powders prepared by solution combustion using different fuels. Each fuel yielded a powder with a unique microstructure. Differences in the microstructures were attributed to different combustion kinetics. Differences in conversion and selectivity were observed with the different fuels.

Tue-P-35

**XAFS with a Laboratory-Based Spectrometer in Catalysis Characterization**

Christopher Schlesiger, Sebastian Praetz, Wolfgang Malzer, Richard Gnewkow and Birgit Kanngießler, *Technische Universität Berlin, Germany*.

Short Summary:

A laboratory-based X-ray Absorption Fine Structure (XAFS) spectrometer is shown, that is capable of measuring in transmission mode with a high efficiency, and therefore, to a certain amount, rendering XAFS analysis not only possible at synchrotron radiation facilities.

Tue-P-36

**Resonant Excitation Reveals Chemical Sensitivity in Platinum L $\beta$  X-Ray Emission Spectra**

Louise M. Debeve and Christopher J. Pollock, *Cornell University, USA*.

Short Summary:

Resonant x-ray emission spectroscopy of platinum compounds uncovers features that were previously unresolvable with non-resonant emission. The valence to core area reveals features corresponding to ligand s, ligand p and platinum 5d contributions. This method offers the potential to directly probe platinum-based catalytic centers during *in situ* chemical reactions.

Tue-P-37

***In-Situ* Study on the Reversible Evolution of CO<sub>2</sub> Hydrogenation Activity Induced By on-Going Surface Modification in a Cu-TiO<sub>2</sub> Catalyst**

Kaixi Deng<sup>1,2</sup> and Jose A. Rodriguez<sup>1,2</sup>, (1)*Stony Brook University, USA*, (2)*Brookhaven National Laboratory, USA*.

Short Summary:

The study identifies a case of a surface reconstruction induced by a mild metal-support interaction. In this work, a relatively complete picture for the structure-activity relationships in the Cu-TiO<sub>2</sub> system under reverse water gas shift reaction conditions has been established.

Tue-P-38

**New Mechanistic Insights into Hydrogenation Reactions from *in Situ* Neutron Scattering Studies**

Zili Wu, *Oak Ridge National Laboratory, USA*.

Short Summary:

Thanks to the special sensitivity of neutron to light elements such as H over X-ray, we show a few recent case studies of selected hydrogenation reactions to highlight the promise of neutron scattering for catalysis research by providing unique insights into catalyst structure, surface species/intermediates and reaction mechanisms.

Tue-P-39

**Characterization of Atomic Structure of Maghemite ( $\gamma$ -Fe<sub>2</sub>O<sub>3</sub>) Nanoparticle through Diffraction Anomalous Near Edge Structure**

Chang-Yong Kim, *Canadian Light Source, Canada*.

Short Summary:

By using linearly polarized synchrotron X-ray, polarization-dependent Diffraction Anomalous Near Edge Structure (DANES) from maghemite nanoparticle has been obtained. The DANES results combined with FDMNES simulation gives clear distinction among possible vacancy ordering in the maghemite. The polarization-dependent DANES can be a novel addition to structural characterization of nanoparticles.

Tue-P-40

**Acidity of Naphtha Reforming Catalyst : 2,6-Di-Tert-Butylpyridine, a New Probe Molecule**

Quentin Rivet<sup>1,2</sup>, Thibaud Nardin<sup>2</sup> and David Farrusseng<sup>1</sup>, (1)*Université de Lyon, CNRS, France*, (2)*IFP Energies Nouvelles, France*.

Short Summary:

This work established the usage of a new probe molecule to characterize the Brønsted acidity of reforming catalysts, the 2,6-di-tert-butylpyridine. The IR analysis of the sorption of this molecule gives insight of the number of acid sites on the catalyst.

<p><b>Tue-P-41</b></p>	<p><b>Using Spatially Resolved Soft XAS/X-Peem to Determine the Redox State of Co Nanoparticles on TiO<sub>2</sub> in the Presence of Oxygen Vacancies</b>  Chengwu Qiu<sup>1,2</sup>, Yaroslav Odarchenko<sup>3</sup>, Qingwei Meng<sup>4</sup>, Shaojun Xu<sup>1</sup>, Paul Olalde-Velasco<sup>5</sup>, Francesco Maccherozzi<sup>5</sup> and <u>Andrew M. Beale</u><sup>1,2</sup>, (1)UK Catalysis Hub, United Kingdom, (2)University College London, United Kingdom, (3)Finden Ltd, United Kingdom, (4)Guangdong University of Technology, China, (5)Diamond Light Source, United Kingdom.  Short Summary:  Using X-PEEM coupled with soft XAS we observe how surface O<sub>vac</sub> on TiO<sub>2</sub> can readily reduce individual Co<sub>3</sub>O<sub>4</sub> nanoparticles to CoO/Co<sup>0</sup>, smaller particles being more reduced than larger ones. O<sub>vac</sub> promote reduction at the edge of the NPs more than the centre and prevent total reoxidation after treatment in syn-gas.</p>
<p><b>Tue-P-42</b></p>	<p><b>Multi-Technique Approach to Understanding Complex Structure-Activity Relationships in Supported Metal Oxide Nanoparticles</b>  <u>Lisa Allen</u><sup>1,2</sup>, Andrew M. Beale<sup>1,2</sup>, Ines Lezcano-Gonzalez<sup>1,2</sup>, Husn Islam<sup>3</sup>, Nicoleta Muresan<sup>3</sup>, Loredana Mantarosie<sup>3</sup>, David Thompsett<sup>3</sup>, Jillian Collier<sup>3</sup> and Andrew Smith<sup>4</sup>, (1)University College London, United Kingdom, (2)UK Catalysis Hub, United Kingdom, (3)Johnson Matthey Technology Centre, United Kingdom, (4)Diamond Light Source, United Kingdom.  Short Summary:  The structure-activity relationships of a series of PdO/γ-Al<sub>2</sub>O<sub>3</sub> catalysts toward CO and CH<sub>4</sub> oxidation, critical reactions for the use of natural gas, biomethane and their blends as cleaner fuel options, have been investigated via a multi-technique approach to understand how morphology, speciation and dispersity influence activity.</p>
<p><b>Tue-P-43</b></p>	<p><b>Catalyst Regeneration in the Process to Make Phenylmethyldichlorosilane</b>  <u>Krishna Janmanchi</u>, The Dow Chemical Company, USA.  Short Summary:  This presentation will focus on the evaluation of γ-alumina catalyst for Heterogeneous Pseudo-Friedel-Crafts (het-PFC) reaction using benzene and methyldichlorosilane (MeHSiCl<sub>2</sub>) feed and regeneration of the catalyst by reacting the spent catalyst with anhydrous HCl gas.</p>
<p><b>Tue-P-45</b></p>	<p><b>Dynamics of Water in Cu-Loaded Zeolites: A QENS Study</b>  <u>Vainius Skukauskas</u><sup>1</sup>, Emma Gibson<sup>1</sup> and I. Silverwood<sup>2</sup>, (1)University of Glasgow, United Kingdom, (2)ISIS Facility, STFC Rutherford Appleton Laboratory, United Kingdom.  Short Summary:  Quasielastic Neutron Scattering was employed in order to probe the dynamics of water within Cu-loaded zeolites relevant to the direct methane-to-methanol conversion. Both rotational and translational dynamics have been observed, and their variation appears to depend on composition, Cu-content and topology of the framework.</p>
<p><b>Tue-P-46</b></p>	<p><b>In-Situ XAFS, XRD, and DFT Characterization of the Sulfur Adsorption Sites on Cu and Ce Exchanged Y Zeolites</b>  <u>Henry Sokol</u><sup>1</sup>, Amani Ebrahim<sup>2</sup>, Stavros Caratzoulas<sup>3</sup>, Anatoly Frenkel<sup>2</sup> and Ioulia Valla<sup>1</sup>, (1)University of Connecticut, USA, (2)Stony Brook University, USA, (3)University of Delaware, USA.  Short Summary:  In-situ characterization of the Cu and Ce active sites on CuCeY as prepared for adsorptive desulfurization has investigated the reduction of the metal species and their arrangement throughout the zeolite framework. The findings offer insight into the superior sulfur adsorption performance exhibited by this material.</p>
<p><b>Tue-P-47</b></p>	<p><b>A Metal–Organic Framework As a Crystallographically Well-Defined Heterogeneous Catalyst Support in Olefin Polymerization</b>  <u>Timothy Goetjen</u><sup>1</sup>, Zoha Syed<sup>1,2</sup>, Julia Knapp<sup>1</sup>, Ryan Hackler<sup>2</sup>, Xuan Zhang<sup>1</sup>, Massimiliano Delferro<sup>2</sup>, Joseph T. Hupp<sup>1</sup> and Omar K. Farha<sup>1</sup>, (1)Northwestern University, USA, (2)Argonne National Laboratory, USA.  Short Summary:  Metal–organic frameworks (MOFs) provide a unique opportunity to study uniform catalytic species, deriving key insights into active sites and mechanisms in catalytic reactions. A well-defined Cr-based catalyst supported on a MOF is shown to be active for ethylene polymerization and characterized by single-crystal X-ray diffraction yielding important structural information.</p>
<p><b>Tue-P-48</b></p>	<p><b>Palladium Speciation on Ceria Zirconia: A Combined in Situ Study</b>  <u>Lucy Costley-Wood</u><sup>1</sup>, Emma Gibson<sup>1</sup>, Timothy I. Hyde<sup>2</sup>, David Thompsett<sup>2</sup>, Amy Kolpin<sup>2</sup> and Claire Wilson<sup>1</sup>, (1)University of Glasgow, United Kingdom, (2)Johnson Matthey Technology Centre, United Kingdom.  Short Summary:  <b>This project investigates the effect of ageing on petrol engine TWC catalysts, specifically PGMs on doped and undoped ceria zirconias. In situ XRD and other methods aim to link the composition and phase stability of the ceria zirconia to other deactivation mechanisms such as Pd sintering.</b></p>
<p><b>Tue-P-50</b></p>	<p><b>Characterization of a Spent Catalyst from an Industrial Plant for Bio-Ethylene Production</b>  <u>Andréa Marins de Oliveira</u> and Robson Peguin, Braskem, Brazil.  Short Summary:  Spent catalyst characterization gives insights on the impacts of a reaction along timeframe in industrial reactor operation fostering catalyst developments and process improvements. Bio-ethylene production using as raw feedstock ethanol is the focus. This reaction is known for over hundred years but still now, large scale operation has its challenges.</p>

Tue-P-51	<p><b>Electron-Beam Induced Structural Changes on Layered Double Hydroxides and Derived Materials</b>            Liseth Duarte<sup>1</sup>, Li He<sup>1</sup>, Matus Stredansky<sup>1</sup>, Frank Girgsdies<sup>1</sup>, <u>Katarzyna Skorupska</u><sup>1</sup>, Thomas Lunkenbein<sup>1</sup>, Frank Rosowski<sup>2</sup>, Robert Schlögl<sup>1,3</sup> and Walid Hetaba<sup>1,3</sup>, (1)<i>Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany</i>, (2)<i>BASF SE, Germany</i>, (3)<i>Max Planck Institute for Chemical Energy Conversion, Germany</i>.</p> <p>Short Summary:            The influence of beam irradiation on LDH and derived materials was systematically studied. The structural changes were investigated by changes in the electron diffraction patterns of the same position acquired after consecutive beam-exposure. The findings show the importance to understand the possible undesired changes of the materials during TEM investigations.</p>
Tue-P-52	<p><b>Nanofluidic Scattering Spectroscopy for Single Particle Catalysis</b>  <u>Björn Altenburger</u>, Joachim Fritzsche and Christoph Langhammer, <i>Chalmers University of Technology, Sweden</i>.</p> <p>Short Summary:            A new approach to single particle catalysis is being developed that can monitor the activity of industrially relevant sub-10-nm particles. This technique is based on light scattering from nanochannels which can contain single catalytic particles. The applicability of this method is demonstrated on liquid-phase experiments for colored and transparent reactants.</p>
Tue-P-53	<p><b>In Situ Gas Phase Electron Microscopy Studies on the Nanoparticle Stability of Carbon Supported Nickel Catalysts for CO<sub>2</sub> Hydrogenation</b>  <u>Nienke L. Visser</u><sup>1</sup>, Juliette C. Verschoor<sup>1</sup>, Joseph A. Stewart<sup>2</sup>, Jessi E.S. van der Hoeven<sup>1</sup> and Petra E. de Jongh<sup>1</sup>, (1)<i>Utrecht University, Netherlands</i>, (2)<i>TotalEnergies, Belgium</i>.</p> <p>Short Summary:            The interaction between Ni nanoparticles with (functionalized) carbon support materials is investigated to prevent deactivation via particle sintering during CO<sub>2</sub> hydrogenation to methane. This work demonstrates the potential of <i>in situ</i> gas phase transmission electron microscopy to gain fundamental understanding of Ni nanoparticle growth mechanisms under operating conditions.</p>
Americas Halls 1 & 2	<p><b>Catalyst Design and Synthesis Poster Session II</b></p>
Tue-P-54	<p><b>Catalyst Design to Improve Catalytic Performance</b>  <u>Kwangjin An</u>, <i>Ulsan National Institute of Science and Technology (UNIST), Korea, Republic of (South)</i>.</p> <p>Short Summary:            Various studies on how the interfacial properties of nanocatalysts affect the catalytic reaction are introduced. Through a combinatorial approach of catalytic experiments and density functional theory calculations, we study how the size of metal nanoparticles and the oxide surface facets systematically affect the catalytic properties.</p>
Tue-P-55	<p><b>Highly Dispersed Pd Species on NiO for Efficient Cinnamaldehyde Hydrogenation</b>  <u>Rim C.J. van de Poll</u>, Heiner Friedrich and Emiel J. M. Hensen, <i>Eindhoven University of Technology, Netherlands</i>.</p> <p>Short Summary:            Highly dispersed Pd is placed on NiO nanoparticles. Compared to Pd on SiO<sub>2</sub>, Pd on NiO can be more easily reduced, causing higher hydrogenation activity at low reduction temperature. This was investigated with <i>quasi in-situ</i> XPS and CO-IR.</p>
Tue-P-56	<p><b>Nickel Foam Fixed Bed Catalysts for Hydrogenation Reactions: A Novel Activated Metal Catalyst Technology</b>            Radhika G. Rao<sup>1</sup>, <u>Wynter E. G. Osminski</u><sup>2</sup>, René Poss<sup>3</sup>, Meike Roos<sup>3</sup>, Monika Berweiler<sup>3</sup>, Markus Goettlinger<sup>3</sup> and Andrea Heinroth<sup>3</sup>, (1)<i>Evonik Corporation, USA</i>, (2)<i>Evonik, USA</i>, (3)<i>Evonik Operations GmbH, Germany</i>.</p> <p>Short Summary:            Evonik's Metalyst® MC9 is a novel catalyst series that offers high porosity and mechanical strength, which can be used for a variety of hydrogenations in fixed-bed reactors. This Metalyst® series demonstrates higher conversion, selectivity, and lifetime than the traditional Ni catalysts and less attrition than Ni supported on metal oxides.</p>
Tue-P-58	<p><b>Effects of Rapid Microwave Heating on Surface Hydrophobicity of Nitrogen-Doped Carbons</b>  <u>Isao Ogino</u><sup>1</sup>, Takumi Odawara<sup>1</sup>, Hikaru Sugata<sup>1</sup>, Yusaku Yamazaki<sup>1</sup>, Shinichiroh Iwamura<sup>1</sup>, Hironobu Ono<sup>2</sup> and Shin Mukai<sup>1</sup>, (1)<i>Hokkaido University, Japan</i>, (2)<i>Nippon Shokubai, Japan</i>.</p> <p>Short Summary:            We report that microwave heating quickly increases the surface hydrophobicity and crystallinity of both graphene-based carbons and resin-based amorphous carbons while doping the nitrogen species. We demonstrate that this approach enables the synthesis of nitrogen-doped carbon catalysts with substantially improved performance in the oxygen reduction reaction in acidic electrolytes.</p>
Tue-P-59	<p><b>Steering CO<sub>2</sub> Hydrogenation Towards C-C Coupling to Hydrocarbons Using Porous Organic Polymer/Metal Interfaces</b>  <u>Chengshuang Zhou</u><sup>1</sup>, Arun Asundi<sup>1</sup>, Emmett Goodman<sup>1</sup>, Jiyun Hong<sup>2</sup>, Baraa Werghi<sup>2</sup>, Adam Hoffman<sup>2</sup>, Stacey Bent<sup>1</sup>, Simon Bare<sup>2</sup> and Matteo Cargnello<sup>1</sup>, (1)<i>Stanford University, USA</i>, (2)<i>SLAC National Accelerator Laboratory, USA</i>.</p> <p>Short Summary:            We show that porous polymer encapsulation of metal-supported catalysts is capable of driving the selectivity in the CO<sub>2</sub> conversion to hydrocarbons. With this strategy, we achieve an outstanding improvement in C-C coupling that results in orders of magnitude higher turnover frequencies for hydrocarbon formation compared to conventional catalysts.</p>

Tue-P-60	<p><b>Quantifying the Effect of Surface Density of Aminosilanes on the Fraction of Active Sites in SBA-15 for the Aldol Condensation</b>  <u>Jee-Yee Chen</u> and Nicholas Brunelli, <i>The Ohio State University, USA</i>.  Short Summary:  Aminosilica can be designed to use cooperative interactions between amines and surface silanols. No-micropores SBA-15 shows that active sites would increase and loading has impacts for Aldol condensation. Site quantification reveals there are different sites and the work demonstrates the importance of a molecular understanding of cooperative interactions.</p>
Tue-P-62	<p><b>Synthesis of High-Surface Area Tungstated Zirconia By Atomic Layer Deposition on Mesoporous Silica</b>  <u>Ching-Yu Wang</u>, Raymond J. Gorte and John M. Vohs, <i>University of Pennsylvania, USA</i>.  Short Summary:  Atomic layer deposition (ALD) was used to prepare ZrO<sub>2</sub> and WO<sub>3</sub> on the surface of SBA-15 to form tungstated zirconia with Brønsted-acid sites. The ALD synthesis produced films were conformal to the SBA-15 pores. The ALD-synthesized tungstated-zirconia SBA-15 was active in the acid-catalyzed H-D exchange between toluene and D<sub>2</sub>O.</p>
Tue-P-63	<p><b>Pt/Ni Single-Atom Alloys Encapsulated in SiO<sub>2</sub> Nanotubes for Dry Reforming of Methane</b>  <u>Sunkyu Kim</u><sup>1</sup> and Erdem Sasmaz<sup>2</sup>, (1)<i>University of Delaware, USA</i>, (2)<i>University of California, Irvine, USA</i>.  Short Summary:  A SiO<sub>2</sub>-encapsulated Pt/Ni single atom alloy (SAA) structured catalyst presents high coke-resistance under dry reforming of methane due to synergetic combination of the confined morphology and SAA formation. The Pt/Ni atomic ratio of 0.008 shows great stability for SAA structure, where Pt atoms are well distributed on the Ni surface.</p>
Tue-P-64	<p><b>Nanoparticle Size Effects on Phase Stability of Transition Metal Carbides</b>  <u>Anukriti Shrestha</u><sup>1</sup>, Xutao Gao<sup>1</sup>, Jason C. Hicks<sup>2</sup> and Christopher Paolucci<sup>1</sup>, (1)<i>University of Virginia, USA</i>, (2)<i>University of Notre Dame, USA</i>.  Short Summary:  We use DFT calculations of bulk formation and surface energies of Transition metal carbides to map out theoretical phase diagrams that incorporate the effects of particle size. We observe that the trends predicted by our model are generally in agreement with reported particle sizes in experimental synthesis literature.</p>
Tue-P-65	<p><b>Impact of Dopants in Ceria Supports on the Catalytic Performance of Pt Single Atoms</b>  <u>Brandon Burnside</u> and Abhaya Datye, <i>University of New Mexico, USA</i>.  Short Summary:  By doping ceria supports we have demonstrated that the hydrothermal stability is improved while maintaining the reactivity of platinum single atoms and Pt metallic nanoparticles for CO oxidation.</p>
Tue-P-66	<p><b>Catalytic Dehydrogenation of Ethane over MnO<sub>x</sub> Supported on Chabazite Zeolite</b>  <u>Jian Pan</u> and Raul F. Lobo, <i>University of Delaware, USA</i>.  Short Summary:  We have discovered that MnO<sub>x</sub> nanoparticles supported on the small-pore zeolite chabazite (CHA) have very favorable properties for the selective catalytic dehydrogenation of ethane. In this work, we investigate in detail the catalytic properties of MnO<sub>x</sub> supported on CHA, optimize the synthesis condition, and develop structure-property relations for ethane dehydrogenation.</p>
Tue P-126	<p><b>The Effect of Copper Loading on Mfo-5 Support As a Catalyst for CO<sub>2</sub> Hydrogenation to Methanol</b>  <u>Mduduzi Cele</u><sup>1</sup>, Holger Friedrich<sup>2</sup>, Mzamo Shoji<sup>2</sup> and Amanda Mbhele<sup>2</sup>, (1)<i>North-West University, South Africa</i>, (2)<i>University of KwaZulu-Natal, South Africa</i>.  Short Summary:  All catalysts containing copper showed a good activity in CO<sub>2</sub> hydrogenation. The increase of copper did not influence the MOF-5 phase and the distribution was even in all catalysts. The conversion of CO<sub>2</sub> increased with increasing copper loading.</p>
Americas Halls 1 & 2	<p><b>Conversion of Biomass Resources and Polymers Poster Session II</b></p>
Tue-P-67	<p><b>Mechanocatalytic Depolymerization of the Lignin Model Compound Benzyl-Phenyl Ether over Supported Ni and Pd Catalysts</b>  <u>Erin Phillips</u>, Andrew Tricker and Carsten Sievers, <i>Georgia Institute of Technology, USA</i>.  Short Summary:  This work studies the conversion of the lignin model compound benzyl-phenyl ether (BPE). The goal of this reaction is to cleave the α-O-4 bond in BPE to generate toluene and phenol, while shedding light on the effects that particle size, support composition and catalytic surface area have on the reaction.</p>



<p><b>Tue-P-68</b></p>	<p><b>Investigations into the Catalytic Cracking of Pyrolysis Oil Obtained from Plastic Wastes</b>  <u>Snehesh Shivanandra</u><sup>1</sup>, Golam Chowdhury<sup>1</sup>, Marco J. Castaldi<sup>1</sup>, Lucas Dorazio<sup>2</sup>, Jian Shi<sup>2</sup>, James Fu<sup>2</sup> and C. P. Kelkar<sup>2</sup>, (1)City College of New York, CUNY, USA, (2)BASF Corporation, USA.  Short Summary:  We investigate the composition of pyoils obtained from common waste plastics and biogenic feedstock, and show the impact of pyrolysis severity (temperature and residence time) on the conversion, and product yield. Predictions of FCC yields for different pyrolysis products will be discussed along with comparisons to preliminary ACE<sup>®</sup> performance data.</p>
<p><b>Tue-P-69</b></p>	<p><b>Direct Reduction of Esters to Ethers with H<sub>2</sub> over Supported Pd Catalysts: Reaction Mechanisms, Site Requirements, and Particle Size Effects</b>  Claudia Berdugo-Díaz<sup>1</sup>, Yangsik Yun<sup>1</sup>, Jing Luo<sup>2</sup>, David Barton<sup>2</sup>, Ida Chen<sup>2</sup> and David Flaherty<sup>1</sup>, (1)University of Illinois Urbana-Champaign, USA, (2)The Dow Chemical Company, USA.  Short Summary:  We demonstrate the direct reduction of esters to ethers by reactions with H<sub>2</sub> using Pd nanoparticles supported on high surface area Nb<sub>2</sub>O<sub>5</sub>. Rate measurements, selective site titrations, and kinetic isotope effects demonstrate that the reaction requires both metal and acid functions in close proximity and implicates a hemiacetal intermediates.</p>
<p><b>Tue-P-70</b></p>	<p><b>Catalytic Valorization of Furans to Aromatics over Modified Zeolites and Metal Oxides</b>  Guido de Reijer, <u>Christopher Sauer</u> and Per-Anders Carlsson, Chalmers University of Technology, Sweden.  Short Summary:  Sustainable production of chemicals can be satisfied by converting biomass-derived furans into aromatics, i.e., benzene, toluene, and xylenes, using microporous acid catalysts, e.g., modified zeolites or metal oxides, in a continuous flow reactor. Initial findings support the validity of a dual-cycle hydrocarbon mechanism as opposed to the Diels-Alder Cycloaddition-Dehydration mechanism.</p>
<p><b>Tue-P-71</b></p>	<p><b>Effect of Surface Hydrophobicity on the Rate and Selectivity of Phenol Hydrogenation, Observed By <i>Operando</i> <sup>13</sup>C MAS-NMR</b>  <u>Hyunjin Moon</u>, Jason A. Chalmers, Ali Chamas and Susannah L. Scott, University of California, Santa Barbara, USA.  Short Summary:  The use of <i>operando</i> MAS-NMR spectroscopy provides detailed information on the origin of catalytic activity/selectivity in phenol hydrogenation catalyzed by Pd-silica catalysts. The enhanced phenol adsorption leads to ca. 2 times higher phenol conversion rate and selectivity to cyclohexanone for the hydrophobic catalyst compared to the hydrophilic catalyst.</p>
<p><b>Tue-P-72</b></p>	<p><b>High Purity Hydrogen Production from Food Waste Sludge Using Alkaline Catalyst</b>  <u>Jieun Park</u><sup>1</sup>, Hyemin Jung<sup>1</sup>, Ung Gi Hong<sup>2</sup> and Woo-Jae Kim<sup>1</sup>, (1)Ewha Womans University, Korea, Republic of (South), (2)SK gas, Korea, Republic of (South).  Short Summary:  Alkaline thermal treatment of food waste using NaOH as alkaline catalysts produced high-purity H<sub>2</sub> with capturing CO<sub>2</sub> as carbonate. When alkaline thermal treatment is coupled with SMR catalyst (Ni/ZrO<sub>2</sub>) to covert additional CH<sub>4</sub> to H<sub>2</sub>, maximum of 78 % purity of 118.24 mmol H<sub>2</sub>/ is obtained from 1g-food waste.</p>
<p><b>Tue-P-73</b></p>	<p><b>Mechanocatalytic Depolymerization of Poly(Ethylene Terephthalate)</b>  Anuoluwatobi Osibo, Carsten Sievers, Christopher Jones, Andrew Tricker and <u>George Y. Chang</u>, Georgia Institute of Technology, USA.  Short Summary:  Poly(ethylene) terephthalate, in the presence of sodium hydroxide, is depolymerized to its constituent monomer with the use of a ball mill. A ball mill uses mechanical forces to drive chemical reactions, and the surface of the milling balls can provide catalytically active site.</p>
<p><b>Tue-P-74</b></p>	<p><b>Integrating Kinetic Monte Carlo Modeling with Experiment to Clarify Transient Product Distributions Relevant to Polyolefin Hydrogenolysis</b>  <u>Griffin Drake</u> and Yuriy Roman, Massachusetts Institute of Technology, USA.  Short Summary:  Hydrogenolysis is a promising method of deconstructing waste polyolefins into processable alkanes, but its mechanism is obscured by the complex nature of the reaction network. In this study, we integrate model compound experiments with kinetic Monte Carlo modeling to elucidate how process conditions impact the hydrogenolysis mechanism and product distributions.</p>
<p><b>Tue-P-75</b></p>	<p><b>Valorization of Unsaturated Dicarboxylic Acids Obtained from Bio-Fermentation of Organic Municipal Wastes</b>  Jean Caillon<sup>1</sup>, Maxime Ducreux<sup>1</sup>, <u>Gilles Berhault</u><sup>1</sup>, Dorothee Laurenti<sup>1</sup>, Millet Jean-Marc<sup>1</sup> and Jean-Luc Dubois<sup>2</sup>, (1)Université de Lyon, CNRS, France, (2)Arkema, France.  Short Summary:  This work is focused on the valorization of unsaturated dicarboxylic acids obtained from organic municipal wastes. Different strategies for SH addition were investigated for use as polymer additive. A protocol has then been optimized using a thio-Michael reaction while a new approach based on thiourea addition was also developed</p>

- Tue-P-76** **Supported Pt, Ni and Ni Pt Catalysts for Anisole Hydrodeoxygenation: Synthesis, Characterization and Catalytic Activity**  
Daniel E. Pérez and Tatiana E. Klimova, *Universidad Nacional Autónoma de México (UNAM), Mexico*.  
 Short Summary:  
 Synthesis and characterization of monometallic Ni, Pt and bimetallic NiPt catalysts supported on SBA-15. Activity and selectivity in hydrodeoxygenation of anisole as a model compound of bio-oil. Platinum addition to Ni/SBA-15 catalyst improved its activity and selectivity in HDO.
- Tue-P-77** **Co-Processing Biomass Derivatives with Vacuum Gasoil through Hydrocracking**  
Yves Schuurman, *Université de Lyon, CNRS, France*.  
 Short Summary:  
 Co-processing bio-liquids from wood biomass in existing refineries allows fast implementation of liquid biofuels. The aim is to shed light on the impact of bio-liquids on hydrocracking with mineral feed into middle distillates. We found that hydrodeoxygenation took place before the hydrocracking, having no impact on the product distribution.
- Tue-P-78** **Conversion of Bio-Based Levulinic Acid and Its Derivatives to Methyl-N-Ethyl- Pyrrolidone: High Throughput Screening and Reaction Network Analysis**  
 Ghith Al Shaal and Stefan Altwasser, *hte GmbH, Germany*.  
 Short Summary:  
 In this study, we present a design of experiments, based on 45 references to identify the best catalyst system and the ideal parameters that can be applied for the reductive amination of bio-based levulinic acid and its derivatives to methyl-n-ethyl- pyrrolidone.
- Tue-P-79** **Colloidal Nanoparticles for Fundamental Studies in Polyethylene Hydrogenolysis**  
 Matteo Cargnello and Makenna Pennel, *Stanford University, USA*.  
 Short Summary:  
 Colloidal nanoparticles were used to explore particle size and composition effects during polyethylene hydrogenolysis, disentangled from the influence of the support. Such studies address fundamental questions in the field and are inaccessible with catalysts synthesized using traditional impregnation techniques.
- Tue-P-80** **Sustainable Production of Hydrodeoxygenated Palm Oil over Supported Pt Catalysts on Mesoporous Alumina**  
Hwiram Jeong and Young-Woong Suh, *Hanyang University, Korea, Republic of (South)*.  
 Short Summary:  
 Mesoporous alumina supported Pt catalyst, which has a large pore diameter and induces strong-metal interaction, exhibits stable long-term activity in palm oil hydrodeoxygenation.
- Tue-P-81** **High Throughput Experimentation in Catalytic Sugar Conversion**  
 Ghith Al Shaal, Simon Wodarz and Stefan Altwasser, *hte GmbH, Germany*.  
 Short Summary:  
 High throughput experimentation has distinguished itself to be the ideal tool to accelerate R&D and innovation with high degree of reliability and credibility in the catalytic sugar conversion. We present two examples on sugar conversion into added-value chemicals using high throughput technologies.
- Tue-P-82** **Guaiacol Hydrodeoxygenation over Ni-Fe Supported on Nb<sub>2</sub>O<sub>5</sub> and SiO<sub>2</sub> Catalysts**  
 Nina L. A. Souza, Naiara C. Telis, Ana L. M. Alves, Matheus V. A. Ferraz, Tellys Lins Almeida Barbosa and Ricardo R. Soares, *Federal University of Uberlândia, Brazil*.  
 Short Summary:  
 Hydrodeoxygenation of guaiacol, a model compound of lignin widely used due to the methoxy and hydroxyl bonds present, to identify possible products, conversion and selectivity for later application in more complex systems. The catalysts were: Ni, Fe metallic and the bimetallic Ni-Fe all supported on Nb<sub>2</sub>O<sub>5</sub> and SiO<sub>2</sub>.
- Tue-P-83** **Fractionation and Pretreatment of Lignin from Biomass for the Enhanced Production of Platform Chemicals**  
 Daniel Vincent Sahayaraj, Lusi A, Andrew Kohler, Hamed Bateni, 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 pretreatment strategy to drastically reduce the formation of char by 80% and improve aromatic hydrocarbons + alkene yields by >40%.

## Americas Halls 1 & 2

### Electrocatalysis and Photocatalysis Poster Session II

- Tue-P-84** **Impact of Operating Potential on Multicarbon Product Generation for Integrated Photoelectrochemical CO<sub>2</sub> Reduction Cells Using Cu**  
Alex J. King<sup>1,2</sup>, Justin C. Bui<sup>1,2</sup>, Adam Z. Weber<sup>2</sup> and Alexis T. Bell<sup>1,3</sup>, (1)*University of California, Berkeley, USA*, (2)*Liquid Sunlight Alliance, LBNL, USA*, (3)*Lawrence Berkeley National Laboratory, USA*.  
 Short Summary:  
 The implications of the potential dependent product distribution of CO<sub>2</sub> reduction using a Cu catalyst are explored in a photoelectrochemical (PEC) device. Unlike PEC water splitting, operating in an electrochemical current limit regime is advantageous as it offers greater control over device operating potential, enabling stable and improved solar-to-fuel rates.

<p><b>Tue-P-85</b></p>	<p><b>Electrocatalytic Synthesis of Ammonia on Composite Bimetallic Nitride-Perovskite Oxide Cathode</b>  <u>Matthew Ferree</u>, Seval Gunduz, Jaesung Kim, Anne Co and Umit S. Ozkan, <i>The Ohio State University, USA</i>.  Short Summary:  High-temperature (500-600°C) electrocatalytic ammonia synthesis can be carried out using <math>\text{Co}_3\text{Mo}_3\text{N}</math> and LSCF catalyst materials. Combining these materials in a composite cathode merges the benefits of both, resulting in better NRR activity.</p>
<p><b>Tue-P-86</b></p>	<p><b>The Butler-Volmer Equation and Tafel Slope – an Interpretation Based on Transition State Theory and Unidirectional Degrees of Rate Control</b>  <u>Neil Kanth Razdan</u> and Aditya Bhan, <i>University of Minnesota, Twin Cities, USA</i>.  Short Summary:  We develop mathematical foundations for oft-employed Butler-Volmer kinetics and Tafel slope from transition state theory and the principle of microscopic reversibility and, in doing so, rationalize cardinal Tafel slopes (<math>b \sim 118</math> mV/dec) and propose strategies to simultaneously measure anodic and cathodic transfer coefficients at low overpotential.</p>
<p><b>Tue-P-87</b></p>	<p><b>SrTi<sub>1-x</sub>Zr<sub>x</sub>O<sub>3</sub> (x=0.75-1) Solid Solution Synthesis and Its Potential Applications in Energy Vector Production</b>  Leticia M. Torres-Martínez and <u>Angélica González-Grado</u>, <i>Instituto de Ingeniería Civil/Universidad Autónoma de Nuevo León, Mexico</i>.  Short Summary:  SrTi<sub>1-x</sub>Zr<sub>x</sub>O<sub>3</sub> (x=0.75-1) solid solution samples were synthesized via sol-gel method exchanging Ti<sup>4+</sup> by Zr<sup>4+</sup> ions. Optical, crystallographic and morphological properties were analyzed as well as their effect in photoreforming of ethanol to hydrogen performance in aims to find sustainable energy production technologies.</p>
<p><b>Tue-P-88</b></p>	<p><b>Photoreduction of CO<sub>2</sub> at High Pressure: Effect of Co-Catalyst and Conditions</b>  <u>Gianguido Ramis</u><sup>1</sup>, Ilenia Rossetti<sup>2</sup> and Francesco Conte<sup>2</sup>, (1)<i>Università degli Studi di Genova, Italy</i>, (2)<i>Università degli Studi di Milano, Italy</i>.  Short Summary:  The photoreduction of CO<sub>2</sub> has been studied operating under different conditions and investigating the effects of catalyst formulation. Significantly higher productivity than the state of the art was achieved by operating at pressure up to 20 bar. pH was found to play a major role in the product distribution.</p>
<p><b>Tue-P-89</b></p>	<p><b>Atomically Dispersed Ru Catalyst for Stable Hydrogen Evolution Reaction in Alkaline Media</b>  Yang Wang<sup>1,2</sup>, Yida Deng<sup>2</sup> and <u>Jingyue Liu</u><sup>1</sup>, (1)<i>Arizona State University, USA</i>, (2)<i>Tianjin University, China</i>.  Short Summary:  Green hydrogen via water electrolysis requires highly active and stable catalysts. Atomically dispersed Bi atoms stabilize Ru atoms and significantly enhance their HER activity. The as-synthesized Ru/Bi/Co<sub>3</sub>O<sub>4</sub> catalyst delivered ultra-low overpotential of 14 mV@10 mA cm<sup>-2</sup> and lasted 1,200 h of continuous HER without any sign of deactivation.</p>
<p><b>Tue-P-90</b></p>	<p><b>First Principles Based Analysis to Understand Electrooxidation of Ethanol on Platinum</b>  <u>Siddharth Deshpande</u> and Jeffrey Greeley, <i>Purdue University, USA</i>.  Short Summary:  Fundamentally understanding electrocatalytic reactions pertaining to complex carbon and nitrogen based feedstock is important to move towards a sustainable energy future. This work aims to elucidate the observed potential dependent electro-oxidation reaction of ethanol on Pt surfaces. A combination of DFT and Ab-initio molecular dynamic based simulations is utilized.</p>
<p><b>Tue-P-91</b></p>	<p><b>Benchmarking Metal-Organic Framework-Derived Copper Nanoparticle Composite Films for CO<sub>2</sub> Electroreduction</b>  <u>Michael Smith</u>, Bruce E. Koel and Michele Sarazen, <i>Princeton University, USA</i>.  Short Summary:  Metal-organic frameworks (MOFs) are an attractive class of materials for CO<sub>2</sub> electroreduction (CO<sub>2</sub>R) due to their ability to act as catalysts, supports, or as precursors for nanostructured materials. Benchmarking MOFs for CO<sub>2</sub>R requires structure-activity relationship investigations to determine the active site for catalysis and subsequent implications on catalyst activity.</p>
<p><b>Tue-P-92</b></p>	<p><b>Design, Analysis and Simulation of the Acetaminophen Photocatalytic Degradation Process.</b>  José Luis Naranjo, Arick Castillo, Carolina Solís Maldonado, Nayeli Ortiz, Nadia Cruz, Alfredo Cristóbal Salas and <u>Raúl Luna</u>, <i>Universidad Veracruzana, Mexico</i>.  Short Summary:  In this work, the photocatalytic degradation process of an emerging pollutant acetaminophen was analyzed and simulated, using the simulation software Aspen Plus®. A PFR reaction system was conceptually designed from the specific kinetic data of the chemical process, it presents a reaction system on a larger scale.</p>
<p><b>Tue-P-94</b></p>	<p><b>Engineering Catalysis at Solid-Solid Interfaces Using Non-Precious Mixed Metal Oxides for Energy Storage</b>  <u>Samji Samira</u><sup>1</sup>, Siddharth Deshpande<sup>2</sup>, Charles A. Roberts<sup>3</sup>, Ayad Nancy<sup>1</sup>, Jeffrey Greeley<sup>2</sup> and Eranda Nikolla<sup>1</sup>, (1)<i>Wayne State University, USA</i>, (2)<i>Purdue University, USA</i>, (3)<i>Toyota Research Institute - North America, USA</i>.  Short Summary:  A fundamental framework for understanding the factors that influence the growth of lithium-oxygen species on metal oxides is developed. A multifaceted approach coupling atomically-controlled synthesis, electrochemical and characterization studies, and quantum chemical calculations lays the groundwork for studying solid-solid interfacial catalysis for enhancing the efficiency of next-generation energy storage technologies.</p>

Tue-P-95	<p><b>Electrochemical Chlorination Enables Ethylene Oxide Synthesis from Ethanol</b>  <u>Christine Lucky</u>, Taobo Wang and Marcel Schreier, <i>University of Wisconsin-Madison, USA</i>.  Short Summary:  We present the first direct electrochemical chlorination of ethanol to 2-chloroethanol. This pathway uses a radical-mediated chlorination to provide a new route for sustainable ethylene oxide synthesis. Furthermore, it offers a generalizable method to activate <math>sp^3</math> C–H bonds for the electrochemical synthesis of an array of chemicals.</p>
Tue-P-96	<p><b>Electrocatalytic Hydrogenation of Muconic Acid for the Production of Renewable Adipic Acid</b>  <u>Prathamesh Prabhu</u><sup>1,2</sup>, Marco Nazareno Dell'Anna<sup>1,2</sup> and Jean-Philippe Tessonnier<sup>2,3</sup>, (1)<i>Center for Biorenewable Chemicals (CBiRC), USA</i>, (2)<i>Iowa State University, USA</i>, (3)<i>NSF-ERC Center for Biorenewable Chemicals (CBiRC), USA</i>.  Short Summary:  The electrochemical hydrogenation of biobased muconic acid produces the monounsaturated monomer trans-3-hexenedioic acid through homogeneous electronation-protonation. In contrast, the hydrogenation to adipic acid proceeds through a distinct surface-mediated electrocatalytic pathway. Pd/C showed exceptional selectivity to adipic acid, which is likely due to the contribution of a Pd hydride phase.</p>
Tue-P-97	<p><b>Investigating the Structure-Activity Correlation of Bioinspired Manganese Oxides As Electrocatalysts for the Water Oxidation Reaction</b>  <u>Krishani Teeluck</u><sup>1</sup>, Corey Frank<sup>2</sup>, Alicia Manjón Sanz<sup>3</sup> and Charles Dismukes<sup>1</sup>, (1)<i>Rutgers University, USA</i>, (2)<i>National Institute of Standards and Technology, USA</i>, (3)<i>Oak Ridge National Laboratory, USA</i>.  Short Summary:  Water oxidation is the only truly sustainable source of renewable hydrogen, and here we show that a Co-modified bixbyite catalyst increases the electrocatalytic activity of the oxygen evolution reaction as more Co(III) is incorporated into the crystal lattice, likely due to the two empty <math>e_g</math> orbitals allowing two-electron redox chemistry.</p>
Tue-P-98	<p><b>Controlling Hydrogenation Rates in Aqueous Environments Via Applied Potential and Brønsted Acidity</b>  Laura C. Meyer<sup>1</sup>, Udishnu Sanyal<sup>2</sup>, Guanhua Cheng<sup>3</sup>, Katherine Koh<sup>1</sup>, Andreas Jentys<sup>3</sup>, Donald M. Camaioni<sup>1</sup>, <u>Oliver Y. Gutierrez</u><sup>1</sup> and Johannes A. Lercher<sup>1,3</sup>, (1)<i>Pacific Northwest National Laboratory, USA</i>, (2)<i>Washington State University, USA</i>, (3)<i>Technical University of Munich, Germany</i>.  Short Summary:  The conversion of organic compounds driven by electrical potential at low temperature is key for the development of modular decentralized energy conversion systems. This work contributes to understanding how to control rates with applied potential and to use the influence of Brønsted acidity on metal-catalyzed hydrogenation in water.</p>
Americas Halls 1 & 2	<p><b>Fundamentals of Catalysis Poster Session II</b></p>
Tue-P-135	<p><b>Supported Vanadium Catalysts for Selective Sulfur-Oxidative Dehydrogenation of Propane</b>  <u>Allison Arinaga</u>, Selim Alayoglu, Ding Zheng and Tobin J. Marks, <i>Northwestern University, USA</i>.  Short Summary:  Conventional propane oxidative dehydrogenation is limited by overoxidation to <math>CO_x</math>. Using the soft oxidant, <math>S_2</math>, supported vanadium catalysts can achieve high yields of propylene, with isolated sulfided vanadium species being more active and selective than crystalline vanadium sulfide. Furthermore, the <math>S_2</math> oxidant is shown to enhance selectivity compared to <math>O_2</math>.</p>
Tue-P-99	<p><b>A Langmuir-Hinshelwood Deactivation Model of an Ir-Pt Catalyst in Butane Hydrogenolysis</b>  <u>Heng Shou</u>, Ashwin Patel, Cong Nguyen and Byeongjin Baek, <i>SABIC, USA</i>.  Short Summary:  This work presents a Langmuir-Hinshelwood deactivation model of an IrPt catalyst in butane hydrogenolysis. Unlike the conventional wisdom that always uses excessive <math>H_2</math> to mitigate catalyst deactivation, the deactivation rate of the presented system reaches a maximum at a medium <math>H_2</math>-to-butane ratio. Moreover, deactivation may be alleviated at <math>H_2</math>-lean conditions.</p>
Tue-P-134	<p><b>Surface Acidity Impacts on the Structural Evolution of Supported PdAu Catalysts</b>  <u>Welman Curi Elias</u>, Kimberly Heck, Hunter Jacobs, Wenqing Zhang and Michael S. Wong, <i>Rice University, USA</i>.  Short Summary:  While silica supports are standard to study PdAu VA-catalysts, we show the presence of acid sites play an important role on catalyst restructuring. The acidic support had different metallic structures than silica. Moreover, the structures evolved differently under <i>in situ</i> conditions, which is speculated to greater acetate retention on silica.</p>
Tue-P-100	<p><b>Rates and Reversibilities in Interconnected Reaction Networks</b>  <u>Ting Lin</u>, Neil Kanth Razdan and Aditya Bhan, <i>University of Minnesota, Twin Cities, USA</i>.  Short Summary:  Functional forms of unidirectional rates prescribed to single-path reactions do not apply to interconnected networks. Presence of alternative pathways decreases both the forward and reverse unidirectional rates to the product of interest without impacting the functional form of the effective reversibility. Herein, detailed mathematical derivation and physical interpretation are presented.</p>

<b>Tue-P-101</b>	<p><b>Transition-State Vibrational and Thermochemical Scaling Relationships for Dehydrogenations</b>  <u>Sophia Kurdziel</u>, Joshua Lansford and Dionisios G. Vlachos, <i>University of Delaware, USA</i>.</p> <p>Short Summary:  Transition-state vibrational scaling relationships (TSVSRs) scale metal-adsorbate driven modes between local minima and transition states across metal surfaces for <math>AH_x</math> (<math>A = C, N, O</math>) dehydrogenations. TSVSRs, and by extension, thermochemical scaling relationships, offer a potential pathway to estimate vibrational thermochemical contributions without expensive density functional theory calculations.</p>
<b>Tue-P-102</b>	<p><b>Kinetics of Ethylene Epoxidation and in-Situ Enumeration of Active Site Density over Promoted <math>Ag/\alpha-Al_2O_3</math> catalysts</b>  <u>Krishna Iyer</u>, Aditya Bhan and James Harris, <i>University of Minnesota, Twin Cities, USA</i>.</p> <p>Short Summary:  We report the kinetics of ethylene epoxidation and chlorine moderation over promoted <math>Ag/\alpha-Al_2O_3</math> catalysts to elucidate the kinetic interdependencies among the concurrent catalytic cycles occurring in an epoxidation reactor. We also enumerate active site densities over different <math>Ag/\alpha-Al_2O_3</math> formulations to study particle size effects on EO rates and selectivity.</p>
<b>Tue-P-103</b>	<p><b>Untangling the Kinetics of Ethylene Epoxidation through Pressure Transients</b>  Lilliana Brandao, Eric High and <u>Christian Reece</u>, <i>Harvard University, USA</i>.</p> <p>Short Summary:  By combining microkinetic modelling with pressure transients at pressures ranging from ultra-high vacuum to atmospheric pressure we aim to precisely probe the kinetics for ethylene epoxidation over silver catalysts.</p>
<b>Tue-P-104</b>	<p><b>Solvation Effects in Liquid-Phase Esterification Reactions Catalyzed By Hydrogen Form Ion Exchange Resins</b>  <u>Mackenzie R. Todd</u><sup>1</sup>, Jaeryul Park<sup>2</sup>, Luke T. Roling<sup>2</sup> and Thomas J. Schwartz<sup>1</sup>, <i>(1)University of Maine, USA, (2)Iowa State University, USA</i>.</p> <p>Short Summary:  Esterification of butyric acid and butanol catalyzed by solid acid resins was studied while varying solvent polarity and catalyst resin structure. Change in solvent polarity resulted in difference in reaction mechanism. Change in resin structure resulted in difference in turnover frequency due to transition state solvation by the resin.</p>
<b>Tue-P-105</b>	<p><b>The Roles of Acid and Redox Sites during Oxidative Scission of Ketones over <math>VO_x/\gamma-Al_2O_3</math></b>  <u>Bowei Liu</u>, Ran Zhu and Jesse Bond, <i>Syracuse University, USA</i>.</p> <p>Short Summary:  To resolve the mechanistic contributions of Lewis, Bronsted acid, and redox sites during the aerobic methyl ketone oxidative scission, selective site-poisoning experiments were performed using pyridine, 2,6-di-tert-butylpyridine, and ammonia during the oxidation of 3-methyl-2-butanone over <math>\gamma-Al_2O_3</math> supported vanadium oxide catalyst.</p>
<b>Tue-P-106</b>	<p><b>Differentiation between Surface and Vapor-Mediated Deactivation Mechanisms of Noble Metal-Based Catalysts</b>  <u>Jinwon Oh</u><sup>1</sup>, Arik Beck<sup>2</sup>, Emmett Goodman<sup>1</sup>, Anthony Boucly<sup>3</sup>, Luca Artiglia<sup>3</sup>, Jeroen A. van Bokhoven<sup>2</sup> and Matteo Cargnello<sup>1</sup>, <i>(1)Stanford University, USA, (2)ETH Zürich, Switzerland, (3)Paul Scherrer Institut, Switzerland</i>.</p> <p>Short Summary:  There are two fundamental mechanisms of sintering, which are particle migration and coalescence and Ostwald (or atomic) ripening. Previous studies have successfully differentiated them. However, differentiation between surface and vapor phase-mediated ripening has not been reported. In this work, we distinguished two ripening mechanisms using colloiddally engineered catalysts.</p>
<b>Tue-P-107</b>	<p><b>Alpha-C-H Acidity of Carboxylic Acids on Surface of Metal Oxides and Enolization Kinetics</b>  <u>Alexey Ignatchenko</u>, Reem Ibrahim, Jordan Kostera, Jared Jorolemon, Christian Leonardo and Lilliana Weldelessie, <i>St. John Fisher College, USA</i>.</p> <p>Short Summary:  Carboxylic acids are reversibly enolized upon adsorption on metal oxide surface and react as a nucleophile in a condensation with the second carboxylic acid. Reaction kinetics of acetic and iso-butyric acid enolization on <math>ZrO_2</math> and <math>TiO_2</math> surface have been studied by H/D exchange with <math>D_2O</math>.</p>
<b>Tue-P-108</b>	<p><b>Roles of Lattice and Gaseous Oxygen in the Oxidative Scission of Methyl Ketone over <math>VO_x/\gamma-Al_2O_3</math></b>  Siwen Wang, Ran Zhu, Bowei Liu and Jesse Bond, <i>Syracuse University, USA</i>.</p> <p>Short Summary:  Both lattice and gas phase oxygen play important roles in facilitating the oxidative scission of aerobic ketone oxidation on vanadium oxides surfaces. To provide insight into the contributions of each, we employ an online mass spectroscopic analysis of reaction products during TPSR and transient analysis of products.</p>
<b>Tue-P-109</b>	<p><b>Computational Insights of Water in Catalytic Reduction of Nitrite</b>  <u>Yu Yan</u> and Bin Wang, <i>University of Oklahoma, USA</i>.</p> <p>Short Summary:  The nitrite and NO reduction have been studied here using DFT calculations. The reaction mechanism is revealed through calculations of free energy profile which shows that water can accelerate the reactions by stabilizing the surface species, enabling proton shuttling, and serving as proton donors.</p>



<p><b>Tue-P-110</b></p>	<p><b>Low Temperature Ethylene Oxidation over Pt/Silica: Role of Water-Resistant Pt Sites in Hydrophobic Mesopores</b>  <u>Shazia Sharmin Satter</u><sup>1</sup>, Kiyotaka Nakajima<sup>2</sup> and Atsushi Fukuoka<sup>2</sup>, (1)<i>The University of Kansas, USA</i>, (2)<i>Hokkaido University, Japan</i>.  Short Summary:  Pt nanoparticles on hydrophobic mesoporous silica oxidize trace ethylene at 0 °C more effectively than those of silica gel. FTIR measurements combined with a gas-flow system revealed that high activity of Pt nanoparticles inside hydrophobic mesopores is attributed to efficient removal of H<sub>2</sub>O from active Pt surface.</p>
<p><b>Tue-P-111</b></p>	<p><b>Controlled Bimetallic Catalyst Synthesis Using Galvanic Displacement, Electroless Deposition Methods and Application for Renewable Chemical Production</b>  <u>Weijian Diao</u>, <i>Villanova University, USA</i>.  Short Summary:  Using controlled synthesis methods including galvanic displacement (GD) and electroless deposition (ED), different series of bimetallic catalysts including Pt-Ru, Pd-Ag, Ag-Ir have been prepared with controllable composition and structure. Bimetallic catalysts synthesized by GD and ED methods have shown supreme performance for different applications including selective hydrogenation/oxidation reactions.</p>
<p><b>Tue-P-112</b></p>	<p><b>Support Effects on Hydrogenation Reaction-Understanding the High Activity of Pd Supported on Graphene</b>  <u>Alaba Ojo</u>, Deependra Shakya, Donna Chen, John R. Regalbuto, Julian Stetzler and Narayan Acharya, <i>University of South Carolina, USA</i>.  Short Summary:  The higher hydrogenation TOF of Pd/graphitic carbons relative to other carbon supports and silica has been hypothesized to be due to its higher hydrogen storage capacity. We have performed H<sub>2</sub> temperature programmed desorption (TPD experiments) on Pd catalysts supported on pyrolyzed (cheap) and commercial graphene supports to investigate this hypothesis.</p>
<p><b>Tue-P-113</b></p>	<p><b>NiMo Carbide Supported on Chemically Prepared Activated Carbon from Algal Derived Hydrochar for Hydrodeoxygenation of Algal Biocrude Oil</b>  Shima Masoumi and <u>Ajay Dalai</u>, <i>Saskatchewan University, Canada</i>.  Short Summary:  The objective of this present study is to develop novel heterogeneous catalyst using activated algal hydrochar as a support and its application for hydrodeoxygenation of algal biocrude oil to produce high quality biofuels.</p>
<p><b>Tue-P-114</b></p>	<p><b>Observation and Structure-Insensitivity of Hydroxyls on Gold</b>  <u>Yue Qi</u><sup>1</sup>, Yiteng Zheng<sup>2</sup>, Simon G. Podkolzin<sup>1</sup> and Bruce E. Koel<sup>2</sup>, (1)<i>Stevens Institute of Technology, USA</i>, (2)<i>Princeton University, USA</i>.  Short Summary:  Hydroxyls on Au can be directly observed spectroscopically, that their O-H stretching vibration is insensitivity to the size of Au structures. This vibration is a qualitative indicator of the surface functional properties, that will be useful in developing more efficient Au-based catalysts for selective hydrocarbon oxidation and other industrial applications.</p>
<p><b>Americas Halls 1 &amp; 2</b></p>	<p><b>Modelling, Simulation, and Machine Learning in Catalysis Poster Session II</b></p>
<p><b>Tue-P-115</b></p>	<p><b>DFT Modelling of Acid-Base Active Centers on KOH-Doped Anatase TiO<sub>2</sub> for Alpha-Deprotonation of Carboxylates</b>  <u>Jared Jorolemon</u> and Alexey Ignatchenko, <i>St. John Fisher College, USA</i>.  Short Summary:  KOH doping significantly enhances anatase TiO<sub>2</sub> catalytic activity for the decarboxylative ketonization of carboxylic acids used in biofuel upgrading. DFT study show how newly created OH groups are able to deprotonate alpha carbon of the most abundant bidentate carboxylate and activate it for the rate limiting step, condensation.</p>
<p><b>Tue-P-116</b></p>	<p><b>Performance Modeling of Hydrogen-Based Membrane Palladium-Film Reactors</b>  <u>Juan Donoso</u><sup>1</sup> and Michael S. Wong<sup>2</sup>, (1)<i>Rice University, USA</i>, (2)<i>Nanotechnology Enabled Water Treatment (NEWT) Center, USA</i>.  Short Summary:  Using advanced optimization routines and first principles of reaction engineering, we developed an algorithm to simulate the adsorption-reaction mechanism in a membrane catalyst-film reactor. The results obtained for the defluorination of PFOA in the system exemplify the ability of the method to test reaction mechanisms and obtain kinetic data.</p>
<p><b>Tue-P-118</b></p>	<p><b>Theory-Infused Neural Network for Interpretable Reactivity Prediction</b>  <u>Shih-Han Wang</u>, Hemanth Somarajan Pillai, Siwen Wang, Luke E.K. Achenie and Hongliang Xin, <i>Virginia Polytechnic Institute and State University, USA</i>.  Short Summary:  We developed a theory-infused neural network (TinNet), which integrates deep learning algorithms with the well-established <i>d</i>-band theory of chemisorption for reactivity prediction. TinNet not only achieves prediction performance on par with purely regression-based ML methods, but also opens the black box of ML and reveals the nature of chemical bonding.</p>

<b>Tue-P-119</b>	<p><b>Electrical Double Layer Capacitance and Polarizability Modelled in Classical Molecular Dynamics</b>  <u>Bolton Tran</u>, Scott Milner and Michael Janik, <i>The Pennsylvania State University, USA.</i></p> <p>Short Summary:  We present in this work a novel classical MD simulation of the electrode-electrolyte interface under biased potentials. We measured 1) the double layer's dielectric constant to be abnormally low (2.7), in good agreement with recent experimental measurement, and 2) the capacitance of the interface.</p>
<b>Tue-P-120</b>	<p><b>A Practical Way to Enhance the Synthesis of <math>\text{N}_8^-</math> from an <math>\text{N}_3^-</math> Precursor</b>  <u>Safa Alzaim</u>, Joshua Young and Xianqin Wang, <i>New Jersey Institute of Technology, USA.</i></p> <p>Short Summary:  Using <i>ab initio</i> calculations, a practical and rational way to produce <math>\text{N}_8^-</math> PN from <math>\text{N}_3^-</math> is determined. A TD-DFT calculation was used to calculate the absorption spectrum of <math>\text{N}_3^-</math> and predict a method of yield enhancement via illumination under UV light, which was confirmed with the experimental results.</p>
<b>Tue-P-121</b>	<p><b>Using Machine Learned DFT Surrogates to Model High Throughput Experimental Catalysis Workflows</b>  <u>Kirby Broderick</u> and Zachary Ulissi, <i>Carnegie Mellon University, USA.</i></p> <p>Short Summary:  A workflow is designed to aggregate hydrogen binding energy predictions across chemical systems, and these values are combined with the output of a high-throughput nanoparticle-based experimental catalysis hydrogen evolution workflow in a Sabatier-like plot. The resulting relationship significantly shrinks the space of potentially active catalysts to screen.</p>
<b>Tue-P-122</b>	<p><b>Accelerating Research with the Catalyst Property Database</b>  <u>Sean Tacey</u>, Qiyuan Wu, Carrie Farberow and Kurt Van Allsburg, <i>National Renewable Energy Laboratory, USA.</i></p> <p>Short Summary:  When data—such as computed reaction energetics—is used in catalyst design, it is almost always generated by researchers themselves, even if similar data has been published previously. The <a href="#">Catalyst Property Database</a> (CPD) seeks to reduce this duplication of effort by creating a centralized, searchable database of quality catalyst property data.</p>
<b>Tue-P-123</b>	<p><b>Descriptor for <math>\text{O}^*</math> and <math>\text{OH}^*</math> Adsorption on Pure Rutile Oxide Surfaces</b>  <u>Benjamin Comer</u><sup>1</sup>, Jiang Li<sup>2</sup>, Frank Abild-Pedersen<sup>2</sup>, Michal Bajdich<sup>1</sup> and Kirsten T. Winther<sup>1</sup>, (1)<i>Stanford University, USA</i>, (2)<i>SLAC National Accelerator Laboratory, USA.</i></p> <p>Short Summary:  In this work we show the integrated crystal orbital Hamiltonian populations (ICOHP) obtained from bulk calculations are a good descriptor of adsorption energies of <math>\text{O}^*</math> and <math>\text{OH}^*</math> on rutile oxide surfaces (RMSE 0.2-0.35 eV.) Thus, bulk calculations may be sufficient to screen materials for their OER/ORR activity.</p>
<b>Tue-P-124</b>	<p><b>Reactive Neural Network Potentials for Zeolites with Density Functional Theory Accuracy</b>  <u>Andreas Erlebach</u>, <u>Martin Šípk</u>, Christopher Heard, Petr Nachtigall and Lukáš Grajciar, <i>Charles University, Czech Republic.</i></p> <p>Short Summary:  We demonstrate the development of reactive Machine Learning Potentials (MLP) for various classes of zeolites. The new MLPs retain the accuracy of quantum mechanical simulations while speeding up the calculations by at least three orders of magnitude, allowing realistic modeling of zeolites under <i>operando</i> conditions.</p>
<b>Tue-P-125</b>	<p><b>Analysis of Kinetic Dependencies of Catalyst Deactivation Based on the Three-Factor Kinetic Equation</b>  <u>Zoë Gromotka</u><sup>1</sup>, Gregory Yablonsky<sup>2</sup>, Nickolay Ostrovskii<sup>3</sup> and Denis Constales<sup>1</sup>, (1)<i>Ghent University, Belgium</i>, (2)<i>Washington University in St. Louis, USA</i>, (3)<i>Euro Gas, Serbia.</i></p> <p>Short Summary:  We used the three-building block scheme to derive the three-factor kinetic equation. We then performed a mathematical parametric study on this equation to determine how the rate may be manipulated using the apparent parameters of the main cycle. We looked at how parameters from the main cycle may manipulate deactivation.</p>
<b>Tue-P-127</b>	<p><b>Trends in Methane Oxidation on Rutile Oxide Under Emission Conditions</b>  <u>Geun Ho Gu</u>, Gi Joo Bang and Yousung Jung, <i>Korea Advanced Institute of Science and Technology (KAIST), Korea, Republic of (South).</i></p> <p>Short Summary:  The oxidation of the methane is important for the incomplete combustion of methane. Here, we demonstrate the experiment-validated microkinetic model for methane oxidation on rutile oxides. We develop the volcano map and elucidate the design principles in emission conditions. Furthermore, we implement machine learning (ML) to rapidly perform high-throughput screening.</p>
<b>Tue-P-128</b>	<p><b>The Effect of Hartree-Fock Exchange on Scaling Relations and Reaction Energetics for C–H Activation Catalysts</b>  <u>Vyshnavi Vennelakanti</u>, Aditya Nandy and Heather Kulik, <i>Massachusetts Institute of Technology, USA.</i></p> <p>Short Summary:  By studying direct methane-to-methanol conversion with density functional theory using 3d transition metal catalysts, we show that the choice of functional can alter relative energetics, catalyst performance, and conclusions on whether a reaction is spin-conserved. For closed shell intermediates, however, a single approximate functional can lead to useful conclusions.</p>

<p><b>Tue-P-129</b></p>	<p><b>Modeling of Hydrogenolysis of Light Alkanes on Ru</b>  <u>Tianjun Xie</u>, Gerhard R. Wittreich and Dionisios G. Vlachos, <i>University of Delaware, USA</i>.  Short Summary:  We have built the first robust microkinetic models (MKM) of ethane and propane hydrogenolysis on Ru, which yielded fundamental mechanistic insights. We will discuss how to leverage the information to understand the hydrogenolysis of long hydrocarbons.</p>
<p><b>Tue-P-130</b></p>	<p><b>A Computational Investigation of the H-SSZ-13 Surface Reactivity</b>  <u>Philipp Huber</u> and Philipp N. Plessow, <i>Karlsruhe Institute of Technology (KIT), Germany</i>.  Short Summary:  The reactivity of Brønsted and Lewis acid sites at the (101) and (001) surfaces of H-SSZ-13 is investigated computationally using DFT calculations corrected by highly accurate DLPNO-CCSD(T) calculations on cluster models. Concerted and stepwise DME formation were studied as catalytic probe reactions.</p>
<p><b>Tue-P-131</b></p>	<p><b>Cesium Enabled Ethanol Production from CO<sub>2</sub> Hydrogenation on Cu/ZnO(000-1) and Cu-M/ZnO(000-1) Surfaces</b>  <u>Xuelong Wang</u><sup>1</sup>, Wenjie Liao<sup>2</sup>, Jose A. Rodriguez<sup>1</sup> and Ping Liu<sup>1</sup>, <i>(1)Brookhaven National Laboratory, USA, (2)Stony Brook University, USA</i>.  Short Summary:  The deposition of Cs on Cu/ZnO(000-1) is found to enable the ethanol synthesis from CO<sub>2</sub> hydrogenation. Theoretical study reveals that synergy among Cs, Cu, and ZnO at the interface plays an essential role, being able to promote the CO<sub>2</sub> adsorption and conversion toward methanol and ethanol.</p>
<p><b>Tue-P-132</b></p>	<p><b>A Predictive Partial Least Square Model for Inline Monitoring of Biomass Reactions Via ATR-FTIR Spectroscopy.</b>  <u>Jakub Konkol</u> and George Tsilomelekis, <i>Rutgers, The State University of New Jersey, USA</i>.  Short Summary:  Through multivariate regression modeling, vibrational spectroscopy can be used to analyze complex reaction media for inline analysis of biomass upgrading reactions. Built from simple binary mixtures, predictive models can be generated to analyze real reaction mixtures, supporting the screening of catalysts and eventually operando analysis of on heterogenous catalysts.</p>
<p><b>Tue-P-133</b></p>	<p><b>A Machine Learning Approach to Pore Volume Prediction in Catalyst Manufacturing</b>  <u>Matteo Perno</u>, <i>Technical University of Denmark, Denmark</i>.  Short Summary:  This study compares the performance of 5 machine learning models trained using real-world data from 5 catalysts. The models are designed to predict each catalysts' pore volume. The results indicate that Light Gradient Boosting Machines and Extreme Gradient Boosting Machines can predict catalyst pore volume with high accuracy.</p>

# Wednesday May 25, 2022 Poster Program

<b>Americas Halls 1 &amp; 2</b>	<b>Catalysis for Chemical Synthesis and Functionalization Poster Session</b>
<b>Wed-P-3</b>	<b>Catalytic Oxidation of Nitric Oxide at Industrial Nitric Acid Conditions</b> Jithin Gopakumar and <u>Magnus Rønning</u> , <i>Norwegian University of Science and Technology (NTNU), Norway</i> . Short Summary: Nitric oxide oxidation at nitric acid plant conditions has been a highly researched topic in the industry. Only three early patents are ever published. My research focusses on using low cost Manganese supported on Zirconia catalyst to oxidize NO to NO <sub>2</sub> at partial industrial nitric acid conditions.
<b>Wed-P-4</b>	<b>Highly Selective Dehydra-Decyclization of Cyclic Ethers to Conjugated Dienes over ZrO<sub>2</sub></b> <u>Mengjie Fan</u> <sup>1</sup> , Yichen Ji <sup>1</sup> , Sai Praneet Batchu <sup>2</sup> , Omar Abdelrahman <sup>3</sup> , Stavros Caratzoulas <sup>2</sup> , Raymond J. Gorte <sup>1</sup> and John M. Vohs <sup>1</sup> , (1) <i>University of Pennsylvania, USA</i> , (2) <i>University of Delaware, USA</i> , (3) <i>University of Massachusetts Amherst, USA</i> . Short Summary: Our research demonstrates ZrO <sub>2</sub> as catalyst favors production of C <sub>4</sub> ~C <sub>5</sub> conjugated dienes from corresponding cyclic ethers, which has potential to substitute the current petroleum-based production. A thermodynamically favorable surface intermediate isomerization on ZrO <sub>2</sub> is the key. Catalyst performance can be further improved by utilizing ALD technique.
<b>Wed-P-5</b>	<b>Partial Oxidation of Benzyl Alcohol Using Gold-Copper Nanoparticles: Investigating Effects of Bound Ligands, Support, and Composition</b> Joseph Brindle and <u>Michael M. Nigra</u> , <i>University of Utah, USA</i> . Short Summary: Gold-copper bimetallic nanoparticles are synthesized using a facile one-pot synthesis method. The nanoparticles are then used in solution as unsupported catalysts for benzyl alcohol oxidation. Additionally, the nanoparticles are also supported on three different supports for catalysis testing. Results indicate that the metallic composition and support influence catalytic activity.
<b>Wed-P-6</b>	<b>Valorization of Furfural Using Ruthenium (II) Complexes Containing Phosphorus-Nitrogen Ligands Under Homogeneous Transfer Hydrogen Condition.</b> <u>Sebastian Parra Melipan</u> <sup>1</sup> , Gonzalo Valdebenito <sup>1</sup> and Pedro Aguirre <sup>1,2</sup> , (1) <i>Universidad de Chile, Facultad de Ciencias Químicas y Farmacéuticas, Chile</i> , (2) <i>Universidad de Santiago de Chile, Facultad de Química y Biología, Chile</i> . Short Summary: The catalysts reported 100% conversion and high selectivity's in the furfural hydrogenation using 2-propanol and formic acid. The reaction studied in a basic medium competes with the Cannizzaro reaction, obtaining furfuryl alcohol and furoic acid. The formic acid as the hydrogen source yields furfuryl alcohol with 100% selectivity.
<b>Wed-P-7</b>	<b>Reduction of Dimethyl Oxalate to Ethylene Glycol Via Heterogeneous Ag-Based Catalysts: Reaction Kinetic and Surface Spectroscopic Investigation</b> <u>Nicolas Gleason-Bouré</u> and Christopher T. Williams, <i>University of South Carolina, USA</i> . Short Summary: Ethylene glycol (EG) is an important industrial chemical that is predominately produced from non-renewable resources. The hydrogenation from dimethyl oxalate (DMO) is a novel synthesis route to sustainable produce EG from more sustainable sources. This research will look at the benefits of silver catalysts for this reduction method.
<b>Wed-P-8</b>	<b>Elucidation of Isorecticular MIL-101 Deactivation Mechanisms for Liquid-Phase Styrene Oxidation By Hydrogen Peroxide</b> <u>Rachel Yang</u> and Michele Sarazen, <i>Princeton University, USA</i> . Short Summary: Isorecticular MIL-101(Cr, Fe) is investigated as a modular platform to quantify differences in reactivity, selectivity, and deactivation for liquid-phase styrene oxidation by hydrogen peroxide at mild conditions. Disparate reactivities, deactivation mechanisms, and regeneration potentials for Cr and Fe are elucidated as a function of intrinsic metal and bulk material properties.
<b>Wed-P-9</b>	<b>Experimental Analysis of Operating Conditions for Radio Frequency Plasma Catalysis of Ammonia</b> <u>Sebastian Bastek</u> , Vincent Dieterich, Sebastian Fendt and Hartmut Spliethoff, <i>Technical University of Munich, Germany</i> . Short Summary: The goal of this research is to study the impact of operating conditions (H <sub>2</sub> /N <sub>2</sub> ratio, temperature, pressure, catalyst) on plasma catalysis of ammonia using radio frequency discharge plasma. The experiments are performed under mild operating conditions using an in-house built plasma catalysis lab set-up.
<b>Wed-P-10</b>	<b>Pd-Based Yolk-Shell Nanocrystals for Acetylene Semi-Hydrogenation Reaction</b> <u>Zihao Yan</u> and Huiyuan Zhu, <i>Virginia Polytechnic Institute and State University, USA</i> . Short Summary: Herein, we introduce our recent work on developing Pd-based yolk-shell nanocrystals through applying strong metal-support interaction via a reverse route (SMSIR). Factors, including shell thickness and core composition, have been optimized to achieve a 95% ethylene selectivity in the acetylene semi-hydrogenation reaction.

Wed-P-11	<p><b>Quantifying Solvent and pH Effects on Rh Catalyzed Benzaldehyde Hydrogenation</b>  <u>Thuy T. Le</u><sup>1</sup>, Abhi Karkamkar<sup>1</sup> and Johannes A. Lercher<sup>1,2</sup>, (1)<i>Pacific Northwest National Laboratory, USA</i>, (2)<i>Technical University of Munich, Germany</i>.</p> <p>Short Summary:  Benzaldehyde hydrogenation on Rh/TiO<sub>2</sub> was performed in solvents of different polarity and pH to determine dependencies of reaction orders and reaction rates on these properties. With detailed kinetics modeling, we can quantitatively understand the relevant mechanism and underlying thermodynamics of these effects to enable prediction and control of catalytic performance.</p>
Wed-P-12	<p><b>Synthesis of Hierarchical ZSM-5 and Its Evaluation in Catalytic Cracking of Various Hydrocarbons</b>  <u>Ebrahim Mohiuddin</u>, Loyiso Nqakala, Philani Mpungose and Masikana Mdleleni, <i>University of the Western Cape, South Africa</i>.</p> <p>Short Summary:  This study on the synthesis of ZSM-5 as catalysts in the catalytic cracking of hydrocarbons showed that hierarchical ZSM-5 was successfully synthesised using a steam assisted method. It showed better conversion and selectivity to propylene when compared to a microporous ZSM-5 and converted long chain hydrocarbons with high propylene selectivity.</p>
Wed-P-13	<p><b>Acidity-Activity Relationships in the Tert-Butylation of Phenol over Sulfated Metal Oxides</b>  <u>Adam Zuber</u> and George Tsilomelekis, <i>Rutgers, The State University of New Jersey, USA</i>.</p> <p>Short Summary:  Tert-butylation of phenol was carried out via select sulfated metal oxides with significant yield towards the mono-alkylated products. Spectroscopic studies and acidity measurements were correlated with kinetic data, resulting in an acidity-activity relation. This study has revealed that the relative ratio of Lewis and Bronsted acidity corresponds well with reactivity.</p>
Wed-P-14	<p><b>Ethanol Oligomerization into Alcohols and Esters over MgAl Mixed Oxides Doped with Low-Loadings of Cu</b>  <u>Paolo Cuello Penalzoa</u><sup>1</sup>, Yi Du<sup>2</sup>, Michael Lanci<sup>2</sup> and George Huber<sup>1</sup>, (1)<i>University of Wisconsin-Madison, USA</i>, (2)<i>ExxonMobil Research and Engineering, USA</i>.</p> <p>Short Summary:  We synthesized and tested a 0.3wt%Cu/Mg<sub>x</sub>AlO<sub>y</sub> catalyst in the ethanol coupling reaction, obtaining yields up to 75% for diesel fuel precursor molecules. We demonstrate that we can obtain selectively from ethanol C<sub>4+</sub> alcohols, C<sub>6+</sub> esters and other higher oxygenates suitable for upgrading into diesel fuel via subsequent processes.</p>
Wed-P-15	<p><b>Harmonic Acidity and Basicity of Yttria-Stabilized Zirconia in Dehydration of 4-Methyl-2-Pentanol</b>  <u>Jae-Hong Lee</u> and Young-Woong Suh, <i>Hanyang University, Korea, Republic of (South)</i>.</p> <p>Short Summary:  This study reports that the well-dispersed yttria on zirconia surface, which retains the harmony of acidity and basicity, exhibits the promoted catalytic performance in 4-methyl-2-pentanol dehydration to acquire the 4-methyl-1-pentene which is the desired <math>\alpha</math>-olefin.</p>
Wed-P-16	<p><b>Silica-Alumina As Catalyst for Melt Polycondensation of L-Lactic Acid</b>  <u>Mateus Paiva</u><sup>1</sup>, Juliene França<sup>2</sup>, Silvia Dias<sup>2</sup> and José Dias<sup>2</sup>, (1)<i>Université de Lille, CNRS, Centrale Lille, France</i>, (2)<i>University of Brasilia, Brazil</i>.</p> <p>Short Summary:  The present study describes the relevant acid properties of silica alumina for its application as a heterogeneous catalyst in the melt polycondensation reaction of L-lactic acid, which resulted in the formation of crystalline polymeric materials with good thermal / mechanical properties and molar mass above 18 000 g mol<sup>-1</sup>.</p>
Americas Halls 1 & 2	<p><b>Catalysis for C<sub>1</sub> and SynGas Chemistry Poster Session III</b></p>
Wed-P-17	<p><b>Bifunctional Catalysts for Energy Efficient Conversion of CO<sub>2</sub> to Dimethyl Ether</b>  <u>Hai-Ying Chen</u>, Josh A. Pihl, Todd J. Toops and Sreshtha Sinha Majumdar, <i>Oak Ridge National Laboratory, USA</i>.</p> <p>Short Summary:  This study investigates various preparation approaches to develop highly active, selective, and durable bifunctional catalysts for the direct conversion of CO<sub>2</sub> to dimethyl ether. The results support continued effort to explore alternative catalyst configurations to overcome the long-term durability challenges that such type of bifunctional catalysts are facing.</p>
Wed-P-18	<p><b>Structure-Activity Relationship for the Reduction of CO<sub>2</sub> on Ce<sub>x</sub>Cu<sub>1-x</sub>O<sub>2</sub> Catalysts</b>  <u>Jorge Moncada</u> and Jose A. Rodriguez, <i>Brookhaven National Laboratory, USA</i>.</p> <p>Short Summary:  A correlation between the catalytic activity and structure/composition of the inverse CeO<sub>x</sub>/CuO catalysts has not been made in a systematic way under CO<sub>2</sub> hydrogenation conditions. Here, it was found how particular oxidation states driven by solid solution cerium atomic loading drive the reactivity for the CO<sub>2</sub> reduction reaction.</p>



<p><b>Wed-P-19</b></p>	<p><b>CO<sub>2</sub> Hydrogenation Catalysis for the Design of Dual Function Materials (DFMs) for Combined Capture and Utilisation</b>  <u>Loukia-Pantzechroula Merkouri</u>, Tomas Ramirez Reina and Melis Duyar, <i>University of Surrey, United Kingdom</i>.  Short Summary:  Dual Function Materials (DFMs) are combinations of adsorbent and catalyst capable of both capturing CO<sub>2</sub> and converting it to fuels and chemicals, in the same reactor with the help of a co-reactant. We further extend this idea to the development of switchable DFMs for the synthesis of methane and syngas.</p>
<p><b>Wed-P-20</b></p>	<p><b>Zinc Based High Temperature Methanol Synthesis Catalysts Enabling Direct Synthesis of Olefins and Aromatics from CO<sub>2</sub></b>  <u>Michael Nikolajsen</u>, Martin Høj and Jakob M. Christensen, <i>Technical University of Denmark, Denmark</i>.  Short Summary:  Zinc spinel structures and supported zinc oxide on zirconia are capable of producing methanol at relatively high temperatures. Therefore, they are good candidates to be used in combination with zeolites in a fixed bed reactor to utilize CO<sub>2</sub> from plastic incineration.</p>
<p><b>Wed-P-21</b></p>	<p><b>In-Situ Exsolution of Bimetallic CoFe Nanoparticles on (La,Sr)FeO<sub>3</sub> Perovskite: Its Effect on Oxidative Coupling of Methane</b>  <u>Jaesung Kim</u><sup>1</sup>, Yu Jin Kim<sup>2</sup>, Matthew Ferree<sup>1</sup>, Seval Gunduz<sup>1</sup>, Anne Co<sup>1</sup>, Minkyu Kim<sup>2</sup> and Umit S. Ozkan<sup>1</sup>, (1)<i>The Ohio State University, USA</i>, (2)<i>Yeungnam University, Korea, Republic of (South)</i>.  Short Summary:  The exsolution of bimetallic CoFe nanoparticles on the surface of LSCF perovskite can be achieved by exposing it to CH<sub>4</sub> at elevated temperatures. The <i>in-situ</i> grown CoFe nanoparticles provide superior electrocatalytic characteristics for oxidative coupling of methane.</p>
<p><b>Wed-P-22</b></p>	<p><b>Insight into W/ZSM-5 Catalysts in Methane Dehydroaromatization</b>  <u>Mustafa Caglayan</u><sup>1</sup>, Samy Oud-Chikh<sup>1</sup>, Genrikh Shterk<sup>1</sup>, Edy Abou-Hamad<sup>1</sup>, Tuiana Shoinkhorova<sup>1</sup>, Alla Dikhtiarenko<sup>1</sup>, Abhishek Dutta Chowdury<sup>2</sup> and Jorge Gascon<sup>1</sup>, (1)<i>King Abdullah University of Science and Technology (KAUST), Saudi Arabia</i>, (2)<i>Wuhan University, China</i>.  Short Summary:  Our current study investigates the methane dehydroaromatization activity of W-loaded ZSM-5 catalysts during high-temperature reaction-regeneration cycles. The catalysis performance tests and a set of detailed characterizations reveal that if W dispersion-distribution on zeolites can be tuned, it can be a promising alternative to Mo/ZSM-5 catalysts in methane dehydroaromatization reaction.</p>
<p><b>Wed-P-23</b></p>	<p><b>Catalytic Descriptors for CO<sub>2</sub> Methanation Reactivity and Selectivity on Transition Metals</b>  <u>Michelle Nolen</u><sup>1</sup>, Sean Tacey<sup>2</sup>, Stephanie Kwon<sup>1</sup> and Carrie Farberow<sup>2</sup>, (1)<i>Colorado School of Mines, USA</i>, (2)<i>National Renewable Energy Laboratory, USA</i>.  Short Summary:  Atomic-scale modelling of transition-metal active sites at the clean-surface limit exposes intrinsic properties that can explicate catalytic performance. CO<sub>2</sub> conversion routes on transition-metal methanation catalysts were modelled with DFT methods, and results indicate that CO<sub>2</sub> activation routes are strong functions of O-affinity and product selectivity corresponds to distinct activation routes.</p>
<p><b>Wed-P-24</b></p>	<p><b>Enhanced Activity in the Aerobic, Selective Oxidation of Methane over Pt-Based Nanoalloy catalysts</b>  <u>Singobile Mahlaba</u>, Junfeng Guo, Gerard Leteba and Eric van Steen, <i>University of Cape Town, South Africa</i>.  Short Summary:  Alloying platinum with Group 11 elements in the form of Pt<sub>3</sub>Me nanoparticles significantly enhances the activity of platinum in the selective aerobic oxidation of methane yielding formaldehyde, when performing the reaction in the presence of water. This will be related to the surface structure of these alloys.</p>
<p><b>Wed-P-25</b></p>	<p><b>Liquid Fuel Production By CO<sub>2</sub> Hydrogenation - Sodium Impregnated ZnFe<sub>2</sub>O<sub>4</sub> and Zeolites</b>  <u>Eun Cheol Ra</u> and Jae Sung Lee, <i>Ulsan National Institute of Science and Technology (UNIST), Korea, Republic of (South)</i>.  Short Summary:  The catalytic process of converting CO<sub>2</sub> back to liquid fuel can be an important solution to solve global warming and environmental problems. In this presentation, a single catalyst and zeolite combined catalyst perform both reactions in a sequence, and produce C<sub>5+</sub> hydrocarbons with high CO<sub>2</sub> conversion rate.</p>
<p><b>Wed-P-26</b></p>	<p><b>Highly Active Single Atom Alloys for the Conversion of CO<sub>2</sub> and CH<sub>4</sub> to CH<sub>3</sub>OH.</b>  <u>Scott Bamonte</u><sup>1</sup>, Inosh Perera<sup>1</sup>, Harshul Khanna<sup>1</sup>, Meilin Li<sup>1</sup>, Seth March<sup>1</sup>, Shubhashish Shubhashish<sup>1</sup>, Pu-Xian Gao<sup>1</sup>, Ashley Head<sup>2</sup>, Dmitri Zakharov<sup>2</sup>, Anatoly Frenkel<sup>1,2</sup> and Steven Suib<sup>1</sup>, (1)<i>University of Connecticut, USA</i>, (2)<i>Brookhaven National Laboratory, USA</i>.  Short Summary:  From our finding single atom alloy have outperformed industrial standards and bulk nano particles of the same materials for the conversion of C1`s to methanol. We have used advanced characterization techniques such as E-TEM, Ap-XPS, and EXAFS to determine how the catalyst is evolving under reaction conditions.</p>

Wed-P-27	<p><b>Altering the Cobalt-Support Interaction in Fischer-Tropsch Synthesis</b>  <u>Michela Martinelli</u><sup>1</sup>, Mohammad Mehrbod<sup>2</sup>, Donald C. Cronauer<sup>3</sup>, A. Jeremy Kropf<sup>3</sup> and Gary Jacobs<sup>2</sup>, (1)University of Kentucky, USA, (2)University of Texas at San Antonio, USA, (3)Argonne National Laboratory, USA.</p> <p>Short Summary:  The effect of direct reduction for cobalt catalyst on reducibility, dispersion and FTS activity was investigated with different cobalt precursors (acetate, nitrate and chloride) and supports (Al<sub>2</sub>O<sub>3</sub> and SiO<sub>2</sub>). Direct reduction of certain cobalt salts improves dispersion over traditional air calcination/reduction; remarkable improvements were observed using nitrate, SiO<sub>2</sub> and Pt-promoter.</p>
Wed-P-28	<p><b>Direct Partial Oxidation of Methane to Methanol: New Learnings in an Old Challenge</b>  Partha Nandi<sup>1</sup> and Steven Suib<sup>2</sup>, (1)Corporate Research, ExxonMobil Research and Engineering, USA, (2)University of Connecticut, USA.</p> <p>Short Summary:  We present a new mechanistic understanding of direct partial oxidation of methane to methanol using tri-Cu-oxo sites via a series of control experiments. Our results indicate that direct partial oxidation mechanism using tri-Cu-oxo sites as mimics of methanemonooxygenase (MMO) is different than what was originally hypothesized.</p>
Wed-P-29	<p><b>Accelerating the Decarbonization of Steel and Cement Production with High-Throughput Screening of Gtl Catalysts for Efuels Production</b>  Anton Nagy<sup>1</sup> and Hendrik van Rensburg<sup>2</sup>, (1)ILS-Integrated Lab Solutions GmbH, Germany, (2)Drachaid Research Services Ltd, United Kingdom.</p> <p>Short Summary:  Conversion of CO, CO<sub>2</sub> and H<sub>2</sub> rich flue gases from cement- or steel-production to eFuels represents a promising decarbonization route. Implementation of High-throughput screening tools can significantly shorten the R&amp;D time required to determine the impact of varying H<sub>2</sub>/CO/CO<sub>2</sub> ratios as various poisons resulting from these processes on GTL catalyst performance.</p>
Wed-P-30	<p><b>Base-Free CO<sub>2</sub> Hydrogenation to Formic Acid over Pd Supported on Defective Carbon Nitride Modified By Microwave and Acid Treatments</b>  <u>EunHyup Kim</u> and Jae Sung Lee, Ulsan National Institute of Science and Technology (UNIST), Korea, Republic of (South).</p> <p>Short Summary:  Graphitic carbon nitride (g-C<sub>3</sub>N<sub>4</sub>) is synthesized via pyrolyzing urea by hybrid microwave annealing (HMA) to support Pd catalyst for direct CO<sub>2</sub> hydrogenation to formic acid under a base-free condition. It produces fragmented C<sub>3</sub>N<sub>4</sub> with abundant defects along their edges, because of the high annealing temperature in an extremely short time.</p>
Wed-P-31	<p><b>Hierarchical Approach to Novel Catalysts for Low Temperature Oxidative Coupling of Methane</b>  <u>Sung Jin Lee</u>, Changhyeok Choi and Yousung Jung, Korea Advanced Institute of Science and Technology (KAIST), Korea, Republic of (South).</p> <p>Short Summary:  We present a systematic approach to designing new catalysts for selective activation of methane under 300°C. Catalysts found in this work show promises toward selective ethylene formation, overcoming the tradeoff between methane activation and C2 selectivity that occurs on highly active catalysts such as IrO<sub>2</sub>.</p>
Wed-P-32	<p><b>Enhanced Catalytic Performance in Methane Dehydro-Aromatization over Mo/HZSM-5 Physically Mixed with NiO</b>  <u>Kihun Nam</u>, Haewon Ryu and Do Heui Kim, Seoul National University, Korea, Republic of (South).</p> <p>Short Summary:  The catalytic activity and stability of Mo/HZSM-5 catalyst on methane dehydro-aromatization was enhanced by physically mixed with bulk NiO and pretreatment process, which is superior with respect to the simplicity and cost of synthesis procedure.</p>
Americas Halls 1 & 2	<p><b>Catalyst Design and Synthesis Poster Session III</b></p>
Wed-P-33	<p><b>CO<sub>2</sub>-to-CO Enhanced By Self-Assembled Monolayers Modulated Ag Bifunctional Catalysts</b>  <u>Zhengyang Yang</u>, Zhiyong Gu and Fanglin Che, University of Massachusetts Lowell, USA.</p> <p>Short Summary:  In this work, we applied DFT method to study the adsorption behavior of 4-MBN SAMs over different Ag surfaces and how 4-MBN SAMs modified Ag can enhance the electro-catalytic performance of CO<sub>2</sub>RR-to-CO over Ag. Results provide the possible strategy of electro-catalyst design via applying the SAMs over the metallic surface.</p>
Wed-P-35	<p><b>Sustainable Bimetallic MOF-74 Synthesis Prepared with Methanol at Room Temperature</b>  <u>José Gabriel Flores Aguilar</u> and Julia Aguilar Pliego, Universidad Autonoma Metropolitana-Azcapotzalco, Mexico.</p> <p>Short Summary:  In this work we report a novel bimetallic MOF-74 synthesis route, at room temperature and employing methanol as solvent. The novel synthesis procedure provides well-structured nanocrystals, environmental sustainability and economic benefits. We employed Zn as metallic center together with other metals (Me), in order to obtain bimetallic ZnMe-MOF-74 materials.</p>

<p><b>Wed-P-36</b></p>	<p><b>Titanium Silicalite-1 Nanosheet Supported Platinum Fornon-Oxidative Ethane Dehydrogenation</b>  Ying Pan, Antara Bhowmick, Yuan Zhang and <u>Dongxia Liu</u>, <i>University of Maryland - College Park, USA</i>.  Short Summary:  We report a catalyst mechanism that overcome both challenges to enable highly stable, active and selective NDE. The catalyst is made of subnanometric Pt species habituated on the two-dimensional (2D) multilamellar titanium silicalite-1 (M-TS-1) zeolite nanosheet support, and it exhibited durable catalytic activity and high ethylene selectivity in the NDE.</p>
<p><b>Wed-P-38</b></p>	<p><b>Strategy for Ultrathin Ferrierite (UTF) Synthesis and Its Application to Dimethyl Ether Carbonylation</b>  <u>Hyun Seung Jung</u> and Jong Wook Bae, <i>Sungkyunkwan University, Korea, Republic of (South)</i>.  Short Summary:  The Ultrathin-FERs were prepared with different CTAB and piperidine ratio (C/p) as template and OSDA materials and utilized for DME carbonylation where the optimum C/p ratio was revealed as ~0.1 in terms of catalyst properties and activity while the effect of the dual-reagent was quantified by molecular dynamics computation.</p>
<p><b>Wed-P-39</b></p>	<p><b>Lithium Promotion of Pt/m-ZrO<sub>2</sub> for Low Temperature Water-Gas Shift</b>  <u>Zahra Rajabi</u><sup>1</sup>, Michela Martinelli<sup>2</sup>, Caleb D. Watson<sup>3</sup>, Donald C. Cronauer<sup>4</sup>, A. Jeremy Kropf<sup>4</sup> and Gary Jacobs<sup>1</sup>, (1)<i>University of Texas at San Antonio, USA</i>, (2)<i>University of Kentucky, USA</i>, (3)<i>UTSA, USA</i>, (4)<i>Argonne National Laboratory, USA</i>.  Short Summary:  The promoting role of lithium on Pt/m-ZrO<sub>2</sub> catalyst for low temperature water-gas shift was investigated. Increasing lithium loading to 0.5% facilitated formate C-H bond scission and significantly accelerated the WGS rate, while higher loadings blocked Pt hindering CO<sub>2</sub> product desorption. The electronic and geometric structure of the catalysts were explored.</p>
<p><b>Wed-P-41</b></p>	<p><b>Synthesis of Ultra-Small PdAu Nanoparticles with Homogenous Alloys on SiO<sub>2</sub> and Al<sub>2</sub>O<sub>3</sub> Via Electrostatic Adsorption</b>  <u>Anhua Dong</u>, Douglas Blom and John R. Regalbuto, <i>University of South Carolina, USA</i>.  Short Summary:  Strong electrostatic adsorption is a simple and effective method to synthesize ultra-small PdAu nanoparticles (&lt;1.6nm) with homogenous alloys due to the strong interaction between metal precursor and the supports. The dispersion of Pd was higher on SEA samples and it increased with a lower molar ratio of Pd/Au.</p>
<p><b>Wed-P-42</b></p>	<p><b>Precision Control of Supported Pd and Pt Nanoparticle Sizes Via Electroless Deposition</b>  <u>Haiying Zhou</u>, Wen Xiong, Yanjiao Yi, John Meynard Tengco and John R. Monnier, <i>University of South Carolina, USA</i>.  Short Summary:  A controlled and scalable method has been developed to synthesize supported nanoparticles with controlled sizes using electroless deposition (ED) to deposit additional metal atoms over existing particles of the same metal made by SEA. A new ED bath for palladium deposition has been successfully formulated using N<sub>2</sub>H<sub>4</sub> as reducing agent.</p>
<p><b>Wed-P-43</b></p>	<p><b>Novel Zeolite Catalysts for Conversion of CO<sub>2</sub></b>  Jerrick Mielby and <u>Søren Kegnæs</u>, <i>Technical University of Denmark, Denmark</i>.  Short Summary:  We have developed several catalytic systems with various metal nanoparticles confined in zeolite materials. The methods are cost-effective and results in a narrow size distribution of small nanoparticles. The materials are very active and selective catalysts in selective hydrogenation of CO<sub>2</sub> into CO, CH<sub>4</sub> and methanol and ethanol.</p>
<p><b>Wed-P-44</b></p>	<p><b>Enhancement of Ni-O-Si Interface Generation Using Surfactant-Assisted Melt-Infiltration Method: Selection of Surfactant and Its Application for CO<sub>2</sub> Hydrogenation</b>  <u>Eui Hyun Cho</u> and Chang Hyun Ko, <i>Chonnam National University, Korea, Republic of (South)</i>.  Short Summary:  Considering catalyst reproducibility and absence of waste liquid, the surfactant-assisted melt-infiltration method was useful. In addition, high loading and effective dispersion of nickel-based catalyst can be achieved by this method, and efficient catalytic activity was exhibited in CO<sub>2</sub> hydrogenation reaction.</p>
<p><b>Wed-P-45</b></p>	<p><b>Earth Abundant Transition Metal Catalysts for Light Alkane Oxydehydrogenation</b>  <u>Muntaseer Bunian</u> and Yu Lei, <i>The University of Alabama in Huntsville, USA</i>.  Short Summary:  This study utilizes a microporous material such as silicalite-1 to disperse Fe using an organic precursor in the tetrahedral sites resulting in reducing the strength of the acid sites and promoting ethane ODH pathway by activating the C-H bond and inhibiting the C-C bond activation.</p>
<p><b>Wed-P-46</b></p>	<p><b>Customized Fe-Cu-Al Catalyst Design and Scale-up for Hydrogen Production from Waste-Derived Synthesis Gas</b>  <u>Hyun-Seog Roh</u><sup>1</sup>, Kyoung-Jin Kim<sup>1</sup>, Ho-Ryong Park<sup>1</sup>, Doo-Wook Kim<sup>2</sup> and Wang Lai Yoon<sup>2</sup>, (1)<i>Yonsei University, Korea, Republic of (South)</i>, (2)<i>Korea Institute of Energy Research, Korea, Republic of (South)</i>.  Short Summary:  Fe-Cu-Al catalysts for H<sub>2</sub> production from waste-derived synthesis gas achieve efficient hydrogen recovery and high CO conversion in the WGS reaction. We confirmed that the concentrations of metal precursors significantly affect the surface area, Fe<sub>3</sub>O<sub>4</sub> crystallite size, and reducibility. The key properties of the best-performing sample were maintained upon scale-up.</p>

<p><b>Wed-P-47</b></p>	<p><b>Fabrication of Aei-Type Aluminosilicate Catalyst with Sheet-like Morphology and Its Catalysis on Propene to Butenes Reaction</b>  <u>Takeshi Matsumoto</u><sup>1</sup>, Takashi Takeuchi<sup>1</sup>, Masato Sawada<sup>1</sup>, Masafumi Kamidate<sup>1</sup>, Ryota Osuga<sup>2</sup>, Yusuke Kunitake<sup>1</sup>, Shuhei Yasuda<sup>1</sup>, Junko N. Kondo<sup>1</sup>, Hermann Gies<sup>1</sup> and Toshiyuki Yokoi<sup>1</sup>, (1)Tokyo Institute of Technology, Japan, (2)Tohoku University, Japan.  Short Summary:  AEI-type aluminosilicates with sheet-like morphology were successfully synthesized by a CGI-assisted synthesis method using CTAB as a CGI. Moreover, a unique catalytic performance of these catalysts for the PTB (Propylene-to-butene) reaction was observed, where a longer catalytic lifetime and higher selectivity for butenes were confirmed as advantages.</p>
<p><b>Americas Halls 1 &amp; 2</b></p> <p><b>Catalyst Manufacturing Poster Session</b></p>	
<p><b>Wed-P-48</b></p>	<p><b>3D Printing As Innovative Strategy to Enhance Catalytic Performance in the Methane Dehydroaromatization Process</b>  Antoine Beauque<sup>1</sup>, Ludovic Pinard<sup>2</sup>, Vesna Middelkoop<sup>3</sup>, <u>Santiago Palencia Ruiz</u><sup>2</sup>, Ben Sutens<sup>3</sup> and Alexander Sachse<sup>2</sup>, (1) Institut de Chimie des Milieux et Matériaux de Poitiers (ICM2P), France, (2)Université de Poitiers, France, (3)Vito NV, Boeretang 200, BE-2400 MOL, Belgium, Belgium.  Short Summary:  The use of 3D catalyst shaping in catalyst production allows for the optimal customization of the catalyst properties required for increased aromatics production in the MDA process. Thus, the 3D shaping appears to be very promising for the scale-up of this challenging reaction.</p>
<p><b>Wed-P-49</b></p>	<p><b>Powder-Based Additive Manufacturing of NiAl Catalysts Via Binder Jetting</b>  <u>Hanh My Bui</u><sup>1</sup>, Tabea Gros<sup>1</sup>, Merle Blum<sup>1</sup>, Markus Tonigold<sup>2</sup>, Richard Fischer<sup>2</sup>, Normen Szesni<sup>2</sup> and Olaf Hinrichsen<sup>1</sup>, (1) Technical University of Munich, Germany, (2)Clariant Produkte (Deutschland) GmbH, Germany.  Short Summary:  The presented work shows a proof-of-principle for direct powder-based printing of NiAl catalysts via Binder Jetting from co-precipitated NiAl catalyst powder. A thorough characterization and a first catalytic test reveal that efficient CO<sub>2</sub> methanation catalysts were successfully 3D printed.</p>
<p><b>Americas Halls 1 &amp; 2</b></p> <p><b>Conversion of Biomass Resources and Polymers Poster Session III</b></p>	
<p><b>Wed-P-50</b></p>	<p><b>Catalytic Pyrolysis of Sorted Polyethylene Reveals Opportunities and Challenges for Economical Chemical Recycling of Mixed Waste Plastic</b>  <u>Cody J. Wrasman</u>, Abhijit Dutta, Joshua Schaidle and Calvin Mukarakate, National Renewable Energy Laboratory, USA.  Short Summary:  Ex-situ catalytic pyrolysis of polyethylene with high species resolution, near 100% mass closure, and catalyst regeneration cycles is used to inform techno-economic models of a commercial scale facility. The modeled results can be used to inform future research needs in the successful scale-up of waste plastic catalytic pyrolysis.</p>
<p><b>Wed-P-51</b></p>	<p><b>Sustainable Catalyst for Synthesis of Sugar Alcohols As Potential Replacement of Raney™ Nickel</b>  <u>Jose Trejo O'Reilly</u>, Dupont, USA.  Short Summary:  Biomass conversion pathway using hydrogenation reaction has been studied at our laboratory. The reaction selected was hydrogenation of Glucose and Fructose to make Sorbitol and Mannitol. AmberLite(tm)/AmberLyst(tm) impregnated with Ni, Pd and Ru were tested under hydrogenation conditions. High selectivity and conversion achieved. IC-MS used for selectivity confirmations.</p>
<p><b>Wed-P-52</b></p>	<p><b>Solvent Optimization for Extraction of High Commercial Value Chemicals from Food Waste</b>  <u>Yagya Gupta</u><sup>1</sup>, Souryadeep Bhattacharyya<sup>2</sup> and Dionisios G. Vlachos<sup>1</sup>, (1)University of Delaware, USA, (2)Georgia Institute of Technology, USA.  Short Summary:  Extraction of antioxidant and antimicrobial activity providing chemicals is economically lucrative. The choice of the solvent is a critical parameter. There is an insufficient fundamental understanding of the solvent selection process for FW extraction applications. This study directly addresses this issue by focusing on solvent selection.</p>
<p><b>Wed-P-53</b></p>	<p><b>Deactivation and Mitigation Strategies in the Sustainable Hydrogen Production from Wastewater Streams Via APR</b>  <u>Giuseppe Pipitone</u><sup>1</sup>, Giulia Zoppi<sup>1</sup>, Andrea Maria Rizzo<sup>2</sup>, Raffaele Pirone<sup>1</sup>, David Chiaramonti<sup>1,2</sup> and Samir Bensaid<sup>1</sup>, (1) Politecnico di Torino, Italy, (2)RE-CORD, Italy.  Short Summary:  This work allowed to detect important deactivating organic and inorganic compounds in the APR of waste streams. The provided outcomes and the investigation on different strategies to moderate their effects are relevant also to other fields related to catalytic biomass valorization routes (e.g. hydrothermal gasification, etc.) sensitive to similar compounds.</p>

Wed-P-54	<p><b>Single-Step Conversion of Ethanol to n-Butene-Rich Olefins or Butadiene over Metal Supported on ZrO<sub>2</sub>/SiO<sub>2</sub> Catalysts with Tailored Metal and Lewis-Acid Sites</b></p> <p><u>Vanessa Dagle</u><sup>1</sup>, Austin Winkelman<sup>1,2</sup>, Libor Kovarik<sup>1</sup>, Mark Engelhard<sup>1</sup>, Nicholas R. Jaegers<sup>1</sup>, Jian Zhi Hu<sup>1</sup>, Yong Wang<sup>1</sup> and Robert A. Dagle<sup>1</sup>, (1)<i>Pacific Northwest National Laboratory, USA</i>, (2)<i>Washington State University, USA</i>.</p> <p>Short Summary: We have developed a metal-supported ZrO<sub>2</sub>/SiO<sub>2</sub> catalyst system with specially tailored metal and Lewis acid sites for producing either BD or n-butenes from ethanol, and with outstanding activity, selectivity, and stability.</p>
Wed-P-55	<p><b>Development of New Ni/KIT-5 Catalysts for Hydrodeoxygenation of Palmitic Acid</b></p> <p><u>Citlalli Zenteno</u> and Diego Valencia, <i>Instituto Mexicano del Petróleo, Mexico</i>.</p> <p>Short Summary: <i>New Ni catalysts supported on mesoporous KIT-5 were synthesized. We prepared the materials by varying the metal loading and using 1-10-phenanthroline as a chelating agent to bind Ni<sup>2+</sup> species prior to impregnation. These materials showed outstanding catalytic performance in the hydrodeoxygenation of palmitic acid</i></p>
Wed-P-56	<p><b>Acid-Catalyzed Synthesis of Butyl-Exchanged Polyoxymethylene Ethers As Renewable Diesel Blendstocks with Improved Fuel Properties</b></p> <p><u>Martha Arellano-Trevino</u>, Anh To, Thomas D. Foust and Daniel Ruddy, <i>National Renewable Energy Laboratory, USA</i>.</p> <p>Short Summary: Acid-catalyzed end-group exchange chemistry employing renewable butanol improves two key diesel fuel properties for high-cetane polyoxymethylene ethers.</p>
Wed-P-57	<p><b>Zeolite Supported Pt-Sn for Depolymerization of Polyethylene By Induction Heating</b></p> <p><u>Bernard Whajah</u><sup>1</sup>, Joseph Heil<sup>2</sup>, James Dorman<sup>1</sup> and Kerry Dooley<sup>1</sup>, (1)<i>Louisiana State University, USA</i>, (2)<i>LeTourneau University, USA</i>.</p> <p>Short Summary: Combining the heating efficiency obtained from induction heating-based depolymerization with a rational design of Pt-Sn/zeolite catalysts, plastic waste was converted to useful products with tunability based on the design of the catalyst. Morphology of the zeolite and promoting Pt with Sn can greatly alter the selectivity of the products.</p>
Wed-P-58	<p><b>Catalytic Hydrodeoxygenation of Methyl Palmitate to Long Chain Hydrocarbons over Copper Phyllosilicate Catalyst</b></p> <p><u>Warot Prasanseang</u> and Tawan Sooknoi, <i>King Mongkut's Institute of Technology Ladkrabang, Thailand</i>.</p> <p>Short Summary: Copper phyllosilicate (CuPS) as a bifunctional catalyst for hydrodeoxygenation of methyl palmitate to linear long-chain <math>\alpha</math>-olefin and paraffin without carbon loss. The hydrodeoxygenation activity was related to the active Cu surface and Brønsted acid sites at the metal-support interface.</p>
Wed-P-59	<p><b>Biogas and Its Utilization into Synthesis-Gas and Hydrogen Rich Fuel Compositions</b></p> <p><u>Svetlana Tungatarova</u><sup>1,2</sup>, Tolkyn S. Baizhumanova<sup>1,2</sup>, Manaphan Zhumabek<sup>1</sup> and Stanislav Kotov<sup>3</sup>, (1)<i>D.V. Sokolsky Institute of Fuel, Catalysis and Electrochemistry, Kazakhstan</i>, (2)<i>al-Faraby Kazakh National University, Kazakhstan</i>, (3)<i>M.Kh. Dulaty Taraz Regional University, Kazakhstan</i>.</p> <p>Short Summary: The results of model biogas reforming on Ni/Mn-based catalysts prepared by solution combustion synthesis are presented. Non-stoichiometric spinels with highly defective catalyst structures were obtained due to very high heating and cooling rates during SCS, which work as active sites and are responsible for the high activity of catalysts.</p>
Wed-P-60	<p><b>The Effect of Ferrierite Post-Synthesis Modifications on the Isomerization of Oleic Acid</b></p> <p>Alexandre F. Young, Donato Aranda, Pedro Nothaft Romano and <u>João M.A.R. de Almeida</u>, <i>Universidade Federal do Rio de Janeiro, Brazil</i>.</p> <p>Short Summary: Ferrierite dealumination techniques applied to the oleic acid isomerization: chemical dealumination with (NH<sub>4</sub>)<sub>2</sub>SiF<sub>6</sub> and vapor calcination followed by acid leaching. Both approaches modify the number of Ferrierite's Brønsted acid sites. Kinetics modeling will be carried to compare reaction parameters when using the parent FER and the modified ones.</p>
Wed-P-61	<p><b>Catalytic Evaluation of Ru/KIT-6 Modified with Titania for the Hydrodeoxygenation of Anisole.</b></p> <p>Brenda Taylor<sup>1</sup>, <u>Jose Antonio De los Reyes</u><sup>2</sup>, Sergio Gomez Torres<sup>2</sup>, Marco A. Sánchez Castillo<sup>3</sup> and Mara Cordero-García<sup>2</sup>, (1)<i>Universidad Autonoma Metropolitana-Azcapotzalco, Mexico</i>, (2)<i>Universidad Autónoma Metropolitana-Iztapalapa, Mexico</i>, (3)<i>Universidad Autonoma de San Luis Potosí, Mexico</i>.</p> <p>Short Summary: Understanding the effects on the activity and selectivity in the HDO of anisole cause by deposit of Titania in KIT-6 in Ru catalysts is importance in the design and selection of new catalytic materials with special characteristics (acidity and surface area).</p>
Wed-P-62	<p><b>High-Purity Hydrogen Production from Alkaline Thermal Treatment of Plastic Waste</b></p> <p><u>Hyerin Seo</u>, Hyemin Jung, Sunwoo Kim and Woo-Jae Kim, <i>Ewha Womans University, Korea, Republic of (South)</i>.</p> <p>Short Summary: We demonstrated that high purity hydrogen is produced from plastic waste by alkaline thermal treatment. When NaOH was added, plastic waste produced 30.35 mmol H<sub>2</sub>/g-plastic at 335 °C, which is significantly higher than conventional steam gasification can produce. We also investigated thermal oxidation of plastics to enhance hydrogen production.</p>



Wed-P-63	<p><b>Mechanocatalytic Depolymerization of Poly(Styrene)</b>  <u>George Y. Chang</u> and Carsten Sievers, <i>Georgia Institute of Technology, USA</i>.  Short Summary:  Poly(styrene) was processed inside a ball mill at ambient conditions to yield styrene, and boric acid was found to enhance the yield significantly. The conversion of a polyolefin to small molecules via mechanocatalytic processing represents a novel approach to the upcycling of plastic waste.</p>
Wed-P-64	<p><b>In-Situ Catalytic Pyrolysis of Disposable COVID-19 Face Masks with Clinoptilolite and H-ZSM5</b>  Ivana Gabriela Esquivel López<sup>1</sup>, Gloria Dimas Rivera<sup>2</sup>, Carolina Solis Maldonado<sup>3</sup>, Javier Rivera de la Rosa<sup>2</sup>, <u>Carlos Lucio Ortiz</u><sup>2</sup>, Alejandro Montesinos Castellanos<sup>1</sup> and Ladislao Sandoval-Rangel<sup>1</sup>, (1)<i>Tecnológico de Monterrey, Mexico</i>, (2)<i>Universidad Autónoma de Nuevo León, Mexico</i>, (3)<i>Universidad Veracruzana, Mexico</i>.  Short Summary:  One effective protection against COVID19 is face masks, although their use resulted in disposal of 130 billion masks worldwide, resulting in PPE wastes. Two natural minerals along with H-ZSM5 were used as catalysts for in-situ catalytic pyrolysis of COVID-19 face masks, evaluating their effects on the obtained products.</p>
Wed-P-65	<p><b>Influence of Several Reaction Parameters on the 1,2-PDO Production By Glycerol Hydrodeoxygenation over Cu-Pd/TiO<sub>2</sub>-Na Catalysts</b>  <u>Alba Ardila</u>, <i>Politécnico Colombiano Jaime Isaza Cadavid, Colombia</i>.  Short Summary:  Here, we report the influence of several reaction parameters (temperature reaction, initial concentration of H<sub>2</sub> and initial concentration of glycerol) for the 1,2-PDO production from the glycerol HDO on aqueous phase over Cu-Pd/TiO<sub>2</sub> catalyst.</p>
Wed-P-67	<p><b>Bimetallic Ir-Ni and Ir-Fe Catalysts for Selective Glycerol Hydrogenolysis.</b>  Aracelis J. Pamphile-Adrian<sup>1</sup>, Pedro P. Florez-Rodriguez<sup>1</sup> and <u>Fabio B. Passos</u><sup>2</sup>, (1)<i>Universidade Federal de Alagoas, Brazil</i>, (2)<i>Universidade Federal Fluminense, Brazil</i>.  Short Summary:  Bimetallic Ir-Ni and Ir-Fe catalysts were prepared and presented a higher activity than monometallic Ir, Ni and Fe catalysts for glycerol hydrogenolysis. The effect of calcination was shown to be important factor in the modification of the catalytic sites for both glycerol conversion and products selectivity.</p>
Wed-P-68	<p><b>Investigating the Catalytic Stability of Molybdenum Carbide Using Real Lignin-Derived Feedstocks</b>  <u>Michael L. Stone</u><sup>1</sup>, Matthew S. Webber<sup>1</sup>, William P. Mounfield<sup>1</sup>, Earl Christensen<sup>2</sup>, Ana R. C. Morais<sup>2</sup>, Yanding Li<sup>1</sup>, Eric Anderson<sup>1</sup>, Gregg T. Beckham<sup>2,3</sup> and Yuriy Roman<sup>1</sup>, (1)<i>Massachusetts Institute of Technology, USA</i>, (2)<i>National Renewable Energy Laboratory, USA</i>, (3)<i>Center for Bioenergy Innovation, USA</i>.  Short Summary:  Hydrodeoxygenation reactivity of a lignin bio-oil derived from reductive catalytic fractionation over molybdenum carbide requires harsher conditions for stable phenolic cleavage than those commonly used in model compound studies. This highlights the necessity for testing promising lignin upgrading catalysts using realistic feedstocks.</p>
Americas Halls 1 & 2	<p><b>Conversion of Fossil Resources Poster Session</b></p>
Wed-P-69	<p><b>Effect of Zn Incorporation into MFI Framework on Ethane Dehydroaromatization Performance</b>  <u>Ye Rim Park</u>, ByungJin Lee and Kwan-Young Lee, <i>Korea University, Korea, Republic of (South)</i>.  Short Summary:  Zn atoms are incorporated into the MFI zeolite framework with various Zn/(Zn+Al) ratio. The influence of the ratio on the catalytic activity over ethane dehydroaromatization was investigated to achieve high BTX yield. The state of Zn species and promoting effect were analyzed by characterization techniques.</p>
Wed-P-70	<p><b>Effects of Alkali Metal Additives on Al<sub>2</sub>O<sub>3</sub> Catalyst in Octanol Dehydration for Linear <math>\alpha</math>-Olefin Production</b>  <u>Young-eun Kim</u><sup>1</sup>, Unho Jung<sup>1</sup>, Hyo Been Im<sup>1</sup>, Dong Hyun Chun<sup>1</sup>, Min Hye Yoon<sup>1</sup>, Ki Bong Lee<sup>2</sup> and Kee Young Koo<sup>1,3</sup>, (1)<i>Korea Institute of Energy Research, Korea, Republic of (South)</i>, (2)<i>Korea University, Korea, Republic of (South)</i>, (3)<i>University of Science and Technology, Korea, Republic of (South)</i>.  Short Summary:  The alkaline earth metal promoted Al<sub>2</sub>O<sub>3</sub> catalyst showed better 1-octene selectivity and yield than pure Al<sub>2</sub>O<sub>3</sub> catalyst in 1-octanol dehydration reaction for linear <math>\alpha</math>-olefin production. This is because the anti-Saytzeff effect enhanced with basic property of alkaline metal additives inhibits the re-adsorption of 1-octene which causes the isomer formation.</p>
Wed-P-72	<p><b>Recycling Plastics Waste to New Plastics and Fuels Using Catalytic Hydrolysis</b>  <u>Troels Kaas Ibsen</u><sup>1</sup>, Martin Høj<sup>1</sup>, Magnus Stummann<sup>2</sup> and Anker D. Jensen<sup>1</sup>, (1)<i>Technical University of Denmark, Denmark</i>, (2)<i>Haldor Topsøe A/S, Denmark</i>.  Short Summary:  Recycling of low density polyethylene (LDPE) has been investigated in a catalytic fluid bed reactor. Increased cracking activity at 400 °C compared to a non-catalytic reaction at 520 °C was observed. However, a large wax fraction was still obtained and higher temperatures are desired to maximize C<sub>5-12</sub> yield.</p>

Wed-P-73	<p><b>Development of Perovskites-Based Catalysts for Solid Oxide Fuel Cell's Anode</b>  <u>Melodj Dosa</u><sup>1</sup>, Alessandro Monteverde<sup>1</sup>, Andrea Felli<sup>2</sup>, Marta Boaro<sup>2</sup>, Leonardo Duranti<sup>3</sup>, Elisabetta Di Bartolomeo<sup>3</sup> and Marco Piumetti<sup>1</sup>, (1)Politecnico di Torino, Italy, (2)Università degli Studi di Udine, Italy, (3)Università di Roma Tor Vergata, Italy.</p> <p>Short Summary:  Perovskites with different compositions were synthesized and characterized by complementary techniques. These materials were studied in order to find new SOFC's anode catalysts due to avoid the carbon deposition. The Ce-based samples exhibits good soot oxidation performance, and they could be proposed as alternative to the actual Ni-YSZ.</p>
Wed-P-74	<p><b>Preparation, Characterisation, and Testing of Supported Nickel Catalysts for Tetralin Hydrogenation.</b>  Ahmed AlAsseel and <u>S. David Jackson</u>, <i>University of Glasgow, United Kingdom.</i></p> <p>Short Summary:  This research shows that development of an enhanced nickel catalyst for tetralin hydrogenation requires optimising both aromatic and olefinic hydrogenation capability, which have significantly different site requirements.</p>
Wed-P-75	<p><b>Understanding Methane Activation and Formation of Ethylene/Acetylene on Mo/ZSM-5 Catalyst</b>  Iqra Ahangar, <u>M. Ali Haider</u> and Kamal K. Pant, <i>Indian Institute of Technology Delhi, India.</i></p> <p>Short Summary:  The density functional theory (DFT) calculations are utilized to study the catalytically active carbide (Mo<sub>x</sub>C<sub>y</sub>) species anchored on the zeolite support in C-H bond activation and C-C coupling reaction to form C<sub>2</sub> intermediates. The mechanistic insights obtained from DFT calculations provides a molecular level design strategy for the active sites.</p>
Wed-P-133	<p><b>CO<sub>2</sub>-Assisted Oxidative Dehydrogenation of Propane over VO<sub>x</sub>-in<sub>2</sub>O<sub>3</sub> Catalysts: Interplays between Acid-Base Interaction and Redox Property</b>  Xiao Jiang<sup>1,2</sup>, Bar Mosevitzky Lis<sup>3</sup>, <u>Stephen Purdy</u><sup>2</sup>, Victor Fung<sup>2</sup>, Katharine Page<sup>2</sup>, Israel E. Wachs<sup>3</sup> and Zili Wu<sup>2</sup>, (1)Aramco Americas: Aramco Research Center - Boston, USA, (2)Oak Ridge National Laboratory, USA, (3)Lehigh University, USA.</p> <p>Short Summary:  By introducing acid, redox-active vanadium oxide (VO<sub>x</sub>), both the activity and stability of basic indium oxide (In<sub>2</sub>O<sub>3</sub>) catalyst for carbon dioxide (CO<sub>2</sub>)-assisted oxidative dehydrogenation of propane (CO<sub>2</sub>-ODHP) can be improved through the interplays between surface acid-base interactions and redox properties.</p>
Wed-P-76	<p><b>First Principles Analysis of Selectivity and Durability of Pt-Based Bimetallic Alloys for Light Alkane Dehydrogenation</b>  <u>Yinan Xu</u><sup>1</sup>, Ranga Rohit Seemakurthi<sup>2</sup>, Zhenwei Wu<sup>2</sup>, Jeffrey T. Miller<sup>1</sup> and Jeffrey Greeley<sup>1</sup>, (1)Davidson School of Chemical Engineering, Purdue University, USA, (2)Purdue University, USA.</p> <p>Short Summary:  The DFT analysis of propane dehydrogenation (PDH) using free energies and microkinetic modeling systematically examines the mechanistic details. We highlight the importance of reasonably strong propylene binding over its isomers. This property may be more crucial for PDH than for ethane dehydrogenation, where fewer pathways of ethylene isomers are found.</p>
Wed-P-77	<p><b>Tuning CO<sub>2</sub>-Assisted Selective Cleavage of C—C/C—H Bonds in Ethane with Interfacial Active Sites</b>  <u>Zhenhua Xie</u><sup>1,2</sup>, Shyam Kattel<sup>3</sup> and Jingguang Chen<sup>1</sup>, (1)Columbia University, USA, (2)Brookhaven National Laboratory, USA, (3)Florida A&amp;M University, USA.</p> <p>Short Summary:  The current work identifies different oxygen-containing interfacial configurations and the mechanisms of how they control the selective cleavage of the C—C/C—H bonds of ethane. It highlights opportunities for using different interfacial structures in simultaneously upgrading abundant shale gas and greenhouse gas CO<sub>2</sub>.</p>
Wed-P-78	<p><b>Parametric Optimization of Microwave Assisted Methane Dehydroaromatization Process</b>  <u>Pranjali D. Muley</u>, Victor Abdelsayed, Hari Paudel and Daniel J. Haynes, <i>National Energy Technology Laboratory, USA.</i></p> <p>Short Summary:  Microwave assisted methane dehydroaromatization has the potential to overcome challenges facing the traditional catalytic processes demonstrated through enhanced reaction rates, overcoming equilibrium limitations, and improving selectivity to desired products. Parametric optimization results show that microwave assisted process reduces required reaction temperatures and increases catalyst activity.</p>
Wed-P-79	<p><b>Naphtha Reforming Catalyst : A Study of the Combination of Model Reactions</b>  <u>Quentin Rivet</u><sup>1,2</sup>, Thibaud Nardin<sup>2</sup> and David Farrusseng<sup>1</sup>, (1)Université de Lyon, CNRS, France, (2)IFP Energies Nouvelles, France.</p> <p>Short Summary:  This study describes the combination of two model reactions, the <i>n</i>-heptane reforming and the 3,3-dimethylbut-1-ene isomerization, to assess the acidity of the reforming catalyst.</p>
Wed-P-81	<p><b>Comparative Investigation of Indium and Gallium Exchanged Chabazite Zeolite for Non-Oxidative Ethane Dehydrogenation</b>  <u>Jian Pan</u>, Jason Lee, Muyuan Li and Raul F. Lobo, <i>University of Delaware, USA.</i></p> <p>Short Summary:  We investigate and compare In and Ga exchanged chabazite zeolite for ethane dehydrogenation to determine catalytic and mechanistic differences. This helps to understand the chemical and catalytic properties of reducible M(III) cations in zeolites, and to elucidate the interplay between Lewis acidity and redox properties in alkane dehydrogenation reactions.</p>

## Americas Halls 1 & 2

### Fundamentals of Catalysis Poster Session III

Wed-P-82

#### Molecular-Level Insight into Facet-Dependent Water Impact on Alkanol Dehydration on TiO<sub>2</sub>

Wenda Hu<sup>1,2</sup>, Jinshu Tian<sup>2</sup>, Anthony Savoy<sup>1</sup>, Yiqing Wu<sup>2</sup>, Fan Lin<sup>2</sup>, Junrui Li<sup>1</sup>, Junming Sun<sup>1</sup>, Jian Zhi Hu<sup>2</sup> and Yong Wang<sup>1,2</sup>, (1) *Washington State University, USA*, (2) *Pacific Northwest National Laboratory, USA*.

Short Summary:

Unraveling the impact of water on alkanol dehydration is imperative in biomass conversion. We found that water has a greater inhibition on isopropanol dehydration over TiO<sub>2</sub> (001) than (101) because water interacts more strongly with isopropoxide than isopropanol and perturbs C-H cleavage more significantly, evidenced by NMR and DFT.

Wed-P-84

#### Studying K<sup>+</sup> Interactions on PdAu/SiO<sub>2</sub> with Crown Ether Modification

Wenqing Zhang<sup>1</sup>, Michael S. Wong<sup>1</sup>, Hunter Jacobs<sup>1</sup>, Welman Curi Elias<sup>1</sup> and Kimberly Heck<sup>2</sup>, (1) *Rice University, USA*, (2) *Nanotechnology Enabled Water Treatment (NEWTE) Center, USA*.

Short Summary:

To improve understanding of K<sup>+</sup> in catalysis, in this study, we developed a method to precisely control the amount of potassium ions by adding known amounts of 18-crown-6 crown ether to the catalyst and assess how potassium ions impact model PdAu particle structure and consequent changes in performance.

Wed-P-85

#### Understanding the Bestowing of Enantioselectivity on Heterogeneous Catalysts Via the Addition of Chiral Modifiers

Zihao Wang, Yufei Ni and Francisco Zaera, *University of California, Riverside, USA*.

Short Summary:

In-situ ATR-IR and catalytic studies revealed that, under reaction conditions, 1-(1-naphthyl)ethylamine, a chiral modifier, adsorbs on Pt catalysts through its amine group (with the possible breaking of a N-H bond) rather than via the aromatic ring, as commonly believed. This may better explain the enantioselectivity it bestows to hydrogenation reactions.

Wed-P-86

#### Support Functionalization As an Approach for Modifying Activation Entropies of Catalytic Reactions on Atomically Dispersed Metal Sites.

Gregory Zakem<sup>1</sup>, Jordan Finzel<sup>1</sup>, Insoo Ro<sup>1,2</sup> and Phillip Christopher<sup>1</sup>, (1) *University of California, Santa Barbara, USA*, (2) *Seoul National University of Science and Technology, Korea, Republic of (South)*.

Short Summary:

Atomically dispersed Rh on  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> exhibited decreased entropic barriers for CO desorption and ethylene hydroformylation, with no change in enthalpic barriers, after functionalization with phosphonic acids (PAs). This demonstrated an apparent deviation from the enthalpy-entropy compensation effect. Additionally, entropic barriers were found to decrease with increasing PA tail length.

Wed-P-87

#### Catalytic Carbon Dioxide Hydrogenation to Light Olefins over Various Cobalt Loadings Supported By Cerium Oxide Nano-Rods

Nicole Foley and Cheng Zhang, *Long Island University (Post), USA*.

Short Summary:

The aim of this study is to investigate the catalytic activity of CeO<sub>2</sub>-NR supported cobalt catalysts with varying cobalt loadings up to 10%. The best performing catalyst corresponded to the largest cobalt loading tested.

Wed-P-88

#### Acetic Acid Adsorption and Reactions on Pt and Ni

Lotanna Ezeonu<sup>1</sup>, Jason P. Robbins<sup>1</sup>, Ziyu Tang<sup>1</sup>, Xiaofang Yang<sup>2</sup>, Bruce E. Koel<sup>2</sup> and Simon G. Podkolzin<sup>1</sup>, (1) *Stevens Institute of Technology, USA*, (2) *Princeton University, USA*.

Short Summary:

We investigated the differences in performance of silica supported Pt and Ni catalysts for acetic acid hydrodeoxygenation using surface science experiments and DFT calculations. We found that acetic acid adsorption and surface reactions on both metals are similar; hence we attributed the lower activity of Ni to its lower reducibility.

Wed-P-89

#### Thermodynamic Properties of Iron Oxide Thin Film Oxygen Carriers Prepared By Atomic Layer Deposition

Kai Shen, Julian Paige, Ohhun Kwon, Raymond J. Gorte and John M. Vohs, *University of Pennsylvania, USA*.

Short Summary:

The results of this study demonstrate that thin films of reducible iron oxides supported on a high surface area refractory metal oxide have properties that vary significantly from those of the corresponding bulk oxide which make them interesting candidates for use in chemical looping and other applications.

<p><b>Wed-P-134</b></p>	<p><b>Enhanced Activity in Wet Gas-Phase 2-Propanol Oxidation Caused By Carbonates and Hydroxides on Co-Containing Perovskites</b>  <u>Maik Dreyer</u><sup>1</sup>, Daniel Cruz<sup>2,3</sup>, Patrick Zeller<sup>2,4</sup>, Ulrich Hagemann<sup>5,6</sup>, Markus Heidelmann<sup>5,6</sup>, Steven Angel<sup>1</sup>, Anna Rabe<sup>1</sup>, Nicolas Cosanne<sup>7</sup>, Sharif Najafshirtari<sup>1</sup>, Nils Hartmann<sup>5</sup>, Hartmut Wiggers<sup>1,6</sup>, Christof Schulz<sup>1,6</sup>, Axel Knop-Gericke<sup>2,3</sup>, Robert Schlögl<sup>2,3</sup> and Malte Behrens<sup>1,8</sup>, (1)University of Duisburg-Essen, Germany, (2)Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany, (3)Max Planck Institute for Chemical Energy Conversion, Germany, (4)Helmholtz-Zentrum Berlin für Materialien und Energie, Germany, (5)Interdisciplinary Center for Analytics on the Nanoscale (ICAN), Germany, (6)CENIDE, Center for Nanointegration Duisburg-Essen, Germany, (7)University of Kiel, Germany, (8)Christian-Albrechts-Universität zu Kiel, Germany.</p> <p>Short Summary:  We provide fundamental insights into the effect of water on gas-phase oxidation of 2-propanol, which results in slower deactivation with an enhanced activity during the cooling of a transient experiment. The reason is the buildup of hydroxides and carbonates as seen in NAP-XPS.</p>
<p><b>Wed-P-90</b></p>	<p><b>Theoretical Investigation of the State of Hydroxylated Alumina Surfaces</b>  <u>Chen Jiachen</u>, Dimitry I. Sharapa and Philipp N. Plessow, <i>Karlsruhe Institute of Technology (KIT), Germany.</i></p> <p>Short Summary:  This paper explained previous experimental observation, such as the presence of hydrogen on <math>\alpha</math>-Al<sub>2</sub>O<sub>3</sub>(0001) surface at high temperatures. The presence of additional water will facilitate the decomposition of the hydroxylated surfaces and lead to water desorption.</p>
<p><b>Wed-P-93</b></p>	<p><b>Investigating the Effect of Metal Nuclearity on Activity for Ethylene Hydrogenation By Metal-Organic-Framework-Supported Oxy-Ni(II) Catalysts</b>  <u>Qining Wang</u><sup>1</sup>, Zihan Pengmei<sup>2</sup>, Riddish Umesh Pandharkar<sup>2</sup>, Laura Gagliardi<sup>2</sup>, Joseph T. Hupp<sup>1</sup> and Justin Notestein<sup>1</sup>, (1)Northwestern University, USA, (2)University of Chicago, USA.</p> <p>Short Summary:  The nuclearity and siting of oxy-Ni(II) catalyst were systematically adjusted on a metal-organic framework, NU-1000. The effects of those adjustments were investigated using ethylene hydrogenation as a probe reaction, where oxy-Ni(II) species of nuclearity greater than one were found to be beneficial for achieving high catalytic activity.</p>
<p><b>Wed-P-94</b></p>	<p><b>Selective Oxidation of Ethanol over Zeolite-Supported Gold Catalysts</b>  <u>Yiteng Zheng</u><sup>1</sup>, Yue Qi<sup>2</sup>, Jun Zhi Tan<sup>1</sup>, Simon G. Podkolzin<sup>2</sup> and Bruce E. Koel<sup>1</sup>, (1)Princeton University, USA, (2)Stevens Institute of Technology, USA.</p> <p>Short Summary:  Au/ZSM-5 catalysts are active and selective in ethanol selective oxidation. The obtained information on the effects of Si/Al ratio, Au loading and testing of physical mixtures will be useful in the development of more efficient catalysts for selective oxidation of other primary alcohols.</p>
<p><b>Wed-P-95</b></p>	<p><b>Acylation of Naphthalenic Compounds Using Zeolite Catalysts: Equilibrium or Deactivation Limited?</b>  <u>Abraham Martinez</u><sup>1</sup>, Michael Boreen<sup>1</sup>, Stacey I. Zones<sup>2</sup> and Alexander Katz<sup>1</sup>, (1)University of California, Berkeley, USA, (2)Chevron Energy Technology Company, USA.</p> <p>Short Summary:  The acylation of 2-methoxynaphthalene using acetic anhydride is investigated using extraordinarily mild conditions with acid zeolites. We observe an unprecedented mole balance (<math>\geq 95\%</math>) only when operating under rigorous anhydrous conditions, contrary to prior reports suggesting deactivation-based limitations. Under our conditions, the reaction is equilibrium limited with <math>K_{eq} = 0.11</math> at 40 °C.</p>
<p><b>Wed-P-96</b></p>	<p><b>Identification of the Adaptive Local Configurations and Reaction Mechanisms on Single-Atom Ir/TiO<sub>2</sub> Catalysts for CO Oxidation</b>  <u>Liping Liu</u>, Coogan Thompson, Ayman M. Karim and Hongliang Xin, <i>Virginia Polytechnic Institute and State University, USA.</i></p> <p>Short Summary:  This study identified the local structures and reaction mechanisms of adsorbed Ir<sub>1</sub>/TiO<sub>2</sub> catalysts towards CO oxidation, which is critical for designing high-performance catalysts atom-by-atom on TiO<sub>2</sub> and even other oxides.</p>
<p><b>Wed-P-97</b></p>	<p><b>Zeolites Ga(Nb,Ta)Sibea: Acid-Base Characteristics and Catalytic Performance in the Oxidative Dehydrogenation of Propane to Propylene with CO<sub>2</sub></b>  Pavlo Kyriienko<sup>1</sup>, Svitlana Orlyk<sup>1</sup>, Yannick Millot<sup>2</sup> and <u>Stanislaw Dzwigaj</u><sup>2</sup>, (1)L.V. Piszczewsky Institute of Physical Chemistry, NAS of Ukraine, Ukraine, (2)Sorbonne Université, France.</p> <p>Short Summary:  In this work, we have investigated the influence of the nature of heteroelements (Ga, Ta, Nb) incorporated into the framework of siliceous SIBEA zeolite on their acid-base characteristics and catalytic performance in the PODH-CO<sub>2</sub>.</p>
<p><b>Wed-P-98</b></p>	<p><b>Pt Single-Atom Promotion of Industrial Co-Mo-S Hydrodesulfurization Catalysts</b>  <u>Lars Pilsgaard Hansen</u>, Christian F. Weise, Hanne Falsig, Poul Georg Moses and Michael Brorson, <i>Haldor Topsøe A/S, Denmark.</i></p> <p>Short Summary:  A remarkable boost in HDS activity of 46% was obtained by incorporation of 1wt% Pt into a standard industrial Co-Mo-S catalyst. The promotional effect of Pt is examined at the atomic-level by combining HRSTEM, XANES and DFT-studies and, specifically, the desulfurization of refractory 4,6-DMDBT molecules will be modeled and discussed.</p>

## Americas Halls 1 & 2

### Homogeneous and Molecular Catalysis Poster Session

Wed-P-100

#### Reaction Mechanism of Pd-Catalyzed CO-Free Carbonylation Reaction Uncovered By in Situ Spectroscopy: The Formyl Mechanism

Robert Geitner<sup>1,2</sup>, Andrei Gurinov<sup>2</sup>, Tianbai Huang<sup>3</sup>, Stephan Kupfer<sup>3</sup>, Stefanie Gräfe<sup>3</sup> and Bert M. Weckhuysen<sup>2</sup>, (1)Technical University Ilmenau, Germany, (2)Utrecht University, Netherlands, (3)Friedrich Schiller University Jena, Germany.

Short Summary:

Homogeneous CO-free carbonylation reactions enable laboratory-scale carbonylations, using surrogates like formaldehyde. We studied the mechanism of Pd-catalyzed carbonylations using in situ NMR spectroscopy. The NMR study revealed the existence of Pd-formyl species and enabled the kinetic modelling of all intermediates. Surprisingly, methyl formate is the key intermediate, not CO.

Wed-P-101

#### One-Pot Hydroformylation/Oxirane Ring Opening of Limonene Oxide: A Sustainable Access to Biomass-Based Multi-Functional Fragrances

Mileny P. de Oliveira, Fábio G. Delolo, Jesus A. A. Villarreal, Eduardo N. dos Santos and Elena V. Gusevskaya, Universidade Federal de Minas Gerais, Brazil.

Short Summary:

One-pot process to upgrade bio-renewable limonene oxide includes its hydroformylation and parallel cleavage of the oxirane ring. Either acetic acid or acetic anhydride can be used as acylating agents. The method allows for the substrate functionalization simultaneously at two remote reactive sites to approach novel products with multiple fragrance functionalities.

Wed-P-102

#### Air-Tolerant Nickel-Catalyzed Cyanation of Aryl/Heteroaryl Halides Enabled By Pmhs, a Green Reductant

Renee Sifri and Caleb Hethcox, Merck, USA.

Short Summary:

We report an air tolerant nickel catalyzed cyanation of aryl/heteroaryl bromides aided by polymethylhydrosiloxane (PMHS). PMHS is a green and homogenous reductant that renders this reaction tolerant to air, thus minimizing mass transfer difficulties and oxygen sensitivity commonly associated with the use of heterogenous reductants in cross coupling reactions.

Wed-P-103

#### Bayesian Reaction Optimization of *Rac*-Lactide Polymerization Catalyzed By Aluminum Complexes

Yang Huang, Maverick Lin, Rong Tong and Hongliang Xin, Virginia Polytechnic Institute and State University, USA.

Short Summary:

Polymerization reaction optimization is experimentally costly due to the tremendous chemical search space built with reaction variables. Bayesian optimization (BO) is employed to tackle this challenge on Aluminum-complex catalyzed *rac*-lactide polymerization. Our BO model demonstrates the exceptional performance of a much higher search efficiency than the traditional random search approach.

Wed-P-104

#### Clarification of the Mechanism of NO Reduction with Ammonia (SCR) on Zeolite Catalysts

Konstantin Khivantsev<sup>1</sup>, Ja Hun Kwak<sup>1</sup>, Miroslaw Derewinski<sup>1</sup>, Nicholas R. Jaegers<sup>2</sup>, Janos Szanyi<sup>1</sup>, Hristiyan Aleksandrov<sup>3</sup> and Georgi Vayssilov<sup>3</sup>, (1)Pacific Northwest National Laboratory, USA, (2)University of California, Berkeley, USA, (3)University of Sofia, Bulgaria.

Short Summary:

Nitrosyl ions in zeolites (formed from NO+O<sub>2</sub>) react with ammonia at low temperature to form nitrogen. Reaction proceeds through diazo intermediates and not nitrosamine. The role of Cu(II) ions is to provide the pool of nitrosyl ions through Cu(II) reduction by NO radical to form Cu(I) and nitrosyl ions

## Americas Halls 1 & 2

### Modelling, Simulation, and Machine Learning in Catalysis Poster Session III

Wed-P-105

#### Including Anharmonicity in Adsorbate Partition Functions: Effect on the Thermodynamic Properties of Carbon Monoxide on Pt(111) and Methanol on Cu(111)

Katrín Blöndal<sup>1</sup>, Khachik Sargsyan<sup>2</sup>, David Bross<sup>3</sup>, Branko Ruscic<sup>3</sup> and Franklin Goldsmith<sup>1</sup>, (1)Brown University, USA, (2)Sandia National Laboratories, USA, (3)Argonne National Laboratory, USA.

Short Summary:

A method to generate adsorbate partition functions with anharmonic effects included via Monte Carlo phase space sampling is presented. The method can improve the prediction accuracy of thermodynamic properties and rate parameters in catalytic reaction mechanisms, as demonstrated with application on the CO on Pt(111) and CH<sub>3</sub>OH on Cu(111) systems.

Wed-P-106

#### Computational Modeling of Catalytic Adsorption and Reaction Mechanism of Mo/HZSM-5-Based Microwave Catalysts: A Density Functional Theory Study

Hari Paudel<sup>1</sup> and Daniel J. Haynes<sup>2</sup>, (1)Leidos Inc/NETL DOE, USA, (2)National Energy Technology Laboratory, USA.

Short Summary:

We present metal species formation and their adsorption in ZSM-5 with different Al substituted sites in the HZSM-5 framework. The effect of concentration of the Bronsted acid sites on the adsorption strength and reaction kinetics will also be examined. Change in electronic structures due to carbide formation will be discussed.



Wed-P-107	<p><b>From Highly Coordinated Nanoporous Material to Amorphous Solid: On the Dehydration of a Metal-Organic Framework for CO<sub>2</sub> Capture</b></p> <p><u>Jian Lian</u> and Samira Siahrostami, <i>University of Calgary, Canada</i>.</p> <p>Short Summary: We determine the crystal structure of intermediate states from HMOF to MOF. Our calculations reveal that the dehydration of the bare HMOF leads to the precipitation of the network into an amorphous structure. This work also points out the dynamical aspects of the dehydration mechanism.</p>
Wed-P-108	<p><b>Methane Activation on <math>\alpha</math>-Fe<sub>2</sub>O<sub>3</sub>: A DFT Study</b></p> <p><u>Tiago Goncalves</u> and Samira Siahrostami, <i>University of Calgary, Canada</i>.</p> <p>Short Summary: We aim to investigate how different iron species (Fe<sub>III</sub> and Fe<sub>IV</sub>) enhance or hinder the activation of methane on <math>\alpha</math>-Fe<sub>2</sub>O<sub>3</sub>, and how copper influences the kinetic rates of carbon dioxide formation from formate by comparing <math>\alpha</math>-Fe<sub>2</sub>O<sub>3</sub> with CuFe<sub>2</sub>O<sub>4</sub>, using spin-polarized density functional theory (DFT) calculations.</p>
Wed-P-109	<p><b>In-Operando Nanoplasmonic Sensing of Single Catalytic Particles Enabled By Deep Learning</b></p> <p><u>Henrik Klein Moberg</u> and Christoph Langhammer, <i>Chalmers University of Technology, Sweden</i>.</p> <p>Short Summary: We use deep denoising auto-encoders to improve the LOD of our nanoplasmonic sensing apparatus to simultaneously measure catalytic activity and LSPR readout of single nano-particles in operando. Thus, we enable the possibility to draw direct correlations between nanoplasmonic readout and catalytic activity of single catalytic nanoparticles for generic catalytic reactions.</p>
Wed-P-111	<p><b>CO Organization at Ambient Pressure on Stepped Pt Surfaces: First Principle Modeling Accelerated By Neural Networks</b></p> <p><u>Vaidish Sumaria</u> and Philippe Sautet, <i>University of California, Los Angeles, USA</i>.</p> <p>Short Summary: Step and kink sites at Pt surfaces have a crucial importance in catalysis. We employ High-dimensional Neural-Network Potential trained using first-principle calculations to determine the adsorption structure of CO in ambient conditions on these surfaces. Basin Hopping is used to explore the global minima and several low energy metastable structures.</p>
Wed-P-112	<p><b>Surface Steps Dominate the Water Formation on Pd(111) Surfaces</b></p> <p><u>Elisabeth M. Dietze</u>, Lin Chen and Henrik Grönbeck, <i>Chalmers University of Technology, Sweden</i>.</p> <p>Short Summary: We are clarifying the active sites and main reaction pathways for water formation over different Pd surfaces for various temperatures, total pressures and gas-phase compositions, which is of high importance to develop selective catalysts.</p>
Wed-P-113	<p><b>The Influence of Coverage on Entropy: Changes in Vibrational Frequencies of CO on Pt (111)</b></p> <p><u>Jongyoon Bae</u>, Andrew A. Peterson and Franklin Goldsmith, <i>Brown University, USA</i>.</p> <p>Short Summary: We investigated often-neglected coverage effect on adsorbate entropy in comparison to its effect on adsorbate enthalpy using <i>ab initio</i> methods including density functional theory, equilibrium thermochemistry calculations, and transient kinetic modeling.</p>
Wed-P-114	<p><b>Collaborative Automated High Throughput <i>in silico</i> Reaction Screening of Polyolefin Catalysts for Enhanced Reactivity and Polymer Tacticity</b></p> <p><u>Thomas Mustard</u>, <i>Schrödinger, Inc, USA</i>.</p> <p>Short Summary: First-principles simulation has become a reliable tool for the prediction of structures, mechanisms, and reaction energetics in homogeneous catalysis. Unfortunately, this is an arduous process. To democratize the fundamental understanding, design, and discovery of novel catalysts, an automated reaction workflow has been developed.</p>
Wed-P-115	<p><b>Computational Insights into Pd Nucleation on Gamma-Al<sub>2</sub>O<sub>3</sub> Surface</b></p> <p><u>Tso-Hsuan Chen</u>, Stavros Caratzoulas and Dionisios G. Vlachos, <i>University of Delaware, USA</i>.</p> <p>Short Summary: This is the first work that investigates entropic effects on the thermodynamics and kinetics of nucleation of Pd atoms on gamma-Al<sub>2</sub>O<sub>3</sub> support.</p>
Wed-P-116	<p><b>Uncertainty in Predicting Thermodynamic Properties of TiO<sub>2</sub> Polymorphs</b></p> <p><u>Olga Vinogradova</u>, Pinwen Guan, Siying Li and Venkatasubramanian Viswanathan, <i>Carnegie Mellon University, USA</i>.</p> <p>Short Summary: We use metrics of uncertainty quantification to assess the sensitivity of first principles density functional theory to accurately predict trends in bulk oxide polymorph stability and thermodynamic properties at finite temperature and pressure.</p>
Wed-P-117	<p><b>Identification of Collective Variables Using Graph Neural Networks</b></p> <p><u>Martin Šípka</u> and Lukáš Grajciar, <i>Charles University, Czech Republic</i>.</p> <p>Short Summary: In this work, we propose a new way of collective variables identification. We work with variational autoencoders that are built on pre-trained representations rather than handpicked descriptors. We construct a CV mapping that has all the expected invariances and explores the structures even beyond simple reactant-product classification.</p>

Wed-P-118	<p><b>Identification of Universal Predictors of the Coverage-Dependent Behavior of Biomass-Derived Aromatic Chemicals</b>  <u>Alyssa Hensley</u><sup>1,2</sup>, Naseeha Cardwell<sup>2</sup> and Jean-Sabin McEwen<sup>2</sup>, (1)Stevens Institute of Technology, USA, (2)Washington State University, USA.</p> <p>Short Summary:  Accurate kinetic modeling of catalysts requires knowledge of adsorbate coverage effects, which are exceedingly complex for large adsorbates. Using density functional theory and linear regression, we demonstrate that aromatics' coverage effects are universally predicted from the near-zero coverage behavior, reducing the cost of their determination by an order of magnitude.</p>
Wed-P-119	<p><b>CO Oxidation over Atomically Dispersed Pt<sub>1</sub>/TiO<sub>2</sub>: Atomic-Level Insights into Reaction Pathways and Site-Sensitivity</b>  Selin Bac and Shaama Mallikarjun Sharada, <i>University of Southern California, USA.</i></p> <p>Short Summary:  Reaction mechanisms of CO oxidation over Pt<sub>1</sub>/TiO<sub>2</sub> is observed. Energetic span model and dynamics studies reveal Eley-Rideal as the preferred mechanism out of twelve distinct pathways. Due to evident site distributions of single Pt atoms, site-sensitivity of Mars-van Krevelen mechanism is sought. Atomic level insights on reaction progress are shown.</p>
Wed-P-120	<p><b>First-Principles Analysis of the Ammonia Decomposition Reaction on High Entropy Alloy Catalysts</b>  <u>Zuhal Cakir</u><sup>1</sup>, Liangbing Hu<sup>2</sup>, Chao Wang<sup>3</sup> and Jeffrey Greeley<sup>4</sup>, (1)Purdue University, USA, (2)University of Maryland - College Park, USA, (3)Johns Hopkins University, USA, (4)Davidson School of Chemical Engineering, Purdue University, USA.</p> <p>Short Summary:  We systematically develop a model of high entropy alloy catalysts and subsequently extending these ideas to incorporate multiple elements. We develop tools to efficiently sample different binding sites and to investigate the free energy landscape for simple adsorbates, choosing the ammonia decomposition reaction as a probe reaction.</p>
Wed-P-121	<p><b>Distributed Hydrogen Production Via Bioethanol Autothermal Reforming on Structured Catalysts</b>  Vittoria Troisi, Veronica Piazza, Abdelrahman Mostafa, Roberto Batista da Silva Junior, Alessandro Stagni, Alessio Frassoldati, Alessandra Beretta and Gianpiero Groppi, <i>Politecnico di Milano, Italy.</i></p> <p>Short Summary:  In this work a model for the prediction of ethanol reactivity in an autothermal reformer is developed. The results show that the CPO of ethanol follows a concerted hetero-homogeneous mechanism. Modelling analysis provides a tool to optimize the operative conditions which maximize hydrogen production while minimizing undesired coke precursors.</p>
Wed-P-123	<p><b>Effects of Adsorption Site Coordination on Activity, Selectivity and Reaction Mechanisms of CO<sub>2</sub> Reduction on Cu Catalysts</b>  <u>Lucas G. Verga</u> and Juarez L. F. Da Silva, <i>University of São Paulo, Brazil.</i></p> <p>Short Summary:  We employed density functional theory calculations to study the impact of the adsorption site coordination on the catalytic properties of Cu surfaces for the CO<sub>2</sub> reduction reaction. We observed coordination-dependent reaction mechanisms and used generalized coordination numbers as descriptors for the differences in activity and selectivity of Cu surfaces.</p>
<b>Americas Halls 1 &amp; 2</b>	<b>Reaction Engineering Poster Session</b>
Wed-P-66	<p><b>The Effects of n-Butene in Iso-Butene Selective Oxidation Reaction</b>  Yo Han Choi, Jinsuk Lee and <u>Hyun Chul Choi</u>, <i>Hanwha Total Petrochemical, Korea, Republic of (South).</i></p> <p>Short Summary:  It has been known that n-butenes play important role in iso-butene selective oxidation reaction. In order to confirm the quantitative effect of n-butenes on the iso-butene oxidation reaction, many reaction experiments were conducted at various concentrations of n-butenes (trans-2-butene, 1-butene).</p>
Wed-P-124	<p><b>Electrified Thermal Water Splitting</b>  <u>Olivia Fjord Sloth</u> and Ib Chorkendorff, <i>Technical University of Denmark, Denmark.</i></p> <p>Short Summary:  A novel cycling process for thermal water splitting driven by electrical heating is introduced: By heating nanoparticles at high temperatures, O<sub>2</sub> desorbs from the surface. The reduced nanoparticles are then cooled by H<sub>2</sub>O, allowing the alloy to phase-separate and reform the metal oxide, while H<sub>2</sub> evolves. The cycle is repeated.</p>
Wed-P-125	<p><b>Laboratory-Scale Platform for Validating Novel Industrial Ammonia Oxidation Catalysts</b>  <u>Noah Zecher-Freeman</u> and Chao Wang, <i>Johns Hopkins University, USA.</i></p> <p>Short Summary:  A laboratory-scale ammonia oxidation reactor system is able to replicate the high efficiency of the industrial process without the need for a specialized reactor. The same platform has been used to validate the performance of novel Pt-based high entropy alloy catalysts, with NOx selectivity up to 80%.</p>

<b>Wed-P-126</b>	<p><b>Nanofurnaces for Catalysis Powered By Induction Heating</b>  <u>Paul Camus</u>, Fanny Casteignau, Agathe Dujardin, Federico Galli and Nadi Braidy, <i>Université de Sherbrooke, Canada</i>.  Short Summary:  We develop a PTFE microreactor heated by induction to prove the concept of the hybrid nanocatalyst using CO-oxidation and reverse-Water Gas Shift as test reactions. We will present the preliminary catalysis results using this novel approach, including temperature maps of the bed, conversion and explain the catalyst behavior.</p>
<b>Wed-P-127</b>	<p><b>Fundamental Investigation of Pulsed Flows in Bubbling Fluidized Beds: An Application to Heterogeneous Catalysis</b>  Davide Cafaro<sup>1</sup>, Daniele Micale<sup>1</sup>, Riccardo Uglietti<sup>1</sup>, Kaiqiao Wu<sup>2</sup>, Mauro Bracconi<sup>1</sup>, Marc-Olivier Coppens<sup>2</sup> and <u>Matteo Maestri</u><sup>1</sup>, (1)<i>Politecnico di Milano, Italy</i>, (2)<i>University College London, United Kingdom</i>.  Short Summary:  This work proposes the fundamental investigation of catalytic pulsed fluidized beds with a multiscale reactive particle-tracking methodology. The analysis shows how the pulsed flow parameters can affect both the fluid dynamic and reactive performances, providing insights for the development of novel catalytic processes.</p>
<b>Wed-P-128</b>	<p><b>Kinetic Study of Ammonia Formation on Iron-Based Catalysts at Industrial Operating Conditions</b>  <u>Cristina Pizzolitto</u>, Matteo Guiotto, Alberto Biasin and Pierdomenico Biasi, <i>CASALE SA, Switzerland</i>.  Short Summary:  The present work focuses on the investigation of ammonia catalysts activity under different operating conditions in order to capture and compare their performance with clean and poisoned gas streams. The goal is to collect experimental evidences useful for the development of a new kinetic model of NH<sub>3</sub> formation.</p>
<b>Wed-P-129</b>	<p><b>Process Design of a Direct Route from Bioethanol to Ethylene Oxide</b>  <u>Ilenea Rossetti</u><sup>1</sup>, Antonio Tripodi<sup>1</sup> and Gianguido Ramis<sup>2</sup>, (1)<i>Università degli Studi di Milano, Italy</i>, (2)<i>Università degli Studi di Genova, Italy</i>.  Short Summary:  A novel route for the one-pot oxidation of ethanol to ethylene oxide was designed. Starting from original reaction kinetics, a staged, cooled reactor was designed with the full separation sequence. This lets foresee a conversion of 90% of bioethanol into Ethylene Oxide (&gt;99% purity) and 7.7% into marketable ethylene-glycol.</p>
<b>Wed-P-130</b>	<p><b>A Multiscale Euler-Euler Approach for the Reactive Investigation of Industrial Fluidized Units</b>  <u>Daniele Micale</u>, Riccardo Uglietti, Mauro Bracconi and Matteo Maestri, <i>Politecnico di Milano, Italy</i>.  Short Summary:  This work proposes a multiscale methodology which couples the detailed description of the chemical kinetics with the Eulerian-Eulerian CFD modeling approach. The method provides accurate predictions even at Courant conditions close to one, allowing for the fundamental investigation, design and scale-up of industrial fluidized systems.</p>
<b>Wed-P-131</b>	<p><b>Surfactant-Mediated Lithium Orthosilicate Enables Rapid High-Temperature CO<sub>2</sub> Absorption</b>  <u>Anthony Wallace</u><sup>1,2</sup>, Charles Coe<sup>2</sup>, Michael Smith<sup>2</sup>, Rocco D'Ascanio<sup>2</sup>, Simon Brooks<sup>2</sup> and Joseph Mendez<sup>2</sup>, (1)<i>Georgia Institute of Technology, USA</i>, (2)<i>Villanova University, USA</i>.  Short Summary:  Lithium-based ceramics, notably Li<sub>4</sub>SiO<sub>4</sub> (LOS), have been evaluated as potential CO<sub>2</sub> sorbents for removing CO<sub>2</sub> from steam reforming and water gas shift product streams [1,2]. Here, a novel surfactant-enhanced synthesis yields high-performing LOS with unique properties enabling rapid sorption-enhanced catalysis to produce H<sub>2</sub>.</p>
<b>Wed-P-132</b>	<p><b>Rich H<sub>2</sub> Catalytic Oxidation As a Novel Methodology for the Evaluation of Mass Transport Properties of 3D Printed Catalyst Supports</b>  <u>Federico Sascha Franchi</u>, Matteo Ambrosetti, Mauro Bracconi, Riccardo Balzarotti, Gianpiero Groppi and Enrico Tronconi, <i>Politecnico di Milano, Italy</i>.  Short Summary:  We present a novel methodology for the evaluation of mass transfer coefficients for advanced catalyst substrates made of high temperature 3D printed resin, based on rich H<sub>2</sub> combustion over a Pd/CeO<sub>2</sub> coated catalyst. This method reduces times and costs enabling experiment-based screening and optimization of 3D printed cellular substrates.</p>
<b>Wed-P-71</b>	<p><b>Microwave Catalysis for Chemical Reactions</b>  <u>Dushyant Shekhawat</u>, Christina Wildfire, Daniel J. Haynes, Douglas Kauffman, Mark Smith, Victor Abdelsayed, Chris Marin, Pranjali D. Muley and Candice Ellison, <i>National Energy Technology Laboratory, USA</i>.  Short Summary:  Microwave-assisted reaction chemistry is a very promising multidisciplinary area of scientific research for more energy-efficient production of valuable chemicals, fuels, and carbon products. Microwave effects can result in greatly enhanced reactions rates, generation of completely different products, and changes in product selectivity or position of chemical equilibria.</p>

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**27th North American  
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## Mechanism Understanding for NO<sub>x</sub> storage, release and reduction on Pt doped Ceria based Catalysts

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### Introduction

Due to strengthening legislations on exhaust emissions of lean-burn gasoline and diesel engines, there is a need for further optimisation of existing emission after-treatment catalytic converters for automotive applications. New regulations focus primarily on NO<sub>x</sub> abatement at low temperature.[1] High surface area ceria is successfully employed as an excellent support of PGMs in commercial catalytic LNT systems for automotive emission control. Platinum supported on ceria shows enhanced NO<sub>x</sub> storage at low temperatures, together with improved hydrocarbons light-offs. Ceria also possesses a high OSC with unique redox properties that can be further enhanced using dopants. The main function of these dopants is to allow the catalyst to function outside of the normal working temperature range and widen the operating conditions to increase catalyst efficiency.[2] To this end, Samarium was selected due to its reported effect on Pt reducibility and the platinum-ceria interaction, to allow greater activation during rich purge. Sm doped catalysts (10 wt.%) were synthesised on a range of ceria-based catalysts with increasing loadings of Pt (0-1 wt.%). The objective of this study was to investigate the effect of the dopant on the performance of the different catalysts, and, to understand morphological changes on the surface.

### Materials and Methods

Catalytic benchmark testing was performed using lean/rich switching conditions to best represent real-driving conditions. 20 cycles using a switching frequency of 120s lean to 10s rich were performed. Lean: 12% O<sub>2</sub>, 5% CO<sub>2</sub>, 5% H<sub>2</sub>O, 60 ppm NO, 400 ppm C<sub>3</sub>H<sub>6</sub> and 1500 ppm CO. Rich: 1.5% O<sub>2</sub>, 5% CO<sub>2</sub>, 5% H<sub>2</sub>O, 60 ppm NO, 1500 ppm C<sub>3</sub>H<sub>6</sub> and 3% CO (balance Ar). Cycles were completed at 150, 200, 250 and 300°C. Experiments were run with a space velocity of 30000 h<sup>-1</sup>, using a flow rate of 200 ml/min. Measurements were performed online using a Pfeiffer OmniStar<sup>TM</sup> Vacuum Mass Spectrometer. H<sub>2</sub>-TPR experiments were performed using a MicroActive AutoChem II 2920 Chemisorption Analyser. The catalysts were pretreated for 1 hour at 500°C in 10% O<sub>2</sub>/He (35ml/min). Hydrogen uptake was measured during a heating rate of 10°C/min, from 0°C to 1000°C under 5%H<sub>2</sub>/Ar (35ml/min).

### Results and Discussion

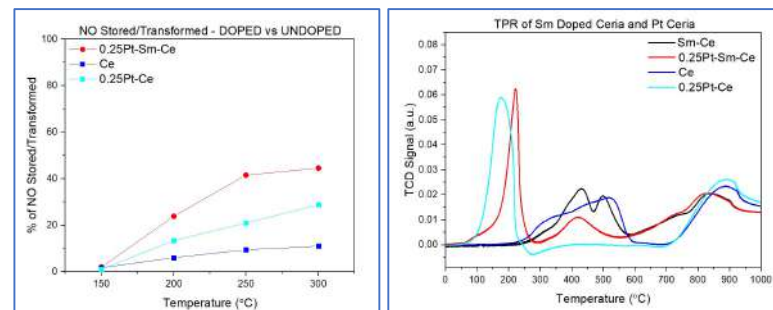
Results from lean/rich cycles illustrated in Figure 1, show that the addition of Sm dopant on to a 0.25wt.% Pt-Ceria catalyst increases the NO<sub>x</sub> stored in lean conditions, at 200°C, from 14% to 24%, of the total NO<sub>x</sub> fed. The presence of Sm dopant (not presented) also increases the amount of HC (C<sub>3</sub>H<sub>6</sub>) oxidised at low temperatures (150-300°C). It was also noted that the effect the dopant on the lean NO<sub>x</sub> storage and HC oxidation is more prevalent when 0.25wt.% Pt loading is present on the Ce surface, compared to higher loadings (1 wt.%). This dopant effect is also evident from H<sub>2</sub>-TPR results depicted in Figure 2 below. The bare Ce support exhibits a set of H<sub>2</sub> consumption peaks ranging from ~200 – 600°C, which correspond

to the surface reduction of ceria. This is followed by a bulk reduction shown in the range of ~700°C and above. Upon the addition of 10wt.% Sm, (Sm-Ce) the surface reduction profile is modified to produce more intense peaks at certain temperatures. There is also a shift in the bulk reduction temperature ranges and peak profiles which may indicate mixed phase reduction. In the presence of Pt, (0.25Pt-Ce) an initial set of peaks, from ~50 – 250°C, is visible. This is likely attributed to the surface reduction of ceria in close contact with the metal, as well as the platinum reduction. The bulk reduction remains unaffected. The incorporation of Sm into the lattice (0.25Pt-Sm-Ce) does not significantly modify the initial reduction temperature range, however, it does indicate that there is a clear effect on the Pt-Ceria interaction. Low temperature peaks are more clearly separated and a further peak, occurring at intermediate temperatures (~300 – 550°C), can be seen.

From these results it is clear that the presence of Sm can modify Ce-based catalysts both with and without the presence of a noble metal. The link between this structural modification and the increase in NO<sub>x</sub> storage capacity will be discussed further.

### Significance

Initial lean/rich activation testing shows that as the presence of the doping element, Samarium, on Pt-Ceria increases the NO<sub>x</sub> storage capacity of the catalyst at low temperatures (150-300°C) and subsequently decreases the temperature needed for NO<sub>x</sub> reduction. This is particularly important for the application of these catalysts to reduce NO<sub>x</sub> during cold start operation. These advances can aid future catalyst development in the hopes of hitting NO<sub>x</sub> emission targets set out in the Euro 7 protocol.



**Figure 1 & 2 (LtoR).** (1) NO stored/transformed during lean gas flow at a temperature range from 150-300°C for 3 catalysts (Ce,0.25Pt-Ce & 0.25Pt-Sm-Ce). (2) H<sub>2</sub>-TPR profile over a temperature range from 0-1000°C for 4 catalysts (Ce, Sm-Ce, 0.25Pt-Ce, 0.25Pt-Sm-Ce).

### References

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2. Q. Sun, Z. Fu, and Z. Yang, Effects of rare-earth doping on the ionic conduction of CeO<sub>2</sub> in solid oxide fuel cells, *Ceram. Int.*, Volume 44, 2018, Pages 3707–3711.