

2018 Pacific Coast Catalysis Society Meeting

Monday, Sept. 10, 2018

Johnson Hall

Oregon State University, Corvallis, Oregon

8:15	<u>Frank Abild-Pedersen</u> ^{*,†} , Tej S. Choksi [*] , Verena Streibel [*] [*] SUNCAT Center for Interface Science and Catalysis, [†] SLAC National Accelerator Laboratory, Stanford University Predicting Catalytic Properties of Transition Metal Nano Particles – Effects of Local Morphology and Atomic Composition
9:00	<u>Neeru Chaudary</u> , Alyssa J.R. Hensley, Yong Wang, and Jean-Sabin McEwen Washington State University Elucidating the Effect of the Lateral Interactions on the Adsorption of Bio-Oil Model Compounds on Pt (111)
9:20	Charles T. Campbell University of Washington Where experiments meet computational catalysis
10:05	break
10:25	Dante Simonetti University of California, Los Angeles Effects of Morphology and Dopants on the CO ₂ Capacity of Nanofibrous Calcium-Oxide Based Materials for Sorption-Enhanced Steam Methane Reforming
10:55	<u>Yifeng Zhu</u> , Oliver Y. Gutierrez, John Fulton, Libor Kovarik, Janos Szanyi, and Johannes A. Lercher Pacific Northwest National Laboratory From Single Atoms to Clusters, Manipulating CO ₂ Reduction Pathways on Rh catalysts
11:15	<u>Nicholas C. Nelson</u> , Manh-Thuong Nguyen, Vassiliki-Alexandra Glezakou, Roger Rousseau, Janos Szanyi Pacific Northwest Laboratory Mapping the water-gas shift reaction network over an oxide-supported transition metal catalyst using operando infrared spectroscopy
12:00	Lunch break



13:20	<u>Feng Chen</u> , ¹ Meng Wang, ¹ Hui Shi, ² Yuanshuai Liu, ² Oliver Y Gutierrez Tinoco, ^{1,*} Donald M. Camaioni, ¹ Johannes A. Lercher ^{1,2} ¹ Pacific Northwest National Laboratory, ² TU München Kinetic and Mechanism Studies for Alcohol Dehydration over Zeolites in Apolar Solvent
13:40	Teh C. Ho Hydrocarbon Conversion Technologies Ultra-Deep Diesel Hydrodesulfurization Catalysis and Process: A Tale of Two Sites
14:25	Konstantinos Goulas Oregon State University Catalysis in Biomass Upgrading: Fundamental and Applied Insights into the Production of Diesel Fuel Replacements
14:55	<u>Christopher Ho</u> and Alexis T. Bell University of California, Berkeley Bimolecular Condensation of Alcohols over Hydroxyapatite: Mechanisms and Site Requirements of C-C and C-N Bond Forming Reactions
15:15	Break
15:35	Norbert Kruse Washington State University Changing Paradigms in the Fischer Tropsch Reaction Mechanism of long-chain Hydrocarbon Production from Carbon Monoxide and Hydrogen
16:20	Sebastian Oener University of Oregon Bipolar junction anionic thin layer water electrolyzers
16:40	Thomas Bligaard SUNCAT Center for Interface Science and Catalysis, SLAC National Accelerator Laboratory, Stanford University TBD
17:25	Poster session and reception



Poster Presentations:

1	<p><u>Dan Huang</u>¹, Matthew Coblyn¹, Bavornpon Jansang², Nichaporn Sirimungkalakul², Thana Sornchamni² and Goran Jovanovic¹ ¹Oregon State University, ²PTT Public Company Limited, Thailand A Dft Study Of Hydrodeoxygenation Reaction Mechanism</p>
2	<p><u>J. Trey Diulus</u> and Gregory S. Herman Oregon State University Surface Chemistry of 2-Propanol on SnO₂(110) Studied with Ambient-Pressure X-ray Photoelectron Spectroscopy</p>
3	<p><u>Maoyu Wang</u>, Zhenxing Feng Oregon State University Mechanistic Study of Oxygen-Reduction activity on Fe substitution LaCo₃ Electrocatalysts</p>
4	<p><u>Lucas Freiberg</u> and Nicholas AuYoung Oregon State University</p>
5	<p><u>Danelle Roan</u>, Kyle Groden, Jean-Sabin McEwen Washington State University Modeling the Reaction Mechanism of Carbon Monoxide Oxidation on a Clean and an Oxidized Cu(110) Surface: A Density Functional Theory Study</p>
6	<p><u>Qin Pang</u>, Hossein DorMohammadi, O. Burkan Isgor, LÍney Árnadóttir Oregon State University Effects of step edges on Cl interactions with α-Fe₂O₃ surface: A Density function theory study</p>
7	<p><u>Sean Seekins</u>, Kingsley Chukwu, LÍney Árnadóttir Oregon State University Density Functional Theory and Ambient Pressure XPS Study of Solvent Effects in the Decomposition of Acetic Acid</p>

8	<p><u>Kingsley Chukwu</u>, Sean Seekins, Liney Árnadóttir Oregon State University First-principles study of the decarboxylation and decarbonylation of acetic acid over Pd (111).</p>
9	<p>Laura Meyer, Udishnu Sanyal, Oliver Y Gutiérrez, Johannes A. Lercher, Pacific Northwest National Laboratory, Richland WA Reaction networks and mechanisms in electrocatalytic hydrogenation of carbonyl compounds</p>
10	<p><u>Kelsey A. Stoerzinger</u>, Scott A. Chambers Pacific Northwest National Laboratory, Richland WA Understanding chemical interactions at solid/gas and solid/liquid interfaces</p>
11	<p>Erum Mansoor and Alexis T. Bell University of California, Berkeley Application of an improved Computational Model to the Dehydrogenation of Light Alkanes Catalyzed by Ga/H-MFI</p>
12	<p>Julie Rorrer and Alexis T. Bell University of California, Berkeley Mechanism and Kinetics of Isobutene Production over Zinc-Zirconium Mixed Oxide</p>
13	<p><u>Aidan Garcia</u>, Michael Ayiania, Kyle Groden, Alyssa Hensley, Jean-Sabin McEwen, Manuel Garcia-Perez Washington State University Characterizing the Binding of Phosphates on Nitrogen-Functionalized Biochars: A Combined Experimental and Theoretical Study</p>
14	<p><u>Teawoo Kim</u> and David P. Fenning University of California, San Diego Strain-controlled Electrochemical CO₂ Reduction to Hydrocarbons and Oxygenates on Planar Copper</p>