Catalysis Club of Philadelphia

Thursday, April 18th, 2018
Crowne Plaza Wilmington North
630 Naamans Road, Claymont, DE 19703

Catalysis Club of Philadelphia Officer Elections

The Catalytic Science of Making Up and Breaking Up Dinitrogen

Speaker: Prof. William F. Schneider
University of Notre Dame

Spectroscopy Characterization of $NiCu_3$/C Nanocrystal Catalysts for Hydrodeoxygenation of 5-Hydroxymethylfurfural

Graduate Student Speaker: Jennifer D. Lee
University of Pennsylvania, Christopher B. Murray Group

Meeting Schedule:
Social Hour .....5:30 PM
Dinner.....6:30 PM
Meeting.....7:30 PM

Meeting Fees:
Members: $40.00
Non-Members: $45.00
Stud. & Retired Members: $25.00

Menu

A tri-colored tortellini appetizer, served with spinach side salad, Crème Brulee Cheesecake, and your choice of entree:

1) Roasted Pork Loin – *Complimented by apple cider demi glaze and golden raisins*
2) Chicken and Salmon – *sautéed chicken and baked salmon with champagne cream sauce*
3) Vegan Pasta Dish – *Cavatappi pasta, oven roasted seasonal vegatables, and marinara sauce*

Meal reservations – Please register online by ***Friday, April 12th*** at http://catalysisclubphilly.org/ or notify your company representative or our Treasurer Lifeng Wang (Lifeng.Wang@pqcorp.com) or Chair Eric Sacia (Eric.R.Sacia@dupont.com)

Membership - Dues for the 2018-19 season will be $25.00 ($5.00 for the local chapter and $20.00 for the national club). Dues for students, post-docs and retirees will be $10.00 ($5.00 for local club and $5.00 for national club).

Catalysis Club of Philadelphia

Thursday, April 18th, 2018

Crowne Plaza Wilmington North

630 Naamans Road, Claymont, DE 19703

Prof. William F. Schneider

The Catalytic Science of Making Up and Breaking Up Dinitrogen

H. Clifford and Evelyn A. Brosey Professor
University of Notre Dame, Department of Chemical and Biomolecular Engineering
Concurrent Professor, Department of Chemistry and Biochemistry

Abstract: The chemistry of nitrogen is inextricably linked with humanity's use of energy. Industrial nitrogen fixation ($N_2 \rightarrow NH_3$) revolutionized the production of fertilizer and enabled the population explosion of the 20th century, consuming several percent of the world's energy annually in the process. NO_X reduction ($NO_X \rightarrow N_2$) is integral to reducing the adverse impacts of automobile use on urban air quality and health. These and other successful technologies all depend at their heart on heterogeneous catalysis. In this presentation, I will discuss the insights we have gained by applying molecular-level models and concepts to nitrogen catalytic chemistry. Examples will be drawn from our work on the selective catalytic reduction of NO_X, a problem that has led us to rethink the factors that govern reactivity in zeolites, from NO and NH_3 oxidation, problems that have caused us to revisit how we model reactions at metal surfaces, and from N_2 reduction, where we are exploring the potential to bypass the constraints imposed by mother nature on the performance of conventional catalysts.

Speaker Details: Bill Schneider's expertise is in chemical applications of density functional theory (DFT) simulations. After receiving his Ph.D. in Inorganic Chemistry from the Ohio State University, he began his professional career in the Ford Motor Company Research Laboratory working on a variety of problems related to the environmental impacts of automobile emissions. At Ford he developed an interest in the catalytic chemistry of NO_X for diesel emissions control, and he has published extensively on the chemistry and mechanisms of NO_X decomposition, selective catalytic reduction, trapping, and oxidation catalysis. In 2004 he joined the Chemical and Biomolecular Engineering faculty at the University of Notre Dame as an Associate Professor. At Notre Dame he has continued his research into the theory and molecular simulation of heterogeneous catalysis, with particular emphasis on reaction environment effects on catalytic materials and their implications for mechanism and reactivity. He was promoted to Professor in 2010 and awarded the H. Clifford and Evelyn A. Brosey Chair in the College of Engineering in 2016. He has co-authored more than 180 papers and book chapters, is a Fellow of the American Association for the Advancement of Science, is a Senior Editor for *The Journal of Physical Chemistry*, and was the 2018 recipient of the Giuseppe Parravano Award of the Michigan Catalysis Society. He makes his home in Granger, Indiana with his three children, Justin, MiMi, and Meredith.

Jennifer D. Lee

Spectroscopy Characterization of $NiCu_3$/C Nanocrystal Catalysts for Hydrodeoxygenation of 5-Hydroxymethylfurfural

Department of Chemistry, University of Pennsylvania, PA, 19104
Advisor: Prof. Christopher B. Murray

Abstract: The development of high-performance catalysts is critical to realizing the transformation of renewable biomass into fuels and chemicals with high yield. The selective hydrodeoxygenation (HDO) of 5-hydroxymethylfurfural (HMF) to 2,5-dimethylfuran (DMF) is an important step in upgrading lignocellulosic biomass, where bimetallic catalysts have shown promising performance. It has also been shown that catalysts consist of well-controlled NCs synthesized *via* solvothermal methods is critical to achieving high DMF selectivity. The high degree of size-, shape- and composition-control could potentially overcome traditional structural heterogeneity and enable a much deeper understanding of the evolution of NC structure that results in superior catalytic performance. This presentation will focus on the spectroscopy characterization of a high-performance HDO catalyst, $NiCu_3$/C, for DMF production. An in-house-built *operando* X-ray absorption spectroscopy (XAS) cell for probing catalysts under reaction conditions will be introduced. Subsequently, we will discuss the structural transformation of $NiCu_3$/C under pretreatment environment and HDO reaction conditions. With the characterization of *operando* XAS combined with X-ray photoelectron spectroscopy (XPS) studies and theoretical calculations, the gradual re-oxidation of catalysts was observed under reaction conditions and the presence of a surface oxide layer (NiO) over a mixed oxide core ($NiCuO_x$) was identified as the active phase for high DMF selectivity. This work aims to advance our understanding of the structure-property correlations that contributes to the superior HDO performance.

Speaker Bio: Jennifer D. Lee is a 5th-year Ph.D. student in the Murray Group at the University of Pennsylvania. She received her B.S. degree in Chemistry from National Taiwan University in 2011 and a Master degree in Chemistry from the same institute in 2013. Her master thesis focused on the synthesis and application of DNA-templated silver nanoclusters. She is currently a Ph.D. candidate in the Department of Chemistry and her research focuses on the preparation and characterization of tailored nanostructures of metal and metal oxides for catalysis and magnetic applications.