Catalysis Club of Philadelphia

Thursday, September 27th, 2018
Crowne Plaza Wilmington North
630 Naamans Road, Claymont, DE 19703

Speaker: Prof. Alan S. Goldman

Catalysis by Pincer-Iridium Complexes. Breaking C-H Bonds, Making C-C Bonds, and Various Combinations Thereof

Department of Chemistry and Chemical Biology
Rutgers University

Post-Doc Speaker: Dr. Ozgen Yalcin

Bridging the Gap between Heterogeneous Catalysts and Bioinorganic Enzymes

Department of Chemical & Biomolecular Engineering
Lehigh University

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
Your choice of 3 entrees:

1) Sliced Roast Sirloin – *Thinly Sliced and Served with a Wild Mushroom Sauce*
2) Roasted Pork Loin – *Rubbed with Whole Grain Dijon, Complimented by a Caramelized Apple and Raisin Chutney*
3) Eggplant Parmigianino – *Eggplant Parmigianino with Layered Mozzarella Cheese and Italian Bread Crumbs*

Meal reservations – Please register online by ***Thursday, September 20th*** 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).

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Professor Alan S. Goldman

Catalysis by Pincer-Iridium Complexes. Breaking C-H Bonds, Making C-C Bonds, and Various Combinations Thereof

Department of Chemistry and Chemical Biology, Rutgers - The State University of New Jersey

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Abstract: Iridium complexes have played a leading role in the organometallic chemistry of alkanes and unreactive C-H bonds since the inception of the field 30 years ago. We have found that "PCP"-pincer-ligated iridium complexes are particularly effective for the dehydrogenation of alkanes and have incorporated this reaction into tandem systems for several catalytic transformations based on dehydrogenation. A closely related class of reactions that we are exploring is dehydrogenative coupling. More recently we have turned attention to iridium Phebox complexes. Although the (PCP)Ir and (Phebox)Ir units are formally isoelectronic, the former operates via C-H activation by Ir(I) while the latter effects dehydrogenation via Ir(III) (as an acetate complex) and possibly Ir(V) intermediates. Such a high-oxidation-state catalytic cycle offers advantages for many potential applications of dehydrogenation. In parallel, however, we find that the low-oxidation-state (+I) chemistry of (Phebox)Ir offers its own novel hydrocarbon chemistry.

1. Gao, Y.; Guan, C.; Zhou, M.; Kumar, A.; Emge, T. J.; Wright, A. M.; Goldberg, K. I.; Krogh-Jespersen, K.; Goldman, A. S. *J. Am. Chem. Soc.* **2017**, 139, 6338–6350.
2. Wilklow-Marnell, M.; Li, B.; Zhou, T.; Krogh-Jespersen, K.; Brennessel, W. W.; Emge, T. J.; Goldman, A. S.; Jones, W. D. *J. Am. Chem. Soc.* **2017**, 139, 8977-8989.
3. Goldberg, K. I.; Goldman, A. S. *Acc. Chem. Res.* **2017**, *50*, 620-626.
4. Kumar, A.; Bhatti, T. M.; Goldman, A. S. *Chem. Rev.* **2017**, *117*, 12357-12384.
5. Gao, Y.; Emge, T. J.; Krogh-Jespersen, K.; Goldman, A. S. *J. Am. Chem. Soc.* **2018**, *140*, 2260-2264.

Speaker Details: Alan Goldman received his B.A from Columbia University in New York in 1980 and his Ph.D. from Columbia in 1985, studying the mechanisms of photoinduced organometallic reactions in the laboratory of Prof. David R. Tyler. He then took an IBM Post-doctoral Fellowship in the lab of Prof. Jack Halpern at the University of Chicago. Goldman began his independent career as an assistant professor at Rutgers University in 1987 where he is currently Distinguished Professor of Chemistry. His research focuses on the development and mechanistic study of transition-metal-catalyzed transformations of small molecules and relevant fundamental chemistry. Goldman has received the Union Carbide Innovation Recognition Award, an Alfred P. Sloan Fellowship, a Dreyfus Teacher-Scholar Fellowship and the inaugural ACS Catalysis Lectureship Award for the Advancement of Catalytic Science.

Graduate Student/Post-Doc Speaker

Bridging the Gap between Heterogeneous Catalysts and Bioinorganic Enzymes

Dr. Ozgen Yalcin

Operando Molecular Spectroscopy and Catalysis Research Laboratory
Department of Chemical & Biomolecular Engineering
Lehigh University
Bethlehem, PA USA

Abstract: To better understand why enzymes are able to perform redox reactions at mild reaction conditions and heterogeneous solid oxide catalysts require elevated reaction temperatures for oxidation reactions, the mechanisms and kinetics of methanol oxidation by bioinorganic enzyme mimics and heterogeneous solid oxide catalysts were compared at the molecular level both experimentally and theoretically. The experimental studies employed time-resolved *in situ* spectroscopy to monitor the molecular chemical transformations of the enzyme mimic and solid oxide catalysts as well as the methanol reactant and reaction intermediates. Both reactions proceed via the same V-OCH_3 intermediate. The origin of the difference in reactivity between bioinorganic enzymes and solid oxide catalysts is related to the highly reactive peroxo VO_2 sites only present in bioinorganic enzymes and not present in heterogeneous solid oxide catalysts under high temperature reaction conditions. The DFT calculated normal vibrational modes and reaction steps are in line with the experimental findings. This study bridges the gap between heterogeneous solid oxide catalysts and protein-based vanadate enzymes for methanol oxidation as well as other oxidation reactions.

Speaker Details: Ozgen Yalcin is a post-doctoral researcher in the *Operando* Molecular Spectroscopy and Catalysis Research Laboratory under the supervision of Prof. Israel E. Wachs at Lehigh University. She received her B.S. and M.Sc. in Chemical Engineering from Middle East Technical University (METU), Ankara, Turkey. She received dual PhD degrees from both the Department of Chemical & Biomolecular Engineering at Lehigh University and the Department of Chemical Engineering at Middle East Technical University. Her principal research interests are in heterogeneous catalysis and can be categorized as computational studies of water-gas shift reaction over inorganic metal oxides, and experimental studies of non-carcinogenic alternatives of solid oxide catalysts for high temperature water-gas shift reaction systems. She also has experience in methanol oxidation by bioinorganic enzyme mimics and supported vanadium oxide catalysts. In the future, she wants to contribute to the field of heterogeneous catalysis by applying the rich experiences she gained from academia.