

**SPRING 2023  
CHEMISTRY  
SEMINAR SERIES**



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New Brunswick, NJ*

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PROF. PROKOPCHUK**

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**“Catalytic Alkane Dehydrogenation and  
Related Reactions by Pincer-Metal Complexes.  
New Approaches, New Reactions”**

**Friday, March 3, 2023, 11:30 AM  
Life Science Center II, Room 130**

**Abstract:** The dehydrogenation of alkanes and alkyl groups to give olefins is a reaction of tremendous potential value. Low-oxidation-state organometallic complexes were demonstrated to be effective for this reaction 40 years ago by Crabtree, and great progress has been since then. We have found that “PCP”-pincer-ligated iridium complexes are particularly effective for alkane dehydrogenation, driven with the use of olefinic acceptors or purging H<sub>2</sub> from solution, and we have incorporated these reactions into tandem systems for several dehydrogenation-based catalytic transformations. More recently we have turned our attention to systems that operate based on fundamentally different principles, such as Phebox iridium catalysts. The iridium Phebox unit is formally isoelectronic to (PCP)Ir, but whereas (PCP)Ir operates via C-H activation by Ir(I), (Phebox)Ir 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. For example, we are interested in dehydrogenation achieved by proton-coupled electron transfer (PCET), which could ultimately be driven electrochemically or with O<sub>2</sub> as the ultimate hydrogen acceptor. We have found that (PCP)Ir can operate via PCET but turnovers are limited by over-oxidation. High-oxidation-state catalysts could allow us to circumvent this problem and may generally be more favorable for PCET-based dehydrogenation.

1. Goldberg, K. I.; Goldman, A. S. *Acc. Chem. Res.* **2017** DOI: 10.1021/acs.accounts.6b00621
2. Kumar, A.; Bhatti, T. M.; Goldman, A. S. *Chem. Rev.* **2017** DOI: 10.1021/acs.chemrev.7b00247
3. Shada, A. D. R.; Miller, A. J. M.; Emge, T. J.; Goldman, A. S., *ACS Catal.* **2021** DOI: 10.1021/acscatal.0c05160
4. Zhou, X.; Malakar, S.; Dugan, T.; Wang, K.; Sattler, A.; Marler, D. O.; Emge, T. J.; Krogh-Jespersen, K.; Goldman, A. S. *ACS Catal.* **2021** DOI: 10.1021/acscatal.1c03562
5. Gordon, B. M.; Lease, N.; Emge, T. J.; Hasanayn, F.; Goldman, A. S. *J. Am. Chem. Soc.* **2022** DOI: 10.1021/jacs.1c13309

**Biographical Sketch:** 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. Honors received by Goldman include an Alfred P. Sloan Fellowship, a Dreyfus Teacher-Scholar Fellowship, the inaugural ACS Catalysis Lectureship Award for the Advancement of Catalytic Science, the 2019 ACS Award in Organometallic Chemistry, the 2020 Royal Society of Chemistry Sir Geoffrey Wilkinson Award, and election to Fellowship in the American Association for the Advancement of Science in 2021.