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Wednesday, September 18th, 2024, 5:30PM
225 Fenster Hall
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Newark, NJ, 07103

Dr. David Kaphan



Argonne National Laboratory
Catalysis Group

Electronic Metal-Surface Communication in Surface Organometallic Catalysis

Chemisorption of organometallic complexes on inorganic supports is a powerful strategy for rational catalyst design and for generating model systems for the controlled study of phenomena such as Electronic Metal-Support Interactions (ESMI) in heterogeneous catalysis. While traditional surface organometallic catalysis on inert oxides affords highly reactive, homogeneous-in-function heterogeneous catalysts, the intrinsic role of the surface as an inner sphere ligand in modulating catalyst reactivity is often underappreciated and unleveraged. In this work organometallic molecular precursors are employed to functionalize a variety of surfaces beyond typical supports in surface organometallic catalysis. Redox active materials inspired by Li-ion battery cathodes and anodes such as lithium manganese oxide ($\text{Li}_x\text{Mn}_2\text{O}_4$) and lithium titanate (Li_xTiO_2) are employed as catalyst supports for which the electronic properties of the active site can be continuously

modulated as a function of the degree of lithium intercalation into the support, resulting in rationally tunable catalysts for a variety of transformations. This approach is explored in a variety of catalytic model reactions including oxidative coupling, hydrogenation, and selective olefin trimerization, all of which are responsive to modulation of the global redox state of the catalyst material, and some evidence for dynamic, “redox non-innocent” surface behavior observed. These studies reveal a complex interplay between bond forming elementary steps at the active site and redox interactions with the surface, both of which are dependent on electronic communication between the surface and active site, and can be modulated a function of surface lithiation. Additional examples of metal-surface cooperativity in non-traditional surfaces will also be discussed.

Speaker Bio

Dr. Kaphan obtained his BS from the University of Rochester and his PhD from the University of California, Berkeley. He is a Chemist in the Catalysis Group in the Chemical Sciences and Engineering Division at Argonne National Laboratory and is affiliated as a Scientist in the UChicago Consortium for Advanced Science and Engineering. David’s research concerns fundamental studies in supported organometallic catalysis, capture and conversion of atmospheric carbon dioxide, and chemical upcycling of polymer waste. His primary area of research in supported organometallic catalysis focuses on understanding stereoelectronic communication between organometallic complexes and inorganic support materials that can be leveraged to modulate reactivity and the development of non-traditional functional materials as catalyst support frameworks.

<u>Schedule TBA</u>		<u>Meeting Fees</u>	
Student Presentation	5:30 PM	Professional Members	\$40
Social Hour (Cash Bar)	6:00 PM	Non-members	\$50
Dinner	6:45 PM	Students	\$25 (Student Members = \$10)
Presentation	7:30 PM	Retired/Post-Doc/Unemp.	\$40 (Members = \$30)
		Annual Membership Dues	\$35 (Students = \$15)

Deadline for reservations is 5:00PM Friday, September 13th, 2024

Please RSVP online using the [online form](#).
To renew your membership, please visit this [link](#).