Research Seminar

NUS National University of Singapore

Department of Chemistry
Faculty of Science

Combining Theory and Experiment to Develop Selective C-C Bond Formations via Open-Shell Intermediates

by Professor Osvaldo Gutierrez
University of Maryland, U.S.A

Host: Asst. Prof. Koh Ming Joo | Tue, 7 Jan 2020 16:00 – 17:30 Executive Classroom (S8-03-14)

About Professor Osvaldo Gutierrez

Professor Gutierrez was born in Salamanca, Guanjuato (Mexico) and raised in Sacramento, California. He attended UCLA in 2006 where he worked as an undergraduate at the laboratories of Professor Houk doing research in computational organic chemistry and B.S./M.S. in 2009. He then completed his Ph.D. in 2012 (UC Davis) under the guidance of Professor Tantillo working on mechanism of organometallic reactions. From 2012-2016 he worked as a postdoc. with Professor Kozlowski at the University of Pennsylvania where he used computational and experimental tools to study transition metal-catalyzed processes. He is now at the University of Maryland College Park where his research combines computational and experimental approaches to advance our understanding of iron- and photo-catalyzed reaction mechanisms. Since 2016, his group has published over 16 papers and recognized by the NSF CARREER AWARD in 2018, the University of Maryland's' College of Computer, Mathematics and Natural Sciences Junior Faculty Award in 2019, and recipient of the first Nathan Drake Endowed Junior Fellowship. In this spare time, he enjoys rap music, running, and tasting spicy food.

Abstract

Despite advances in high-throughput screening methods leading to a surge in the discovery of catalytic reactions, our knowledge of the molecular-level interactions in the rate- and selectivity-determining steps of catalytic reactions, especially those involving highly unstable and reactive open-shell intermediates, is rudimentary. These knowledge gaps prevent control, suppression or enhancement, of competing reaction channels that can drive development of unprecedented catalytic reactions. In this talk, I will focus on our use of high-level quantum mechanical calculations, rigorously calibrated against experimental data, to interrogate the mechanisms and to guide the development of new catalysts and reagents for currently sluggish or unselective reactions. In particular, I will focus on our use of combined experimental and computational tools to understand and develop new (asymmetric) iron-catalyzed and (metallo)photoredox-catalyzed carbon-carbon bond formations with relevance to the synthesis of pharmacetuticals.

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