# 2020-2021 POCC Lecture Series

December 17, 2020, 7:30 PM

*Virtual reception to follow the seminar*

## Prof. Osvaldo Gutierrez

University of Maryland, College Park

***Combining Theory and Experiment to Develop Selective Three-Component Fe-Catalyzed Radical Cascades/Cross-Couplings***

Virtual Seminar by Zoom (LINK)

The Philadelphia Organic Chemist's Club

POCClub.org

**Sponsored by Fox Chase Chemical Diversity Center, Inc.**

FCCDC
Fox Chase Chemical Diversity Center, Inc.

Osvaldo was born in Salamanca, Guanajuato (central Mexico) and raised in Sacramento, California. He attended Sacramento City College and transferred to UCLA in 2006 where he worked as an undergraduate at the laboratories of Prof. Ken Houk. He obtained his B.S./M.S. in 2009 and completed his Ph.D. in 2012 (UC Davis) under the guidance of Prof. Dean Tantillo. From 2012-2016 he worked as a postdoc with Prof. Marisa 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 nickel-catalyzed multicomponent cross-couplings.

**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) three-component iron-catalyzed radical cascade/cross-coupling reactions.