EASTERN MICHIGAN UNIVERSITY Chemistry Department

Seminar

Prof. Hrant Hratchian, University of California, Merced Monday, Oct. 28th 4:00-5:00 pm Strong Hall 200

Exploring the Reactivity and Dynamics of Metallacycle Mediated Coupling Reactions

Abstract

The formation of C–C bonds is the most fundamental objective of synthetic chemistry. In recent decades, a myriad of transition metal catalysts have been discovered and successfully employed to produce selective C–C bond formations in high yield and with high efficiency. Despite these advances in reaction discovery, much remains to be learned about *how* these catalysts simultaneously facilitate oxidation/reduction and navigate treacherous potential energy landscapes. One area of focus in our group is the development and application of quantum chemistry models to seek the molecular and electronic structural factors that drive these sorts of catalytic processes. This talk will describe our initial foray to these questions and outline some of our ongoing developments.