WestVirginiaUniversity.

C. Eugene Bennett Department of Chemistry

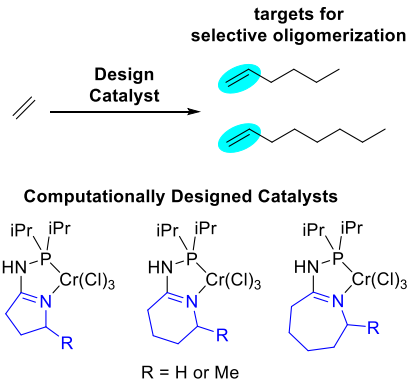
Computational Studies on Organometallic Catalyst Design, Reaction Mechanisms, and Dynamics

Prof. Daniel H. Ess

Brigham Young University

Department of Chemistry and Biochemistry

This talk will describe three of our ongoing computational studies on complex organometallic reactions. 1) Our development and use of a DFT transition-state model that provided quantitative prediction and experimental realization of a new family of molecular Cr catalysts for controllable selective ethylene trimerization and tetramerization. 2). Our use of DFT calculations to understand mechanisms and predict alkane C-H activation and functionalization catalysts based on 5th-row and 6th-row p-block main-group compounds. 3) Our development and use of our DynSuite quasiclassical direct dynamics program to understand dynamical influences during C-H activation reactions with cationic iridium phosphine complexes



Kwon et al. *ACS Catal.* **2018**, 8, 1138-1142.

King, et al. *Organometallics*, **2017**, *36*, 109-113., Fuller et al. *ACS Catal.* **2016**, *6*, 4312-4322.

Date: Wed, Feb 21, 2018

Time: 4:30-5:30 pm

Location: 208 Clark Hall

Students, meet the speaker over coffee and cookies in the Bennett Conference room at 3:30 pm