Iron-Catalyzed Radical Cross-Coupling Reactions: Past and Future

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 radical cross-coupling reactions.

Friday, May 31st at 1:00pm
Mani L. Bhaumik Collaboratory,
Dongwon Yoo Seminar
& Conference Hall (Young Hall 4222)

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