

UNIVERSITY OF RHODE ISLAND
Department of Chemistry
SEMINAR

Room 105 Beupre Center
3:00 p.m., Monday, December 9, 2019

Andy Thomas

MIT

***“Mechanistic Insights Facilitate the
Development of Transition Metal
Catalyzed Processes”***

HOST

Matthew Kiesewetter
Department of Chemistry
401-874-2619

Mechanistic Insights Facilitate the Development of Transition Metal Catalyzed Processes

Despite the widespread use of the Suzuki-Miyaura cross-coupling reaction, the structure of the reactive intermediates underlying the key transmetalation step remained uncertain. We discovered multiple pre-transmetalation intermediates with various boron nucleophiles that were found to transfer their organic groups to palladium, revealing the critical features that affect the transfer of the organic fragment from boron to palladium. These insights led to the development of significantly improved homogenous cross-coupling conditions. In the second part of the talk, a hybrid bisphosphine ligand (SEGFAST) was developed for the LCuH-catalyzed hydroamination reaction of unactivated olefins. The crucial non-covalent interactions necessary for high turnover numbers were discovered using a combination of computational and experimental methods. These synergistic efforts accelerated the catalyst discovery by avoiding the synthesis and empirically testing of a large library of ligands.