Thursday, February 12 2026 @ 4:00 pm – CDI 4.352

Synthesizing Computations and Experiments for Functionalizations and Cross-Couplings

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Abstract: The development of novel organic synthetic methodologies en route to complex small molecules is vital to driving discovery of new materials, dyes, fragrances, and pharmaceuticals. Transition-metal catalysis and metallaphotoredox catalysis have given rise to novel strategies for cross-coupling and functionalization of naturally abundant and synthetically practical functional groups, including alcohols, alkenes, alkanes, and arenes, among others. Computational modeling of organic reactions, when used in tandem with experiments, provides useful insights into reaction mechanisms and allows for cheaper and faster predictions of reactivity trends. Recently, we have reported an arene C—H alkylation by radical-radical cross-coupling, enabling rapid C(sp3)—C(sp2) bond formation from common alcohol and arene precursors. We have performed Density Functional Theory (DFT) calculations to determine the branching mechanistic pathways for this transformation and the origins of heteroselectivity of the cross-coupling. We have further developed a novel piecewise synthesis of vinyl bromides and alkenes from common ketone and alcohol starting materials. I will discuss these projects and some future proposals for synergistic experimental and computational approaches to various problems in organic synthesis.

Biography: Robert was born and raised in Silver Spring, Maryland. He earned his Ph.D. in Chemistry from the University of Maryland, College Park for his computational studies of transition metal-catalyzed and photocatalyzed organic transformations. He joined the MacMillan lab in August 2023 as an NSF MPS-Ascend Fellow to gain hands-on experience and perspective in the field of organic synthesis.

Refreshments will be provided at 3:45 pm in CDI 4.352

Join Meeting in-person at CDI 4.352