

JACQUELYNE READ

Research Assistant Professor of Chemistry
Department of Chemistry, Dartmouth College



Thursday, January 11th

10:30am - 11:30am

Steele 006

“Investigating Substituent Effects on Reactivity, Selectivity, and Noncovalent Interactions: Advancing Reaction Design through Data Science”

Abstract: Different functional groups can strongly influence the course of a given reaction in organic chemistry. This seminar will detail these effects in three main areas: additions of allylmagnesium halides to chiral carbonyl compounds, asymmetric catalysis driven by noncovalent interactions, and photocatalysis initiated by electron donor-acceptor complexes. First, the high reactivity and low diastereoselectivity of allyl Grignard reagents compared to other Grignard reagents in addition reactions to carbonyl compounds will be discussed. A solution to this synthetic challenge will be presented, and the impact for common stereochemical models will be discussed. In the second portion of the talk, the optimization of an enantioselective rearrangement reaction aided by computed noncovalent interaction energies will be discussed. Computational insights led to the design of a better-performing catalyst, and the library of interaction energies was expanded and developed as a diagnostic tool to identify noncovalent interactions in chemical systems. Lastly, the effect of different functional groups on the formation of organic charge-transfer complexes will be discussed, focusing on their ability to absorb visible light and initiate a radical cascade. A machine learning model capable of predicting the formation of these complexes based on computed properties will be presented, and the value of a combined experimental and computational approach to reaction design will be highlighted.