Abstract: Since the development of the first enantioselective organic reactions, chemists have proposed models to explain the origins of the selectivity and inform future developments. With the rise of computational chemistry and especially Density Functional Theory (DFT), it is now possible to identify the reaction intermediates and transition structures, and thus propose mechanisms, for all but the largest chemical systems. Such computations allow us to “look” at complex molecules, determine the factors that affect the reactivity or selectivity of reactions, develop models that support these observations, and predict how to improve on those systems. In this talk, our recent progress toward the development of general models of selectivity in asymmetric organocatalyzed reactions, involving phosphoric acid or phase-transfer catalysts, will be presented. We will demonstrate how the true origins of selectivity are not always obvious from traditional computations, and showcase how our new approach solves this issue.

Biographical Sketch: Pier Alexandre Champagne is an Assistant Professor of Organic Chemistry at the New Jersey Institute of Technology (NJIT). He obtained his Ph.D. in Organic Chemistry from the Université Laval (Québec, Canada) in 2015, with his experimental work on the reactivity of organofluorine compounds under the supervision of Prof. Jean-François Paquin. He then joined Ken Houk’s group at UCLA as a FRQNT postdoctoral fellow, where he focused on DFT investigations of organic reaction mechanisms, mostly focusing on cycloadditions and organocatalysis. After a stint in Michael Organ’s group at the University of Ottawa, he joined NJIT in 2019. His research interests are at the interface of experimental and computational organic chemistry, solving problems in the fields of enantioselective organocatalysis, organosulfur chemistry, and carbocation reactivity.