Learning to Fly in Chemical Reaction Space

TCI SEMINAR

Monday, October 13, 2014
3:00 p.m. Room 9341

Professor Paul Zimmerman
Department of Chemistry
University of Michigan

Research in the chemical sciences has long recognized the value of predicting reaction outcomes. Towards this goal, modern computational chemistry has often been used to characterize individual elementary chemical reaction steps. These techniques can be used to accurately evaluate hypothesized mechanisms for entire reaction sequences by linking together several elementary steps. The success of this procedure, however, is highly dependent on chemical intuition: quantum chemical methods typically only evaluate mechanisms that are previously hypothesized—the right mechanism to study must be determined by the chemist. In order to increase the predictive value of chemical simulation, research in the Zimmerman group has developed powerful new techniques to automatically characterize reaction mechanism. A full description of the methods as well as several applications, including catalytic reactions involving C-H functionalization, will be given in the presentation. Our group's future path of designing new chemical reactivity and catalysts will also be discussed.

Theoretical Chemistry Institute Seminar Series