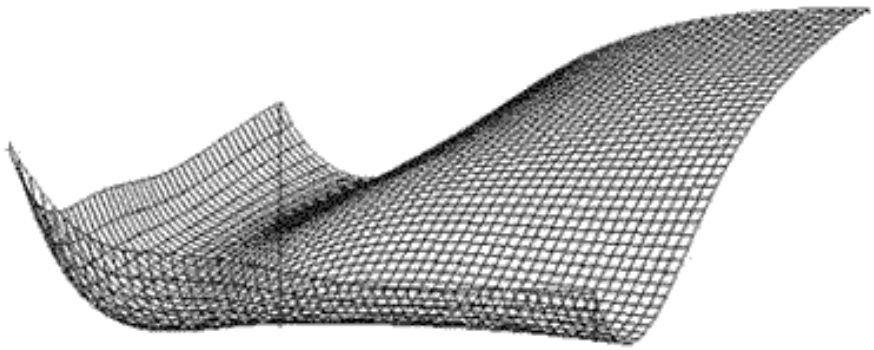
EASTERN MICHIGAN UNIVERSITY

Chemistry Department



Seminar

Prof. Paul Zimmerman, University of Michigan

Monday, Oct. 21st 4:00-5:00 pm Strong Hall 200

Automated Simulation Tools that Predict Chemical Reactivity

Abstract

Quantum chemical methods see widespread use in chemistry due to their ability to investigate a huge variety of molecular systems with high accuracy. These methods have the ability to characterize elementary reaction steps by evaluating equilibrium and kinetics without extensive prior knowledge of the system. Using these techniques, one can hypothesize mechanisms for entire reaction sequences and obtain accurate thermodynamic and kinetic descriptions. The success of this procedure, however, is highly dependent on chemical intuition: quantum chemical methods can only evaluate the energetics of the mechanism, but not the likelihood that the right mechanism was studied. In this presentation, I will show a new way to avoid this problem and automatically characterize reaction mechanisms. This technique starts with the reactants, generates many new structures that are one elementary step away, and then locates the reaction path connecting each pair. After kinetically and thermodynamically feasible elementary steps are found, the procedure is repeated until an entire reaction mechanism is completed. This technique avoids the requirement for significant amounts of chemical intuition as well as the expensive, error prone transition state searches that are notorious in quantum chemistry. The method is massively parallel, allowing full exploitation of modern computing clusters. A full description of the method as well as several examples in the fields of hydrogen storage, synthesis, and transition metal catalysis will be given in the presentation.