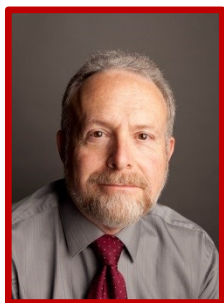


SPRING 2017 CHEMISTRY COLLOQUIA



February 10, 2017

3:00 Reception
548 Hamilton Hall

3:30 Seminar
112 Hamilton Hall

Open to the public

Professor Peter Rossky
Rice University

“Electronic Excited State Relaxation in Complex Systems: Two Stories of Harmony Between Theory and Experiment”

This presentation will focus on progress in our ability to understand, at the level of atoms and on the time scale of femtoseconds, the molecular rearrangements and time-dependent processes that occur following electronic excitation by light when these changes take place in liquid solutions or in unstructured solid materials, including those occurring in biological and synthetic polymeric materials. Computational models and experiment are increasingly able to simultaneously describe these processes, greatly enhancing the information that can be learned about chemistry from the combined theoretical and experimental analysis. In this presentation, two example cases will be discussed with focus on how time-dependent simulations of quantum phenomena can directly inform on mechanisms. The first case is one where both the complex system and electronic process are relatively “simple”: we study the electronic excited state relaxation of photoexcited anionic water clusters to understand the measured cluster size dependence of the ground state recovery rate and how those values come about. In the second, we study far more complex molecular systems based on a simple semiempirical electronic structure method. Analysis of the evolution of electronic excited states in representative conjugated molecular systems, particularly relevant to the function of plastic solar cells, will be discussed, including the processes underlying exciton migration and exciton dissociation, including the impact of interfacial structure and of extrinsic electric fields.

