Title: Nonequilibrium Charge and Energy Transfer in Chemistry

Abstract:

When a molecule changes shape or transfers an electron to one of its neighbours, thermal energy and electric charge flow. These processes are especially important when a molecular system is out-of-equilibrium. Consider the classic example of a photo-excited molecule -- after the light energy is absorbed the system must then find some way to “relax”. Describing these types of processes from a theoretical perspective requires the development and application of simulation methods that lie at the interface of statistical mechanics and quantum dynamics. Combining these areas is essential to accurately capture these fundamental chemical steps in many forefront problems ranging from solar energy conversion and chemical catalysis to biological sensing and signalling. Molecular simulations of this type can help uncover the underlying mechanisms that lie at the heart of many energy conversion problems, and the ultimate goal of my research program is to extend and apply these approaches to study nonequilibrium charge and energy transport. In this talk I will describe the efforts we are making to understand various aspects of laser driven chemical reactions, molecular electronics, and biological light-harvesting systems.