Simulations of Rare Events in Nonadiabatic Systems

Prof. Steven Corcelli
Department of Chemistry and Biochemistry

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Charge transfer processes, including electron transfer, proton transfer, and proton-coupled electron transfer, are ubiquitous and play a vital role in a broad range of chemical and biochemical phenomena. These processes generally involve a breakdown in the Born-Oppenheimer approximation, insomuch as they cannot be fully described by a single, adiabatic potential energy surface. Methods have been developed for the simulation of charge transfer events that involve multiple electronic and/or vibrational energy levels, but these approaches encounter difficulties when the barriers separating reactants and products are high compared to thermal energies (i.e. when the transitions are rare events). I will present new methodologies for simulating charge transfer process that are rare events. These new methods combine the surface hopping approach to nonadiabatic dynamics with transition path sampling that generates trajectories connecting reactants with products, even when the barriers are high.