TCI SEMINAR

A molecular interpretation of Marcus Theory from the Surface Hopping Perspective

Monday, May 6, 2013
3:00 p.m. Room 8335

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In this talk, I will discuss how nonadiabatic transitions and electronic relaxation occur in the context of surface-hopping dynamics for condensed phase systems, and I will discuss in detail when and how we should consider successive events to be correlated. I will then introduce a new way to consider the role of decoherence in condensed phase dynamics, and I will show that this decoherence time scale is crucial for understanding the fundamentals of Marcus theory. My target molecules here will be the Closs systems for energy transfer, where we can establish the absolute validity of Marcus theory. Finally, time permitting, I will discuss the intepretation of electronic momentum and the role of electronic currents in nonadiabatic events, quantities which are often ignored by the Born-Oppenheimer approximation. This talk will merge techniques from electronic structure theory and dynamics, two often separate fields whose intersection is becoming very fruitful for modern research in theoretical chemistry.

Theoretical Chemistry Institute Seminar Series