Constrained DFT for electron transfer and reaction barrier heights"

Abstract:
Electron transfer reactions are the centerpiece of artificial photosynthetic complexes, organic LEDs and essentially all of redox chemistry. This talk will highlight ongoing work being carried out in our group aimed at developing methods that can accurately simulate the reaction dynamics in these types of systems. Specifically, this talk will focus on the electronic structure problem inherent in describing electron transfer: How can we treat charge transfer states on the same footing with the electronic ground state? How do we make connections between a phenomenological picture like Marcus theory and a more rigorous approach like DFT? How do we describe bond formation (in particular proton transfer) that is often intimately connected with the process of electron transfer? Time permitting, we will mention some applications of these methods to organic light emission, photoinduced dynamics and/or redox catalysis.