Simulating Electron Transfer in Biomolecules: the Role of Polarization and Long-range Electrostatic Interactions

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Photo-induced electron transfer is ubiquitous in biological processes, including photosynthesis and respiration. Interestingly, it has been recently shown that magnetosensing by Drosophila flies and possibly by other animals is mediated by flavoproteins cryptochromes, undergoing photoactivation via a series of photo-induced electron transfer events. In this talk, the challenges theoretical chemistry faces when one wants to describe energetics and dynamics of electron transfer in complex heterogeneous media, as proteins, will be discussed. Specifically, the role of environment polarization and long-range electrostatic interactions in accurate evaluation of such quantities as redox potentials, charge-transfer states excitation energies, and electronic couplings, using a cryptochrome protein as a model system, will be addressed. A new software for identifying electron transfer pathways in proteins, eMap, will be introduced.