Theory and simulation of electron transfer in proteins

Dmitry Matyushov
Department of Physics and School of Molecular Sciences
Arizona State University

Electron transport across cellular membrane is a basic component of physiological energy production. The activation barrier for electron tunneling between electron-transfer cofactors largely depends on the spectrum of electrostatic fluctuations produced by the protein-water interface at the protein's active site. The protein-water dynamics are heterogeneous both dynamically and statistically. The following questions are relevant here: (i) Does the interfacial biological water produce electrostatic signatures specific to proteins? (ii) What is the spectrum of interfacial electrostatic fluctuations? (iii) How the protein-mediated chemistry is affected by electrostatics? These questions connect the spectrum of interfacial fluctuations to the issue of whether thermodynamics or dynamics drive biology's performance. Ergodicity is often broken in protein-driven reactions and thermodynamic free energies become irrelevant. The theoretical description of electron transport requires building predictive theoretical algorithms combining the input from atomistic simulations with formal models to predict the kinetics. The resulting activation barrier is affected by both the broad spectrum of fluctuations and the dispersive, multi-scale dynamics of the protein-water interface.