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Theory of Electron Transfer and Transport Pathways in Biomolecules

DAVID BERATAN, Duke University

Electron transfer in proteins and nucleic acids occurs over large distances by a combination of short and long range tunneling mechanisms. Electron tunneling is facilitated by virtual oxidized and reduced states of the bridging macromolecule, and theoretical analysis reveals how a macromolecule's fold, energetics, and fluctuations influence the electron-transfer kinetics. Recent studies of protein electron transfer indicate when and why electron tunneling kinetics is sensitive to the structure of the protein's tunneling pathways. Electron transfer across protein-protein interfaces involves thin structured water layers that play a key role in tunneling mediation as well. Tunneling analysis that takes the dynamical fluctuations of the macromolecules into explicit account provides a unified view that links structure and function in protein electron transfer. In the case of DNA electron transport, a critical role is found for structural fluctuations and transport mediated by carrier injection to intervening bases, even at very short distances.