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How does thermal motion of atoms influence rates of bridge-mediated electron transfer reactions? 1. Dynamical modulation of the effective tunneling coupling. ILYA BALABIN, Duke University, SPYROS SKOURTIS, University of Cyprus, TSUTOMU KAWATSU, DAVID BERATAN, Duke University — Understanding how thermal nuclear motion affects the electron transfer (ET) reaction rates is essential for describing a broad range of vital biological redox reactions as well as designing molecular electronic devices. Theoretical studies of biological ET reaction rates usually assume a) the superexchange ET regime (virtual bridge electronic states), and b) the Franck-Condon approximation (electronic dephasing slower than the time-dependent Franck-Condon factor decay time). We present the first investigation of the electronic dephasing effects and the first quantitative analysis of the modulation of effective tunneling coupling by nuclear dynamics. Molecular dynamics simulations coupled with extended Huckel-level quantum chemical calculations of the effective electronic coupling were performed for the blue copper ET protein azurin. We discuss effects of the donor-to-acceptor distance, tunneling pathway structure, tunneling energy, temperature, and protein motion on the dynamics of the effective tunneling coupling and the ET reaction rate.

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