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Talk Invited Invited Talk

A nonlinear dynamical model for electron transfer

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A theory for electron transfer (ET), particularly relevant to ultrafast processes, is presented [1]. Our model explicitly includes interactions of electronic states with vibrational degrees of freedom. When the energy barrier for ET is small, at the inversion point, electronic frequencies are of the order of vibrational frequencies and electron tunelling is nonadiabatic. The effective electron dynamics becomes nonlinear and energy is dissipated through the phonon bath. While recovering standard theories far from the inversion point, our formalism also captures the main features of fast ETs, when such processes cannot be simply described as thermally activated. ETs in well studied biosystems are discussed, such as photosynthetic reaction centers, where experimental observations can be explained by our approach [2]. As a result of fine tuning between a donor and an extra molecule that acts as a catalyst (coherent electron-phonon oscillator), fast and efficient long distance ET to an acceptor (which is separated from the donor by a large energy barrier) becomes possible.

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[1] S. Aubry and G. Kopidakis, "A Nonlinear Dynamical Model for Ultrafast Catalytic Transfer of Electrons at Zero Temperature", *Int. J. Mod. Phys. B*, **17**, 3908 (2003).

[2] S. Aubry and G. Kopidakis, "A Nonadiabatic Theory for Ultrafast Catalytic Electron Transfer, A Model for the Photosynthetic Reaction Center", *Journal of Biological Physics*, **31**, 375 (2005).