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A nonadiabatic and nonlinear theory for electron transfer

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We propose a general theory both non adiabatic and nonlinear which extends those used for the standard theory of electron transfer (ET) in chemistry but also becomes equivalent to it far from the inversion point. In the vicinity of the inversion point, the model parameters may be finely tuned such that large amplitude electronic oscillations between the donor and an extrasite, associated with large amplitude and collective phonon oscillations at the same frequency, are spontaneously generated (coherent electronphonon oscillator or CEPO). This extrasite is not a true acceptor but could play the role of a catalyst because by the CEPO it may trigger irreversible and ultrafast ET at low temperature toward a third site which is a real acceptor (while in the absence of catalyst, ET cannot occur). Such a trimer system may be regulated by small perturbations and behaves as a molecular transistor. We illustrate this idea by explicit numerical simulations on trimer models of the type donor-catalyst-acceptor. We discuss the relevance of our approach for understanding the ultrafast electron transfer experimentally observed in biosystems such as the photosynthetic reaction center.