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Theories and applications for characterizing electronic coupling factors

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The transport of charges and excitation energy are two processes of fundamental importance in many biological and material systems. One of the fundamental parameters in the transport rates is the electronic coupling, which is essentially an off-diagonal Hamiltonian matrix element between the initial and final diabatic states. We have developed ways to define the diabatic states and calculate the coupling factors, including those for electron transfer (ET) and excitation energy transfer (EET). The fundamental method development and applications will be discussed. For characterizing TEET, the Fragment Spin Difference (FSD) was developed and it can be to calculate the TEET coupling over a general class of systems. TEET in bacterial light-harvesting complex LH2 and the peridinin chlorophyll-a protein (PCP) of dinoflagellates were calculated and analyzed. Our results are in good agreement with experimental results and it offers limits to the photoprotection models. Therefore, with the FSD scheme, it is possible to quantify and analyze the electronic couplings in TEET processes in large systems, and to derive insights and limits of theoretical models.