**Theories and applications for electronic coupling in electronic transfer and excitation energy transfer**

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The transport of charges and excitation energy are two processes of fundamental importance in diverse areas of research. Characterizations of electron transfer (ET) and excitation energy transfer rates are essential for a full understanding of many biological systems and opto-electronic devices. The electronic coupling factor is an off-diagonal Hamiltonian matrix element between the initial and final diabatic states in the transport processes. ET coupling is essentially the interaction of the two molecular orbitals (MOs) where the electron occupancy is changed. Singlet energy transfer (SET) contains a Förster dipole–dipole coupling term as its most important constituent. Triplet energy transfer (TET) involves an exchange of two electrons of different spin and energy; thus, it is like an overlap interaction of two pairs of MOs.

In the past, we have developed or improved the strategies for calculating ET, SET, and TET couplings. In the presentation, I plan to report (1) the theory and development in the characterization of SET coupling with application examples. The fragment excitation difference (FED) is developed to calculate SET coupling, which yields the overall coupling under the Hamiltonian employed, including the through-bond, exchange and orbital overlap effects. With FED and a precise account of the Coulomb coupling, the exchange and overlap effects on SET can be studied. And, (2) our recent progresses in the charge transport properties in tris(8-hydroxyquinolinato)aluminum(III) (AlQ3). With intermolecular configurations derived from crystal structures, we found that most of the commonly seen configurations with $\pi$ -$\pi$ interaction are further stabilized with CH-$\pi$ interactions involving other ligands on AlQ3. The CH-$\pi$ interaction drives the structure of the AlQ3 pair towards a large lowest unoccupied molecular orbital (LUMO) overlap, and a small overlap in the highest occupied molecular orbital (HOMO), accounting for the preference in electron transport. This result provides an insight for the charge transport properties for AlQ3 from the structural perspectives, which is important for designing new materials with desirable charge transfer property.