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Towards Effective Fragment-Based Approach to Computation of Excitation Energy Transfer Couplings

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Excitation energy transfer (EET) phenomenon is responsible for the non-radiative energy transfer between electronically coupled chromophores and its importance for functioning of light harvesting complexes is hard to be overstated.[1] However, the fast and accurate calculation of the EET coupling constants, which govern the energy transfer rates, is still not fully resolved issue.

In this contribution, we present the novel potential fragment-based approach to model EET coupling constants which is based on distributed parameters derived from *ab initio* calculations for isolated molecules. Recently, we developed the distributed multipole model (TrCamm) that can be obtained directly from the transition density matrices of isolated monomers.[2] This model is shown to be superior to the other widely used approximate schemes based on the point dipole approximation (PDA), the distributed transition charges from fitting to transition potential (TrESP) or the transition density cubes (TDC). In the new model we also study the induction, exchange-overlap and charge-hole transfer effects from the perspective of the fragment-based methodology [3]. Also, the polarization effects due to the surrounding medium are treated explicitly in terms of the distributed dipole-dipole polarizabilities.

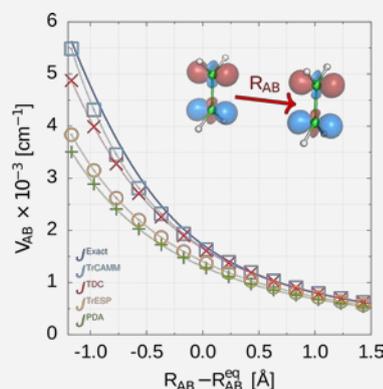


Figure 1. Coulombic part of EET coupling constants of ethylene dimers modelled by various approaches.

[1] C. Curutchet and B. Mennucci, *Chem. Rev.*, **2016**.

[2] B. Błasiak, M. Maj, M. Cho and R. W. Góra, *J. Chem. Theory Comput.* **2015**, *11*, 3259.

[3] B. Błasiak and M. Cho, *J. Chem. Phys.* **2014**, *140*, 164107.