Exciton coupling and energy transfer: From prototypical bichromophores to photosynthetic proteins

Lyudmila V. Slipchenko[1]
[1]*Department of Chemistry, Purdue University, West Lafayette, IN 47907, US*

We investigate exciton coupling in several prototypical bichromophores, such as benzene dimer, diphenylmethane (DPM), and chlorophyll dimers, as well as in photosynthetic proteins such as the Fenna-Matthews-Olson (FMO) complex. Accurate description of interactions between the electronic states is challenging for theory. For instance, in flexible diphenylmethane, a small splitting between the exciton states and a sensitivity of the transition dipole moment to the relative orientation of the aromatic rings leads to curious shapes and crossings of the potential energy surfaces of the exciton states. Exciton couplings are evaluated by using a perturbative approach, in which the coupling strength is estimated by using transition densities of the individual chromophores. By using the effective fragment potential (EFP) and fragment molecular orbital (FMO) methods, we explicitly include and characterize the effect of the protein environment on interactions between the electronic states of chromophores in photosynthetic complexes.