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Vibronic interactions in multi-chromophores

LYUDMILA SLIPCHENKO, Purdue University

Understanding and control of excitation energy transfer and electron-phonon interactions is quintessential for advances in solar energy utilization. Recently, we developed a vibronic model that is capable of predicting vibronic spectra in complex multi-chromophore systems. Parameters to the model are obtained from electronic structure calculations on monomer units of a multi-chromophore. This model can account for multiple vibrational modes, asymmetric wave functions, and inter-chromophore vibrations. Using this model, we explored vibronic spectra in a series of flexible bichromophores with available high-resolution experimental spectra. One of the goals of this work was to understand the effects of asymmetry in monomer units on vibronic interactions in bichromophores. Detailed investigation of diphenylmethane, partially deuterated diphenylmethane, and diphenylethane resulted in intriguing observation that asymmetry leads to a partial localization of one of the exciton states but leaves the other one delocalized. Extension of the developed methodology to modeling spectroscopy and dynamics in synthetic and biological multi-chromophore systems such as photosynthetic proteins will be also discussed.