

Triplet Energy Transfer in Molecules and Materials

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Energy transfer is an extremely important step in solar energy conversion. In order to efficiently harness absorbed light, we must guide the energy both spatially and energetically toward desired products. In this talk we will summarize some of our recent work on triplet energy transfer and the important processes of triplet fusion and singlet fission. Beginning with a diabatic picture of energy transfer, we will outline how localized, physically relevant reactant and product states can be generated using constrained DFT. These diabatic states then form the basis for both adiabatic and non-adiabatic descriptions of energy transfer, fission and fusion. Time permitting, we will illustrate some of the applications of these techniques to organic semiconductors and quantum dots.