Understanding exciton dynamics and photogeneration in molecular semiconductors

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ABSTRACT

Organic electronics is a rapidly growing field of research with an immense potential for energy related applications. In this presentation, I will highlight fundamental physical phenomena and electronic processes unique to these materials and address recent developments in understanding the role of disorder on the electronic and transport properties of molecular semiconductors. I will firstly lay emphasis on the phenomenon of exciton diffusion, which is found to play a role in a remarkably wide range of physical systems, including disordered organic semiconductors, nanocrystalline quantum dots, semiconducting carbon nanotubes and photosynthetic biological systems. One of the key issues in all these systems is the temporal and spatial evolution of exciton transport, responsible for the particular functionality. I will present a temperature dependent theory for singlet exciton hopping transport in disordered semiconductors and test the validity range using kinetic Monte Carlo simulations. The developed model describes in a unified manner the transition from equilibrium to non-equilibrium transport regime and provides a powerful tool for interpreting time-resolved and steady state spectroscopy experiments. In the second part, I will focus on the problem of charge separation in donor-acceptor organic solar cells. Several mechanisms have been suggested to influence charge generation and many contradicting experimental and theoretical reports have appeared over the last decade. By combining spectroscopy and photocurrent experiments with analytical and Monte Carlo simulations, we illustrate how interfacial energetics and transport topology reduce the activation energy required to separate the interfacial electron-hole pair.