Coherent Real-space Charge Transport Across a DonorAcceptor Interface Mediated by Vibrionic Couplings

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Abstract

There is growing experimental and theoretical evidence that vibronic couplings (the interactions between electronic and nuclear degrees of freedom) play a fundamental role for ultrafast excited state dynamics in organic donor–acceptor hybrids. While vibronic coupling has been shown to support charge separation at donor–acceptor interfaces, so far little it is known about its role for the real-space transport of charges in such systems. In my talk, I will present a theoretical study of charge transport in thiophene:fullerene stacks by means of open-system time-dependent density functional tight-binding in combination with Ehrenfest molecular dynamic simulations. Our results support earlier experimental observations by Friend et al. [1] of long-range ballistic charge carrier motion in organic photovoltaic systems and highlights the importance of vibronic coupling engineering as a concept for improving the functionality of hybrid organic devices.

[1] S. Gélinas, A. Rao, A. Kumar, S. L. Smith, A. W. Chin, J. Clark, T. S. van der Poll, G. C. Bazan, and R. H. Friend, *Ultrafast long-range charge separation in organic semiconductor photovoltaic diodes* Science 2014, 343, 512516.