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QE

Quantum Efficiency Seminar und Colloquium

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Elementary processes of organic photovoltaics - What do we learn from a molecular-level perspective?

This talk summarizes our recent molecular-level, quantum dynamical studies of photoinduced exciton transport and exciton dissociation in functional organic polymer materials. As highlighted by recent experiments [1], these processes can be guided by quantum coherence, despite the presence of electron-phonon coupling and static and dynamic disorder. Our approach combines parametrized Hamiltonians, based on electronic structure calculations, with accurate quantum dynamics simulations using the multiconfiguration time-dependent Hartree (MCTDH) method [2]. We will specifically address (i) the dynamics of exciton transfer across a torsional defect that locally breaks the pi-conjugation in an oligo-(p-phenylene vinylene) type fragment [3], and (ii) exciton dissociation in oligothiophene-fullerene complexes [4], i.e., models for P3HT-PCBM heterojunctions, and in novel ordered donor-acceptor assemblies [5]. A unifying theoretical framework is provided by a vibronic coupling Hamiltonian in a monomer-based electron-hole representation [3] that accounts for the intrinsic coherence size of the relevant excitonic states - beyond the standard Frenkel exciton picture - and at the same time accommodates the creation of charge transfer excitons at heterointerfaces. Using these methods, a perspective will be given on the possible role of hot charge transfer excitons in the photocurrent generation.

[1] E. Collini and G. D. Scholes, Science, 323, 369 (2009), C. A. Rozzi et al., Nat. Comm., 4, 1602 (2013).

[2] M. H. Beck, A. Jaeckle, G. A. Worth, and H.-D. Meyer, Phys. Rep. 324, 1 (2000), G. A. Worth, H.-D. Meyer, H. Koeppel, L. S. Cederbaum, and I. Burghardt, Int. Rev. Phys. Chem., 27, 569 (2008).

[3] R. Binder, J. Wahl, S. Römer and I. Burghardt, Faraday Discuss., DOI: 10.1039/C3FD20148A , in press (2013), A. N. Panda, F. Plasser, A. Aquino, I. Burghardt, and H. Lischka, J. Phys. Chem. A, 117, 2181 (2013).

[4] H. Tamura, R. Martinazzo, M. Ruckenbauer, and I. Burghardt, J. Chem. Phys., 137, 22A540 (2012); H. Tamura, I. Burghardt, and M. Tsukada, J. Phys. Chem. C, 115, 9237 (2011).

[5] T. Roland et al., Phys. Chem. Chem. Phys., 14, 273 (2012), J. Wenzel, A. Dreuw, and I. Burghardt, Phys. Chem. Chem. Phys., in press (2013).

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