HL 110: Invited Talk Irene Burghardt

Time: Friday 9:30–10:00 Location: POT 051

Invited Talk HL 110.1 Fri 9:30 POT 051

Quantum dynamics of exciton migration and dissociation in functional organic polymer materials — •Irene Burghardt — Institut f. Physik. u. Theor. Chemie, Goethe Universität Frankfurt

As highlighted by recent experiments, elementary processes in organic photovoltaics can be guided by quantum coherence, despite the presence of electron-phonon coupling and static and dynamic disorder. We present quantum dynamical studies of these processes using the Multi-Configuration Time-Dependent Hartree (MCTDH) method, focusing on (i) the dynamics of exciton migration across a torsional defect that locally breaks the π-conjugation in oligo-(p-phenylene vinylene) type fragments [1], and (ii) exciton dissociation in oligothiophene-fullerene donor-acceptor complexes [2,3], i.e., models of P3HT-PCBM heterojunctions. Here, the primary exciton break-up is found to occur within 50-100 fs and exhibits a pronounced oscillatory decay profile, reflecting vibronic coherence [2]. Furthermore, rapid free carrier generation from the interfacial charge transfer (CT) state is feasible, due to an effective lowering of the Coulomb barrier as a result of charge delocalization, along with the vibronically hot nature of the primary CT state [3].

[1] R. Binder, J. Wahl, S. Römer, I. Burghardt, Faraday Discuss. 163, 205 (2013), A. N. Panda, F. Plasser, A. Aquino, I. Burghardt, H. Lischka, J. Phys. Chem. A, 117, 2181 (2013) [2] H. Tamura, R. Martinazzo, M. Ruckenbauer, I. Burghardt, J. Chem. Phys., 137, 22A540 (2012); H. Tamura, I. Burghardt, M. Tsukada, J. Phys.Chem. C, 115, 9237 (2011) [3] H. Tamura, I. Burghardt, J. Phys. Chem. C, 117, 15020 (2013), J. Am. Chem. Soc. (Comm.), 135, 16364 (2013).