On the study of coupled electronic and nuclear dynamics in photoinduced charge separation

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Early stages of photoinduced charge separation in several photovoltaic materials were studied by combining TDDFT simulations of the quantum dynamics, high time resolution femtosecond spectroscopy, and ultrafast electron diffraction. The role of coherent coupling between electronic and nuclear degrees of freedom is shown to be of key importance in triggering charge delocalization and transfer both in covalently bonded molecules[1] and in non-bonded bulk heterojunctions[2]. The possible exploitation of our findings in order to design and synthesize novel molecular scaffolds[3] for photovoltaic applications is discussed. Further work in progress on ultrafast photoexcitation of polymer-copolymer aggregates and perovskites is presented.

[1] C. A. Rozzi et al., Nat. Comm 4, 1602 (2013)
[2] S. Falke et al., Science 344, 1001 (2014)
[3] S. Pittalis et al., Adv. Func. Mat. (2014)