Intermolecular charge transfer through a conical intersection in organic photovoltaics

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Abstract

The understanding of nonadiabatic dynamics through a conical intersection (CoIn) in donor–acceptor materials is of fundamental importance, since it significantly affects their efficiency in applications such as organic solar cells. So far, however, clear experimental evidence of a conical intersection is challenging to obtain and often just as difficult to interpret.

In this seminar I will present a joint experimental and theoretical study of intermolecular charge transfer through a CoIn in oligomer aggregates, where I will focus on the theoretical modeling of the underlying dynamics. For this purpose, we performed nonadiabatic excited-state molecular dynamics simulations [1] on an oligomer dimer. Our results reveal a complex interplay of symmetry arguments, vibronic couplings and molecular distortions induced by thermal fluctuations.

[1] Nelson, T., Fernandez-Aberti, S., Chernyak, V., Roitberg, A. E. and Tretiak, S. *Nonadiabatic excited-state molecular dynamics modeling of photoinduced dynamics in conjugated molecules.* J. Phys. Chem. B 115, 5402–5414 (2011).