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Early charge separation events in light-harvesting materials

The photoinduced charge-separation events occurring in photovoltaic and light harvesting systems have traditionally been interpreted in terms of the incoherent kinetics of optical excitations and of charge hopping. Although signatures of quantum coherence were recently observed in energy transfer in photosynthetic bacteria and algae[1] still very little is known about the role of quantum coherence at room temperature in technologically relevant organic photovoltaic materials. Recent experiments found evidence for an ultrafast long-range charge separation in such systems but could not differentiate between coherent and incoherent charge-transfer models.[2] By combining TDDFT simulations of the quantum dynamics and high time resolution femtosecond spectroscopy, we provide evidence that the coherent coupling between electronic and nuclear degrees of freedom is of key importance in triggering charge delocalization and transfer both in covalently bonded molecules[2] and in non-bonded bulk heterojunctions[3]. We have exploited the results of our research to design, synthesize and characterize a novel molecular scaffold for photovoltaic applications.[4]


Host: Angel Rubio