Ultrafast dynamics in light-harvesting and photovoltaics: a theoretical and experimental investigation

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It is known that the primary steps of photoinduced energy and charge transfer may occur on extremely fast time scales in many natural and man-made compounds that perform conversion of sunlight into chemical or electrical energy. These processes have traditionally been interpreted in terms of the incoherent kinetics of optical excitations and of charge hopping, but recently signatures of quantum coherence were observed in energy transfer in photosynthetic bacteria and algae [1,2]. We have studied the early steps of photoinduced charge separation in reference systems for artificial photosynthesis and photovoltaics by combining Time-dependent Density Functional Theory simulations of the quantum dynamics and high time resolution femtosecond spectroscopy. Our results show that the coherent coupling between electronic and nuclear degrees of freedom is of key importance for charge delocalization and transfer in both of covalently and non-covalently bonded systems [3,4]. We have exploited the results of our research to design, synthesize and characterize a novel molecular scaffold for photovoltaic applications [5].