Charge transfer and quantum coherence in solar cells and artificial light harvesting system

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In artificial light harvesting systems the conversion of light into electrical or chemical energy happens on the femtosecond time scale, and is thought to involve the incoherent jump of an electron from the optical absorber to an electron acceptor. Here we investigate the primary dynamics of the photoinduced electronic charge transfer process in two prototypical structures: (i) a carotene-porphyrin-fullerene triad, a prototypical elementary component for an artificial light harvesting system and (ii) a polymer:fullerene blend as a model system for an organic solar cell. Our approach [1] combines coherent femtosecond spectroscopy and first-principles quantum dynamics simulations. Our experimental and theoretical results provide strong evidence that the driving mechanism of the primary step within the current generation cycle is a quantum-correlated wavelike motion of electrons and nuclei on a timescale of few tens of femtoseconds. We furthermore highlight the fundamental role played by the flexible interface between the light-absorbing chromophore and the charge acceptor in triggering the coherent wavelike electron-hole splitting.