

Abstract Title : Ultrafast charge generation in a photoexcited polymer-fullerene blend: insights from real-time TDDFT

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Abstract :

The initial quantum dynamics leading to electron transfer from the photoexcited polymer to the fullerene in P3HT-PCBM is investigated ab-initio by time-dependent density functional theory simulations. We find coherent electron transfer between donor and acceptor and oscillations of the transferred charge with a period matching that of observed vibrational modes in ultrafast optical spectroscopy [1]. Our results show that the coherent coupling between electronic and nuclear degrees of freedom is of key importance in triggering charge delocalization and transfer not only in covalently bonded molecules [2] but also in this prototype non-covalently bonded system of relevance for photovoltaics.

[1] SM Falke, CA Rozzi, D Brida, M Amato, A De Sio, A Rubio, G Cerullo, E Molinari, and C Lienau, submitted.

[2] CA Rozzi, SM Falke, N Spallanzani, A Rubio, E Molinari, D Brida, M Maiuri, G Cerullo, H Schramm, J Christoffers, C Lienau, Quantum coherence controls the charge separation in a prototypical artificial light-harvesting system, Nat Commun 4, 1602 (2013).

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