

Partial Charge Transfer States in Fullerene Dye-Sensitized Solar Cells

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In this talk, an analysis of electronically excited states in a triphenylamine – fullerene C₆₀ conjugate (TPA-C₆₀) will be discussed.[1] We present the description of excitonic and charge transfer states that can be accessed in TPA-C₆₀. The main issue to discuss is the role of those states with partial excitonic and charge transfer character (hybrid states). In this regard, hybrid states have been reported to promote charge separation at the donor-acceptor interface.[2] This could have a direct impact in the design of high-efficient dye-sensitized solar cells as materials may be engineered such that their excitations lead to a small number of hybrid states, thus avoiding a premature charge recombination.



1. Martínez J.P., Osuna S., Solà M., Voityuk A. Extent of charge separation and exciton delocalization for electronically excited states in a triphenylamine C₆₀ donor-acceptor conjugate: a combined molecular dynamics and TD-DFT study. *Theor. Chem. Acc.* **2014** (Submitted)
2. Few S., Frost J.M., Kirkpatrick J., Nelson J. Influence of Chemical Structure on the Charge Transfer State Spectrum of a Polymer:Fullerene Complex. *J. Phys. Chem. C* **2014**, 118, 8253-8261