

Charge Transfer States in Bulk Heterojunction Organic Solar Cells

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Organic solar cells (OSCs), unlike inorganic ones, lead to an exciton or strongly bound electron-hole pair after absorption of a photon. The generation of free charges then depends on the exciton binding energy and the absorption properties of the materials used [1]. In the modelling of more efficient OSCs, we have combined a conjugated polymer with a fullerene derivative in bulk heterojunction architectures (see Figure 1). In such architectures, the excitons formed on the absorber polymer are separated through electron transfer process that lead to Charge Transfer (CT) states at the interface of the polymer and fullerene based molecule. We have computed the CT energies in bulk heterojunctions by using Density Functional Theory and its Time Dependent extension, coupled with the Discrete Reaction Field method as implemented in the Amsterdam Density Functional modeling suite [2]. Our preliminary results suggest that organic-photovoltaic blends should perform better when polarizable groups as triethylene glycol chains (TEG) are added to the backbone. Furthermore, our results indicate that the environment stabilizes the charge separation process.

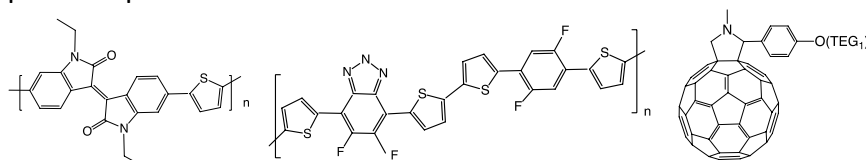


Figure 1. Molecular structure of potential photovoltaic materials used in the modeling of charge transfer and charge separated states. Left, electron-rich type conjugated polymers; (a) polyisindigothiophene (P1TI), (b) polythiophenefluorobenzene (PTFB). Right, acceptor C60 based molecule (PTEG1).

References

[1] L. J. Koster, S. E. Shaheen, J.C. Hummelen, *Adv. Ener. Mat.* 2, 10 (2012), 1246-1253.

[2] "https://www.scm.com".