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Band alignment optimization of bulk rrP3HT/C_{60} heterojunction

ARNAUD MAILLARD, ALAIN ROCHEFORT, Ecole Polytechnique de Montreal, Engineering Physics Department — Organic solar cells could overcome the cost limitation of traditional solar cells by using large-scale fabrication techniques associated with polymers. However, a better understanding of the bulk heterojunctions (BHJs) electronic properties used in these devices is required to reach an efficiency of 10%. DFT and GW computations were used to study BHJs formed by the inclusion of C_{60} in a regioregular poly(3- hexylthiophene) polymer (rrP3HT) crystal. An increasing packing density in the BHJ extent the energy separation between the C_{60}-LUMO and the rrP3HT-HOMO, which is proportional to the open circuit voltage of the device (Voc). This trend is consistent with the induced dipole moment variation observed at a pentacene- C_{60} junction upon reduction of the intermolecular distance [1]. In contrast, an increasing size of rrP3HT crystal domain leads to decrease both Voc and rrP3HT bandgap, in a similar fashion than upon the formation of rrP3HT crystallite along the annealing of BHJs [2].

[1] M. Linares, et al., J. Phys. Chem. C, 114 (2010), 3215.
[2] G. Dennler, et al., Adv. Mater., 21 (2009), 1323.

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