Maximum Open-Circuit Voltage of Ideal Graphene/P3HT Organic Photovoltaic Interfaces

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The use of graphene as an acceptor material represents a recent and compelling alternative to fullerene derivatives and CNTs in bulk heterojunction OPV devices [1]. Despite excellent progress, however, device efficiencies remain low (~1.1 %) for cells made with solution-processable functionalized graphene (SPFGraphene) [1] and several important questions remain unanswered . Here, using a first principles approach combining DFT with hybrid functionals [2], we address the questions of the maximum achievable open-circuit voltage (Voc) and the effects of oxygen functional groups on the Voc. We analyze the atomic structure and energetics of model graphene/P3HT interfaces of over 700 atoms (see Figure 1), and determine a maximum ideal Voc of ~0.7-0.9 eV, in excellent agreement with reduced (annealed) SPFGraphene/P3HT devices [3]. In good agreement with the corresponding non-annealed devices [3], we also find that the presence of the functional groups can raise the Voc of the interface by several tenths of an eV. This effect is likely due to a distortion of the polymer layer, which results in a lowering of its HOMO level, and a simultaneous rise in the energy of the highest occupied graphene state.

This work was supported by the EU FP7/ERC grant no. 239578 and the EU FP7/grant no. 604391 Graphene Flagship.

References

[1] X. Wan, et al., Adv. Mater., **23** (2011) 5342.
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[3] Q. Liu, et al., Adv. Funct. Mater., **19** (2009) 894.

Figures

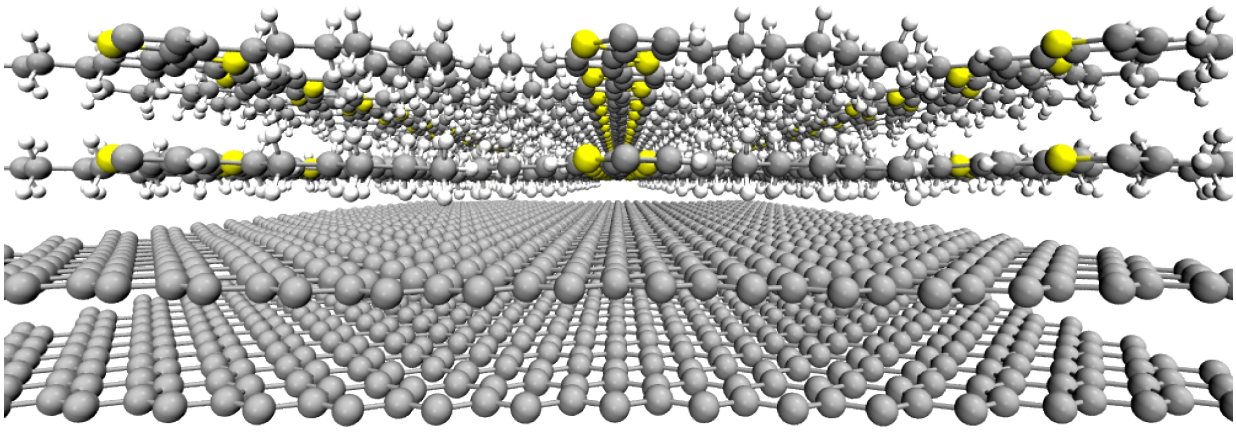

Figure 1: Model graphene/P3HT interface