Simulation of organic solar cell with graphene transparent electrode

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ABSTRACT

We present a simulation study of the performance of organic solar cell (OSC) exploiting graphene as transparent electrode. The approach is based on a multi-scale/multi-physics simulation framework, which is able to provide relevant information regarding the design guidelines of efficient OSC.

INTRODUCTION

Organic solar cells (OSCs) hold promise as next-generation devices for energy conversion, due to their low cost, the large area and their flexibility. Exploiting graphene as transparent electrode in OSCs could represent the killer application of graphene technology [1] because of *i)* its transparency in the whole visible spectrum, *ii)* its flexibility and *iii)* its large conductivity.

In this work, through a multi-scale approach, we will provide design guidelines, assessing the technological issues, which mostly affect device performance, as for example, the quality of graphene and the electrode work-function (WF). Our multi-scale investigation exploits ab-initio calculations to evaluate work-function tuning of graphene contact by means of doping through the deposition of different MoO_3 layers, electromagnetic simulations for light management when pattering the graphene electrode, and device modeling for computing the electrical characteristics of the cell and its main figures of merit.

MODEL

The WF of Graphene on MoO3 has been computed with ab-initio simulations exploiting Quantum ESPRESSO [2], while light-management of patterned electrode has been addressed with COMSOL [3] package. The *I–V* characteristics have been calculated with NanoTCAD ViDES [4], solving self-consistently the electrostatic, the continuity and the exciton diffusion equations [5].

RESULTS

In Fig. 1, the simulated OSC with graphene electrode is shown. In Fig. 2, we show the WF computed with DFT for different MoO_3 thicknesses, and two different geometries of the oxide: oxigen- and Mo-terminated MoO3. On the same picture, we show experimental results, showing good agreement with simulation results. We have then computed the *I–V* characteristics of OSCs with P3HT, PTB7 and Perovskite active layer. In Fig. 3, we show the Fill Factor (FF) and the energy efficiency for the Perovskite case. It is apparent that OSCs are extremely sensitive to the series resistance per unit cell area. WF tuning improves both the fill factor and the efficiency.

CONCLUDING REMARKS

In Fig. 4 we show the efficiency of cells with different HTL materials and the efficiency improvement provided by each cell engineering option, as obtained by our multi scale simulation approach. As can be seen, low contact resistance, work function tuning, and grating can jointly provide a boost in power conversion efficiency. We remark that graphene quality is a serious issue, since a very low defect density is required for an acceptable sheet resistance.

ACKNOWLEDGMENT

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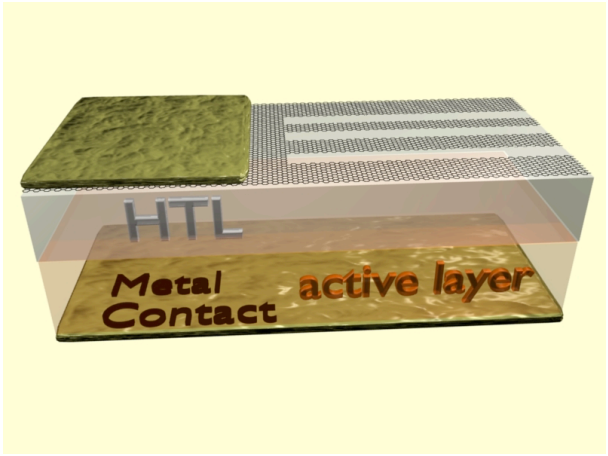

Fig. 1. Sketch of the simulated OSC. When light illuminates the OSC, excitons are generated in the active layer, and then separate at the interface between the active layer and the Hole Transporting layer (HTL). Holes are then collected at the transparent electrode, travelling through the hole-transporting layer (HTL), while electrons are collected at the metal contact.

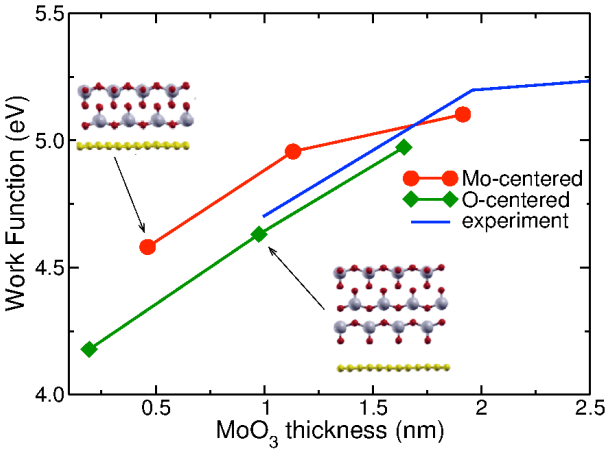

Fig. 2. WF as a function of the MoO_3 layer thickness for both oxygen-terminated MoO_3 top surfaces and Mo-terminated surfaces. The blue solid line represents experiments from [S.W. Tong et al., Adv. Func. Mat. Vol. 21, p. 4430, 2011].

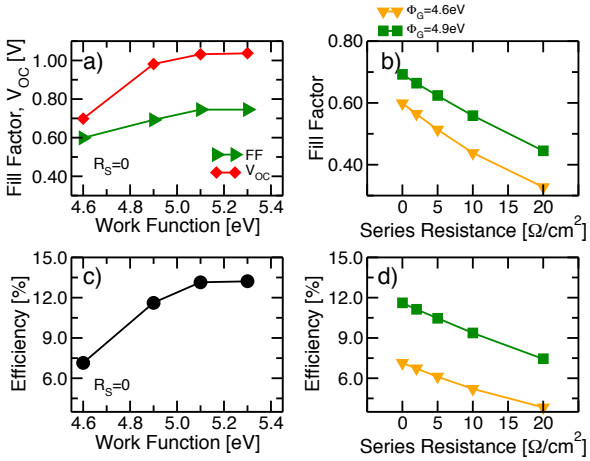

Fig. 3. Simulated results for a) FF, VOC and c) PCE considering different WF for the graphene electrode for the Perovskite-based OSC. Both FF [b)] and PCE [d)] degrade with increasing series resistance.

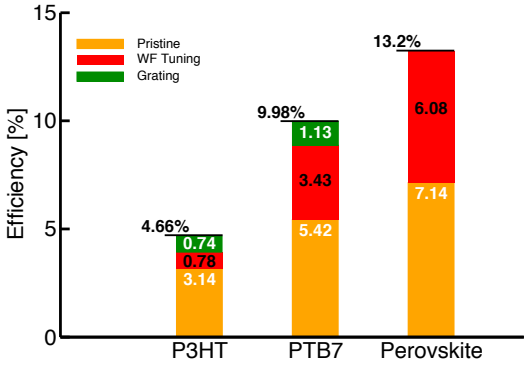

Fig. 4. Power conversion efficiency of the investigated OSC with graphene transparent electrode for different materials as active layer.