Exploring modelling strategies for organic solar cells

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Abstract

The search for ever higher efficiency solar cells is at present focussed on multijunction devices. In this field, there is enormous research on tandems consisting of a wide bandgap top sub-cell coupled to a c-Si bottom sub-cell[1]. An emerging top cell candidate is the organic solar cell, given recent impressive breakthroughs in efficiency and stability[2], thanks in part to non-fullerene acceptors. In this context, we report on approaches to modelling organic solar cells for silicon / organic tandems. The device studied is the three-terminal selective band-offset tandem cell[3]. This innovative design shown in figure 1a is based on the Si interdigitated back contact solar cell[4], which features a number of fabrication and operating advantages over four terminal and two terminal tandems[5]. The wider gap organic top sub-cell consists of donor and acceptor organic phases in an absorber blend, contacted to hole and electron transport layers, which is in development within the French ANR project ORGANIST. The modelling of the organic sub-cell is the main focus of this presentation, and is investigated with increasing of model complexity, while maximising equivalence between the fundamentally dissimilar models by ensuring equal structures and model parameters as far as possible. The modelling of the complete tandem is first described with a simple first approximation which only considers idealised classic drift-diffusion phenomena of inorganic semiconductors, with optical and band structure data from current best estimates of suitable non-fullerene high bandgap organic solar cell materials[6]. It is shown that this approach is sufficient to quantitatively predict tandem efficiencies with suitable approximations for optical and transport parameters. Figure 1b shows the resulting quantum efficiency of a preliminary 27% tandem without device optimisation, and with a non-textured Si IBC. Organic modelling is then developed from standard open access models[7], by moving from the widespread effective medium approach treating the absorber blend as a homogeneous material, to a bulk heterojunction model where the acceptor and donor organic phases are simulated separately. We conclude with lessons learned on the comparative benefits of the modelling approaches for the design and development of high efficiency organic solar cells.

TOPIC 8 : Organiques

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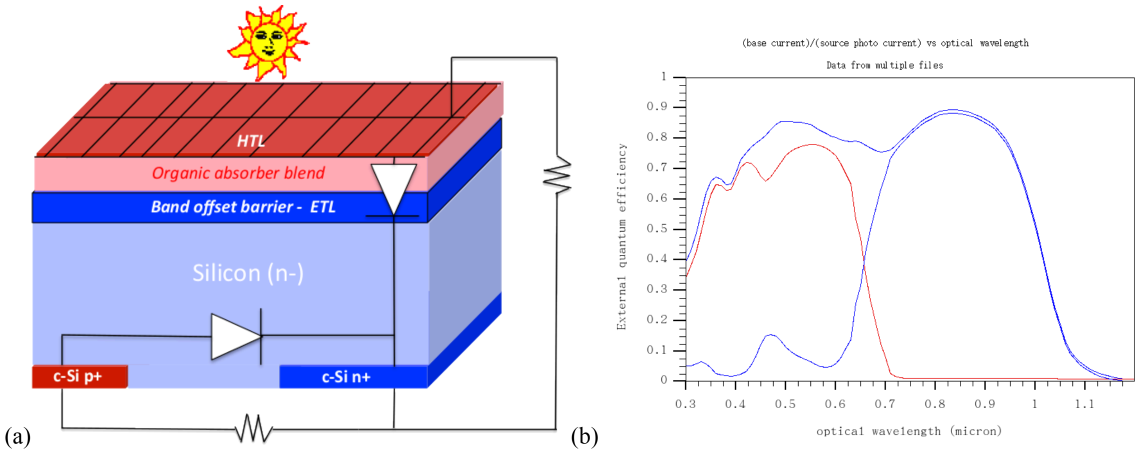

Fig. 1 (a) Schematic of the three terminal band offset barrier tandem here in the organic on silicon embodiment **(b)** external quantum efficiency of the 27% efficiency tandem as described in the text. This results from independent organic cell efficiency of 15.6% AM1.5 for a effective gap of 1.8eV, and untextured Si IBC efficiency 19.8% under AM1.5G reduced to 11.3% IBC efficiency in the tendem due to light absorption by the organic cell.