Organic materials modelling in three terminal Organic/Si tandem solar cells

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Abstract

This paper reports on organic solar cell modelling development, in the context of high efficiency multijunction solar cells for tandem applications. This addresses a gap in solar cell modelling, because while strong elements have been reported in the literature including open access numerical simulation scripts [1], there remains a lack of complete organic solar cell device modelling for multijunction cells.

We choose multijunction silicon based concepts, the dominant technology. Our lower bandgap cell is based on the ZEBRA interdigitated Si cell [2], in industrial production by ISC-Konstanz. The choice of high bandgap subcell is determined by the emergence of organic PV, due to its low material and fabrication costs, abundant feedstock, non-toxicity, and most importantly significant recent progress in performance of over 20% under one sun [3], which is economically viable if developed to the industrial scale.

The structure envisaged is the three-terminal selective band-offset tandem cell [4,5]. This has been experimentally demonstrated by two research projects to date [6,7]. Compared to the four-terminal tandem concept, the selective band-offset barrier [8] design eliminates the need for an intermediate electrode between top and bottom cells, facilitating optical management and subcell interconnection [9], while offering more flexibility than the two-terminal concept. The higher gap subcell is in development within the ANR ORGANIST project and is the main focus of this report. The first structure developed is a planar heterojunction design based on GS-ISO (acceptor) and PBDB (donor) high bandgap materials well suited to the intended high bandgap sub-cell application.

We detail the physics of transport within organic materials within the context of numerical simulation packages (Silvaco ATLAS) contrasted with transport models in crystalline semiconductors. We highlight the properties of excitonic transport and dissociation within these materials, and detail the impact of these models on device simulation, identifying areas for improvement in modelling and cell design.

The result, building on extensive previous theoretical work, is for the first time a three-terminal opto-electronic model of silicon / organic tandem solar cells.

References

[1] L. J. A. Koster, *et al*., "Device model for the operation of polymer/fullerene bulk heterojunction solar cells", Phys. Rev. B 72, 085205, https://dx.doi.org/10.1103/PhysRevB.72.085205

[2] Radovan Kopecek *et al*., "ZEBRA technology: low cost bifacial IBC solar cells in mass production with efficiency exceeding 23.5%", 47th IEEE Photovoltaic Specialists Conference (PVSC), 2020, https://dx.doi.org/10.1109/PVSC45281.2020.9300503

[3] Y. Cui, Y. Xu, H. Yao, *et al.,* Single-Junction Organic Photovoltaic Cell with 19% Efficiency; Adv. Mater. (2021) 2102420; DOI: https://dx.doi.org/10.1002/adma.202102420

[4] Z. Djebbour, W. El-Huni, A. Migan and J-P. Kleider, Patent WO 2017/093695. https://patentscope.wipo.int/search/en/detail.jsf?docId=WO2017093695

[5] J.-P. Kleider, *et al*., "Three-Terminal Tandem Solar Cells Combining Bottom Interdigitated Back Contact and Top Heterojunction Subcells: A New Architecture for High Power Conversion Efficiency", 35th EU PVSEC, 4 to 28 September 2018, Brussels, https://doi.org/10.4229/35thEUPVSEC20182018-1AO.2.4

[6] Philipp Tockhorn *et al*.. "Performance of Monolithic Two- and Three-Terminal Perovskite/Silicon Tandem Solar Cells Under Varying Illumination Conditions" Sol. RRL2023, 2200954, https://doi.org/10.1002/solr.202200954

[7] Hiroyuki Kanda *et al*., "Three-terminal perovskite/integrated back contact silicon tandem solar cells under low light intensity conditions", Interdisciplinary Materials. 2022;1:148–156, https://doi.org/10.1002/idm2.12006

[8] Philip Klipstein *et al*., "High operating temperature XBn-InAsSb bariode detectors", Proc. SPIE 8268, Quantum Sensing and Nanophotonic Devices IX, 82680U, https://dx.doi.org/10.1117/12.910174

[9] J.P. Connolly *et al*., "Recent Results on Carrier Selective Three Terminal Perovskite on Silicon-IBC Tandem Solar Cells", 37th EU PVSEC, 7 to 11 September 2020, DOI : https://dx.doi.org/10.4229/EUPVSEC20202020-1BO.16.6