Realistic limits of perovskite solar cell efficiency

James P. Connolly[1,2a], José Alvarez[1,2], Koffi Ahanogbe[1,2], Jean-Paul Kleider[1,2], Zakaria Djebbour[1,2], Hiroyuki Kanda[3], Mohammad Khaja Nazeeruddin[3], Valentin Mihailetchi[4], Philippe Baranek[5,6], Malte Vogt[7], Rudi Santbergen[7], O. Isabella[7], Ahmed Nejim[8]

[1] *Université Paris-Saclay, CentraleSupélec, CNRS, Laboratoire de Génie Electrique et Electronique de Paris, 91192, Gif-sur-Yvette, France*
[2] *Sorbonne Université, CNRS, Laboratoire de Génie Electrique et Electronique de Paris, 75252, Paris, France*
[3] *Group for Molecular Engineering of Functional Materials, Department of Chemistry and Chemical Engineering, Swiss Federal Institute of Technology, CH-1951 Sion, Switzerland*
[4] *ISC Konstanz e.V., Rudolf-Diesel-Straße 15, Konstanz 78467, Germany*
[5] *EDF R&D, Dept. EFESE, EDF Lab Paris-Saclay, 7 boulevard Gaspard Monge, 91120 Palaiseau, France*
[6] *IPVF, Institut Photovoltaïque d'Île-de-France, 30 route Départementale 128, 91120 Palaiseau, France*
[7] *Delft University of Technology, PVMD Group, Mekelweg 4, 2628 CD Delft, The Netherlands*
[8] *Silvaco Europe Ltd, Cambridgeshire, U.K.*

[(a)] *Correspondence: james.connolly@geeps.centralesupelec.fr tel. +33 783 03 92 70*

Abstract

The perovskite solar cell (PSC) is one of the most dramatic inventions in the field of photovoltaics in the last half century. The device has rapidly risen from a few percent to efficiencies of over 24% [1] in little over a decade. This rapid development is due in part to the wide family of perovskite absorber and of electron and hole tranport materials available which yields great flexibility. The flip-side of this profusion of materials is the challenge in establishing achievable performance potential of real devices. This paper therefore presents a study of the perovskite solar cell materials and applies numerical modelling techniques to evaluate the most promising materials combinations and their efficiency potential. The preliminary device structure is a simple three-layer design consisting of hole transport layer, perovskite aborber, and electron transport layer, on a glass substrate in a p-i-n or "inverted" configuration. A range of materials for these layers is compared and contrasted for this polarity. The structure is then generalised to more complex designs featuring protective buffer layers which prevent damage to the perovskite absorber layer, and two dimensional perovkite layers which have been shown to improve perovskite material stability. The realistic efficiency potential of the materials considered is discused in the context of the common radiative efficiency limit. The study concludes by recommending promising materials combinations for high efficiency PSC compatible with cost effective indutrial fabrication method for single juntion and for multijunction device design in the context of H2020 Solar-ERANET project BOBTANDEM [2]. This work contributes to define efficiencies achievable in this materials systems, both for single junction and multijunction devices which are of great societal interet for cost effective renewable power generation.

References

[1] Jeong, J., Kim, M., Seo, J. et al. Pseudo-halide anion engineering for α-FAPbI3 perovskite solar cells. Nature 592, 381–385 (2021). https://doi.org/10.1038/s41586-021-03406-5
[2] Web : http://bobtandem.geeps.centralesupelec.fr ; Twitter : @BobTandem

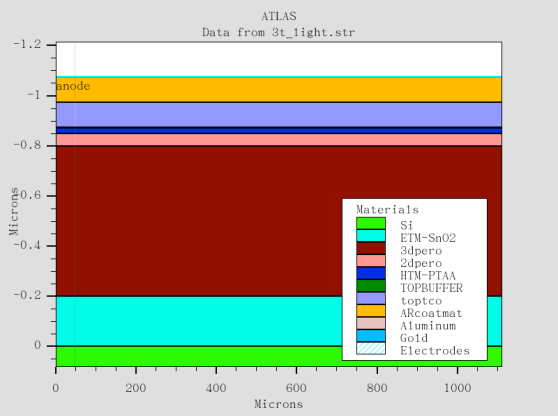

Figure 1 Full set of layers considered in this case on a Si substrate of interest for tandem structures. Defect ditributions are included in absorber and tranport layer materials and interfaces.

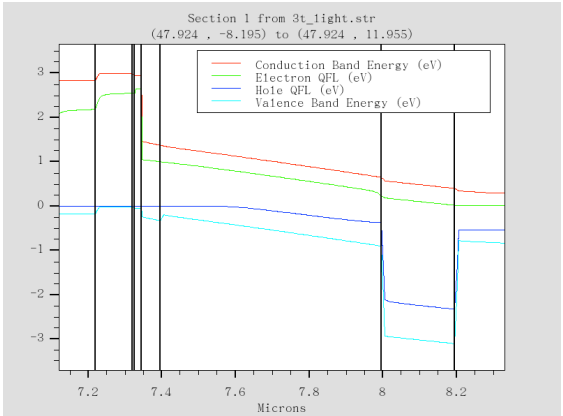

Figure 2 Band structure simulated by two dimensional modelling (Silvaco ATLAS)