Understanding and Optimizing Interface Energetics and Processes: an essential step towards efficient and stable perovskite solar cells

G. Grancini
Dipartimento di Chimica e INSTM, Università di Pavia
Via Taramelli 12, 27100 Pavia, Italy
giulia.grancini@unipv.it

Engineering interfaces in perovskite solar cells is nowadays paramount in the optimization of multilayer perovskite device stack. This stem true for multi-dimensional (2D/3D) perovskite based solar cells, where high efficiency can be combined with promising device durability. However, the exact function of the 2D/3D interface in controlling the device behaviour and the interface physics therein are still vague.
Here I will discuss the 2D/3D functions which can simultaneously act as surface passivant, electron blocking layer, and driving efficient and selective charge extraction. In particular, I will demonstrate that the exact knowledge on the interface energetics is crucial to obtain for a smart interface engineering. As an example, I will discuss the case of thiophene-based 2D perovskite/ 3D perovskite interfaces forming a p-n junction. This leads to a reduction of the electron density at the hole transport layer interface and ultimately suppress the interfacial recombination. As a consequence, we demonstrate that photovoltaic devices with enhanced fill factor (FF) and open-circuit voltage (VOC) of 1.19V which approaches the potential internal Quasi-Fermi Level Splitting (QFLS) voltage of the perovskite absorber, nullifying the interfacial losses. We thus identify the essential parameters and energetic alignment scenario required for 2D/3D perovskite systems in order to surpass the current limitations of hybrid perovskite solar cell performances. This knowledge turns fundamental for device design, opening a new avenue for perovskite interface optimization.

[1] A. Sutanto, P. Caprioglio, N. Drigo, Y. J. Hofstetter, I. Garcia-Benito, V. I. E. Queloz, D. Neher, M. K. Nazeeruddin, M. Stolterfoht, Y. Vaynzof, G. Grancini "2D/3D Perovskite Engineering Eliminates Interfacial Recombination Losses in Hybrid Perovskite Solar Cells", ***Chem*** DOI:10.1016/j.chempr.2021.04.002 (2021)

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