Numerical analysis on the use of carbon nanostructures as additives to perovskite solar cells using SCAPS-1D software

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In the photovoltaic field, it is widely assumed that lead halide perovskite solar cells (PSCs) are the most promising technology capable of meeting both cost and conversion efficiency requirements. Since the pioneering work of Kojima et al in 2009[1], this technology of solar cells has gained significant attention ; its efficiency continues to increase, and it now stands at 26% on a laboratory scale[2]. The electron transport layer (ETL) and hole transport layer (HTL) are among the various factors that impact negatively the performance of PSCs. To improve them, modifying their composition upon doping or incorporating additives are widely investigated, but still remains challenges. Owing to their high chemical stability, low cost and abundance, carbon materials have attracted the attention for their use as additives to the HTL and ETL, or back contacts to replace the expensive metal contact electrodes (usually Au)[3]. Despite the potentitalities, identifying the best carbon material among the wide family of carbons, and the most adequate role in the PSC remains a challenging task. In this study, we have investigated by numerical simulation using SACPS-1D software, the use of carbon mateials with varied properties (e.g., graphene, carbon nanotubes, carbon black, nanoporous carbons) as additives to PSCs. Our simulations show that for regular n-i-p structures stacking as FTO/ETL/$MAPbI_3$/HTL/Ni, a hybrid HTL formed upon the incorporation of a thin carbon layer with a carbon material displaying a bandgap in the range of 3 to 3.5eV significantly improves the open-circuit voltage as well as the fill factor (FF) of the resulting device. As a result, the efficiency of the PSCs also increases by more than 1.8%. From the point of view of the characteristics of the carbon layers, our results underline that carbon black, carbon nanotubes and nanoporous carbon are better additives to the studied HTL compound (spiro-OMeTAD). To summarize, this contribution offers a novel perspective on use of carbon materials in PSCs, and provides new insights into the understanding of the role of carbon materials as additives to PSCs.

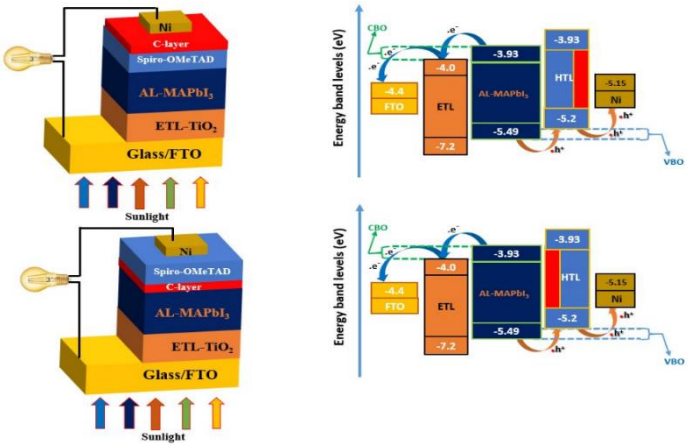

Figure 1.Stacking layers and energy bands alignment of the simulated solar cells.

References :

[1] A. Kojima, K. Teshima, Y. Shirai, et T. Miyasaka, « Organometal halide perovskites as visible-light sensitizers for photovoltaic cells », *J. Am. Chem. Soc.*, vol. 131, nº 17, p. 6050-6051, 2009.

[2] « Interactive Best Research-Cell Efficiency Chart ». https://www.nrel.gov/pv/interactive-cell-efficiency.html.

[3] Z. Li *et al.*, « Laminated carbon nanotube networks for metal electrode-free efficient perovskite solar cells », *ACS Nano*, vol. 8, nº 7, p. 6797-6804, 2014.