Tuning electro-optical properties of perovskite solar cells: the role of MXenes

Antonio Agresti (a)
A. Pazniak(b)§, S. Pescetelli(a)§, D. Saranin(b), D. Rossi(b), M. Auf der Maur(b), A. Di Vito(b), A. Pecchia(c), A. Liedl(d), R. Larciprete(d), A. Di Carlo(a,b))

(a) CHOSE - Centre for Hybrid and Organic Solar Energy, Department of Electronic Engineering, University of Rome Tor Vergata, via del Politecnico 1, 00133, Rome, Italy.
(b) LASE – Laboratory of Advanced Solar Energy National University of Science and Technology "MISiS", Moscow, Russia.
(c) Consiglio Nazionale delle Ricerche-CNR, ISMN, Rome, Italy.
(d) INFN-LNF - Frascati (Rome) Italy.

antonio.agresti@uniroma2.it

Recently bi-dimensional (2D) materials have attracted great attention in several research fields such as batteries, supercapacitor, sensors, catalysis, and photovoltaics. Indeed, from 2D nature derive exceptional physical properties, such as remarkable electrical conductivity and mechanical robustness, high optoelectronic tunability, easy production and solution processability. Thus, the performance of new emerging technologies can be further boosted by exploring the wide range of 2D materials. In this context, the combination between 2D materials and lead halide perovskite photovoltaics was already demonstrated to be a winning strategy for boosting the small area power conversion efficiency (PCE),[1] enlarging the device lifetime [2] and making possible the technology scaling-up from lab-scale device to large area modules.[3] From here the increasing interest by the scientific community in exploiting new 2D materials as efficient additives and/or interlayers in perovskite solar cells (PSCs). This work aims to propose transition metal carbides, nitrides and carbonitrides (MXenes) as promising class of materials for PSC performance improvement. With a general formula $M_{n+1}X_nT_x$ (n = 1, 2, 3), where M represents an early transition metal, X is carbon and/or nitrogen, and T_x stands for surface terminations, MXenes exhibit huge possibilities to tune their electronic properties. As density functional theory predicts, surface termination strongly influences MXenes' Fermi level density of states and the work function ranging from 1.6eV (for OH-termination) to 6.25eV (for O-termination).[4] In particular, we demonstrate the use of $Ti_3C_2T_x$ MXenes for perovskite photovoltaics by fine tuning the interface optoelectronic properties in engineered mesoscopic device. The MXenes-based PSC showed improved performance with respect to the reference one by demonstrating PCE exceeding 20%. A deep optoelectronic and spectroscopic characterization demonstrated the effective role of MXenes in i) tuning the perovskite work function when used as additive in perovskite precursor solution, ii) reduce the device hysteresis affecting the current-voltage (I-V) characteristic when voltage scan is performed from open circuit condition (OC) to short circuit (SC) and viceversa; iii) improving the electron extraction/collection at device photoelectrode (PE) when used as additive for compact and mesoporous TiO_2 precursor solution and/or as interlayer at perovskite/electron transporting layer (ETL) interface. The possibility to tune "on-demand" the MXenes optoelectronic properties, their easy production in liquid form and the stability demonstrated by the related inks open uncountable scenarios for their application in PSC technology and a viable route for perovskite-based photovoltaic diffusion into the market.

References

[1] F. Biccari *et al.*, *Adv. Energy Mater.*, vol. 7, no. 22 (2017).
[2] Y. Busby *et al.*, *Mater. Today Energy*, vol. 9, (2018).
[3] A. Agresti *et al.*, *ACS Energy Lett.*, vol. 2, no. 1 (2017) 279–287,.
[4] Y. Liu, H. Xiao, and W. A. Goddard, *J. Am. Chem. Soc.*, vol. 138, no. 49 (2016) 15853–15856.