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MXenes and emerging 2D materials for perovskite-based photovoltaics

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Recently, the increasing energy demand pushed the scientific community in developing new technologies for the exploitation of the renewable energy sources. As the matter of fact, the word total energy consumption was estimated 153.000 TWh in 2019, increased more than 15% in the last 15 years. In this context, solar energy is the best candidate for satisfying the human being request, since the amount of theoretically exploitable solar energy, which in a year invests the earth's surface is equal to 3.8 YJ. Indeed, in the last decades, new generation photovoltaic promised power conversion efficiency (PCE) comparable to those of silicon photovoltaics by guaranteeing low production costs. In this regards, hybrid photovoltaic technologies such as Perovskite Solar Cells (PSCs) dominated the PV scientific research, by developing efficient and stable devices, produced by employing scalable and low-cost printing techniques, easily embedded in roll2roll or sheet2sheet production lines. However, PSC technology still requires to demonstrate the transfer from lab to fab, pushing the scientific community in finding brilliant solution for drawing a feasible and reliable route toward its commercialization. Indeed, despite perovskite absorber demonstrated outstanding semiconductor properties and low-cost solution processing methods for the fabrication, the use of crystallization processes from the liquid phase tends to the formation of imperfections and defects in the bulk and surfaces that could give rise to non-radiative charge recombination. Moreover, energy levels in halide perovskite semiconductors and materials for the transporting layers cannot be simply controlled by chemical doping as for Si and III-V semiconductors. Here, the use of interface engineering based on bi-dimensional (2D) materials is proposed as an efficient tool for trap passivation and energy level alignment. Beyond graphene and related materials, MXenes ($M_{n+1}X_nT_x$, where M represents an early transition metal, X is carbon or nitrogen, and T_x shows functional termination (OH, O or F, etc.)) are considered as promising material for tuning the surface properties in PSC due to the unique tunability of work function values (from of 1.6 to 6.5 eV), high electronic conductivity and charge carrier mobility. In this work, we demonstrate an effective use of $Ti_3C_2T_x$ MXenes for engineering the energy band alignment in PSCs and passivating bulk and interfacial defects by remarkably improving the device PCE and stability.[1] The here-proposed approach can theoretically be extended to different perovskite absorbers and PSC structures, representing a promising way for further boosting the PCS technology and for speeding its commercialization up.[2]

[1] *A. Agresti et al. Nature Materials, 18 (2019) 1228–1234*
[2] *D. Saranin et al. Nano Energy, 82 (2021) 105771*

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