MXene-based perovskite photovoltaics: a general approach for efficient and scalable devices.

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Recently, a new class of emerging bi-dimensional (2D) materials known as transition metal carbides, nitrides and carbonitrides (MXenes) was successfully employed in full inorganic or organic-inorganic halide perovskite (HP). In particular, $Ti_3C_2T_x$ MXenes have been tested as dopant for electron transporting layer (ETL), to improve the electron collection in planar devices [1] or as interlayer between inorganic perovskite and carbon counter-electrode (CE).[2] In this work we go further to the simple application of MXenes in a specific structure, by suggesting a general approach to boost device performance, suitable for both planar inverted and mesoscopic n-i-p device architectures, independent from the perovskite formulation and easily scalable to large area modules. In fact, as density functional theory predicts, MXenes WF can range from 1.6 eV (for OH-termination) to 6.25 eV (for O-termination), thanks to the surface termination (T_x) strongly influencing the density of states.[3] In addition, we experimentally and theoretically demonstrated perovskite WF tuning when MXenes are used as additive in perovskite precursor solution, for both mesoscopic n-i-p and p-i-n small area devices, without affecting other electronic properties. This approach resulted in strongly improved device power conversion efficiency (PCE) due to the dipole induced by the $Ti_3C_2T_x$ at the perovskite/ETL interface that changes the band alignment between these layers.[4] Moreover, the proposed approach can be applied even to the charge transporting layers, such as TiO_2 in mesoscopic n-i-p or PCBM in inverted PSCs, respectively. Finally, due to the easy solution-based fabrication of MXenes, the proposed approach is easily scalable on large area perovskite modules and panels.

REFERENCES

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FIGURE

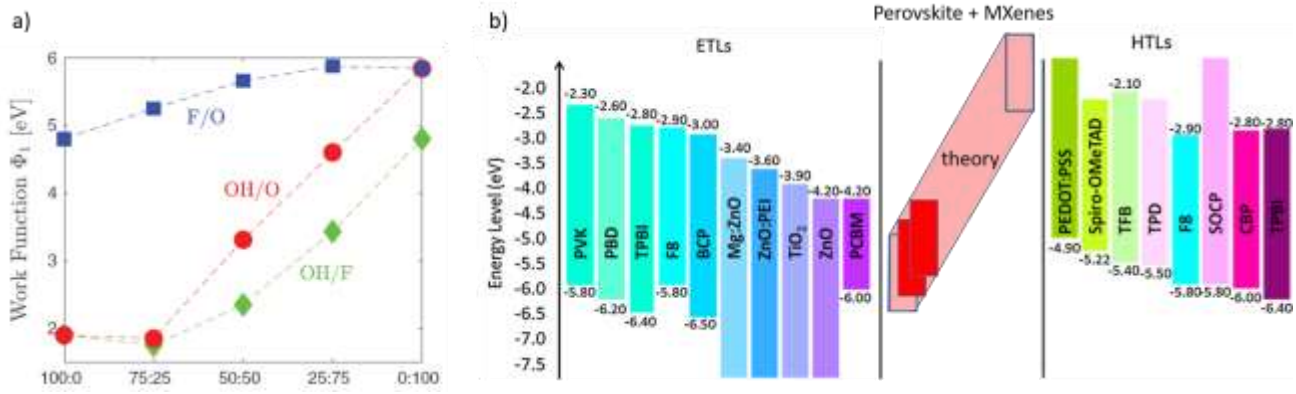

Figure 1: a) Work function values Φ1 derived from density functional theory calculations, for a mixture of OH, O, and F MXene surface terminations at the interface with perovskite (from ref. [3]); b) perovskite WF tuning theoretically predicted and experimentally verified and its energy level alignment with several electron (ETLs) and hole (HTLs) transporting layers (from ref. [4])