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MXENE-BASED PEROVSKITE PHOTOVOLTAICS: A GENERAL APPROACH FOR EFFICIENT AND SCALABLE DEVICES

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ABSTRACT

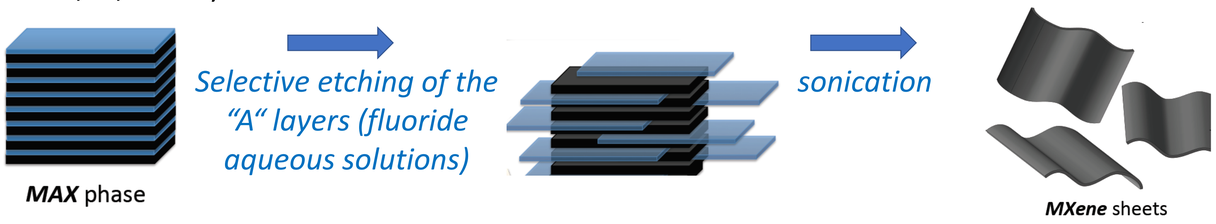
Recently, a new class of emerging **bi-dimensional (2D) materials** known as **transition metal carbides, nitrides and carbonitrides** (MXenes) was successfully employed in full inorganic or organic-inorganic halide perovskite (HP).

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 p-i-n** 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.

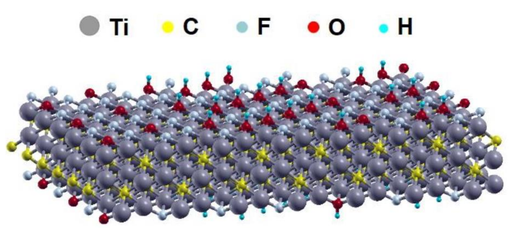
RESULTS

MXENES: PRODUCTION AND WF TUNING

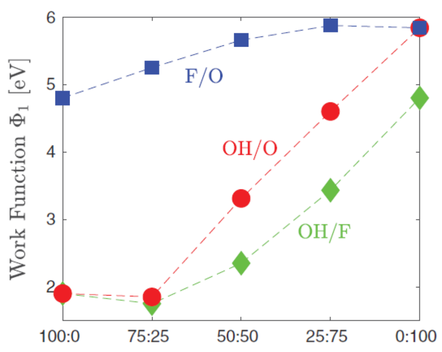
Mxenes have general formula $M_{n+1}X_nT_x$ (n = 1, 2, 3), where **M** represents an early **transition metal**, **X** is **carbon** and/or **nitrogen**, and T_x stands for surface terminations (such as **OH**, **O**, and **F**).



- During the synthesis of MX, their surfaces are naturally functionalized, significantly **shifting** the **WF**;
- WF Tunability, from 1.6 eV (for OH-termination) to 6.25 eV (for O-termination);



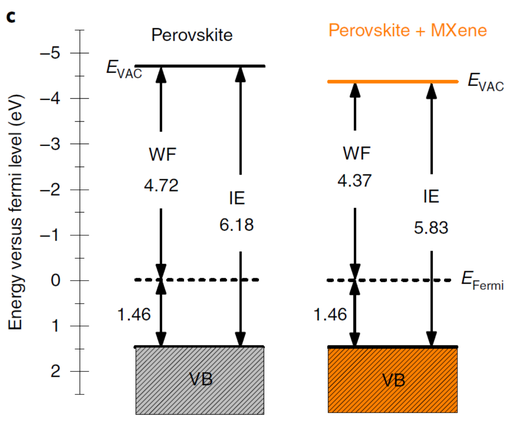
Structure of the MXene slab with mixed F, OH and O functional groups.

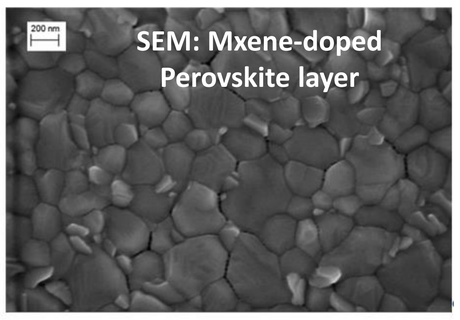


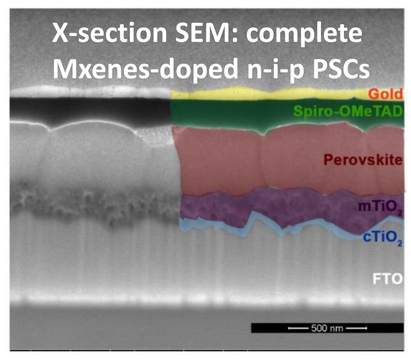
Work function values Φ1 derived for a mixture of OH, O, and F MXene surface terminations at the interface with perovskite.

MXENE-DOPED PEROVSKITE

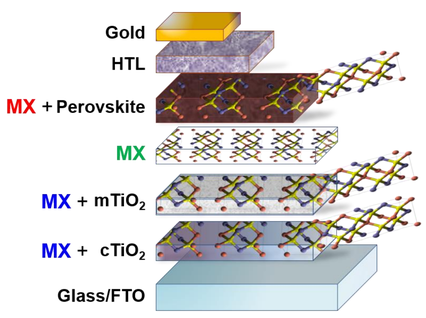
- Charge transfer at the perovskite/MXene interface induces the formation of an **interface dipole** causing an important **shift of** the **WF** and affecting the band alignment of the system.
- **No structural modification** of perovskite crystal structure or of the related electronic properties



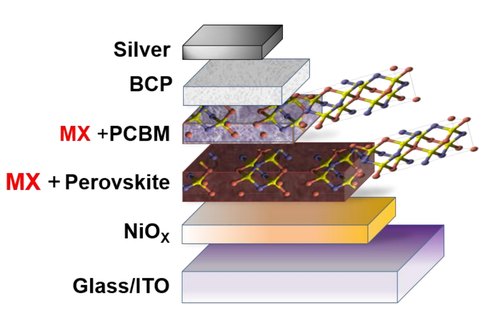




MXENE-BASED PEROVSKITE SOLAR CELLS



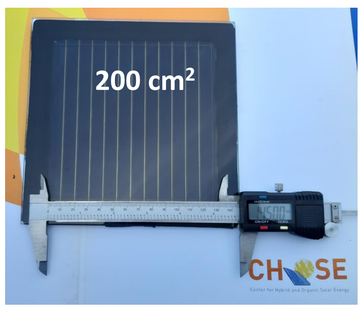
n-i-p mesoscopic Mxene-based PSCs



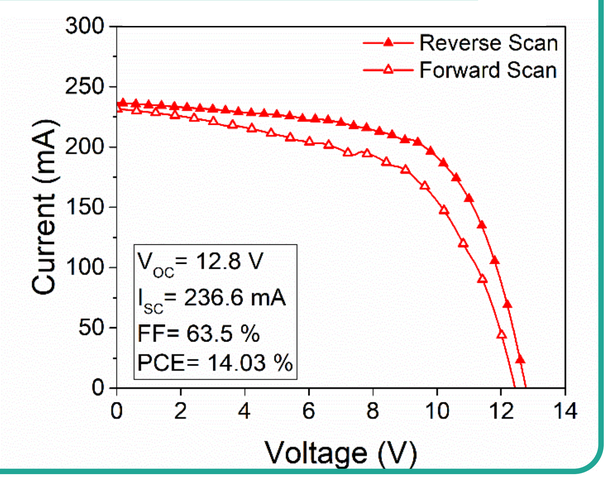
p-i-n planar Mxene-based PSCs

Mxene-doped charge transporting layer and MXene interlayer have been successfully employed to engineer both **mesoscopic n-i-p** and **inverted p-i-n** PSCs by remarkably boosting **PCE** above **20.2%** and **19.4%** respectively.

MXENE-ENABLED PEROVSKITE LARGE AREA MODULES



Mxene in PSC enabled record efficiency **large area module** with **PCE>14%** over **137 cm²** active area.



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