Insights into metal halide perovskite heterostructures and their applications to photovoltaics

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The presentation will review recent results obtained in collaboration between the joint perovskite group in Rennes (FOTON and ISCR CNRS UMR) and the groups of A. Mohite in Houston (Rice University) and M. Kanatzidis in Chicago (Northwestern University). One important building block for stable perovskite solar cells (PSCs) are the 2D multilayered Ruddlesden-Popper phases discovered by J. Calabrese (JACS 1991), recently supplemented by "Alternative cations in the interlayer" (Soe, JACS 2017) and Dion-Jacobson (Mao, JACS 2018) phases. This classification of multilayered perovskites, in relation with the chemistry of the compounds or the crystallographic order along the stacking axis has recently been achieved (Blancon, Nature Nano 2020). Exploring the potential of 2D perovskites for PV and the combination of 2D and 3D perovskites in PSC architectures was a long-term joint project that we started 10 years ago including the first breakthrough on 2D PSC demonstrating their unique stability under operation (Tsai, Nature 2016). This approach is in line with Snaith's recent perspective (Science 2024) on PSCs: "*a growing consensus is forming about the requirements for an ideal perovskite interface: the elimination or repair of surface interface defects, the design of a rational energy landscape to satisfy selective carrier collection, the minimization of strain and stress, and the improvement of physical robustness and adhesion*". When combined in 2D/3D bilayer stacks using new versatile growth methods based on solvent engineering, excellent PSCs device stability can be achieved (Sidhik, Science 2022).

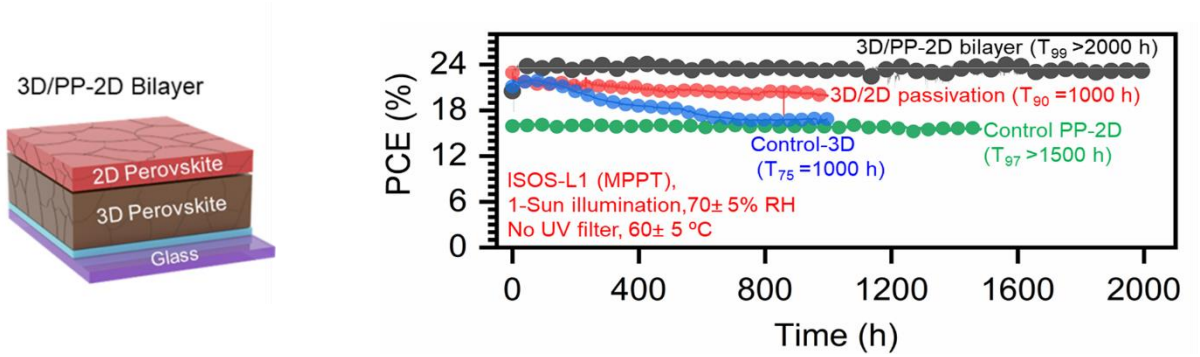

Figure 1 (Sidhik et al, Science 2022): (left) schematic representation of a 2D/3D bilayer PSC with thick layers (right) the 2D/3D bilayer PSC inherits its stability under operation from the corresponding 2D PSC as initially demonstrated in Tsai et al, Nature 2016.

Besides solvent engineering, a deep understanding of electronic properties, including band alignment is required to properly choose each of the 2D and 3D layer compositions. The later also benefits from our lattice matching concept (Kepenekian, Nanoletters 2018), which relies on mechanical energy considerations to select the best pair of 2D/3D or more generally perovskite/perovskite combination. It led recently to record stability for pure $FAPbI_3$ based PSCs (Sidhik, Science 2024).

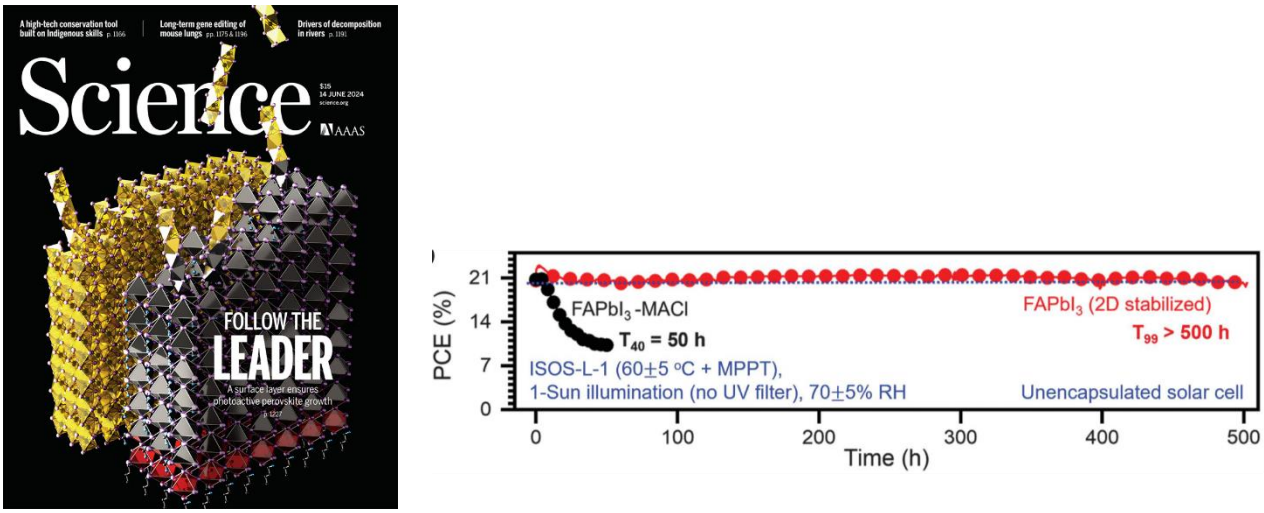

Figure 1 (Sidhik et al, Science 2024): (left) cover of the Science journal, illustrating the templating of pure $FAPbI_3$ by a FA-based n=2 2D perovskite, simultaneously avoiding the formation of the yellow phase (right) stability of the photoconversion efficiency under operation obtained for a 2D/3D PSC containing only FA cations in the perovskite layer

This approach is currently extended to combine more than a pair of perovskite layers of any type (3D, 2D, 1D, 0D…) and into solution-processed photoactive heterostructures for improved stability and efficiency in n-i-p or p-i-n PSC architectures, but also for a variety of optoelectronic devices.