Stabilization of perovskite photovoltaic devices by passivation through Metal Organic Frameworks engineering

Nicolas Pernès[1], Thomas Gomes[1], Yifan Xu[2], Farid Nouar[2], Stéphane Cros[1]

[1] *Univ. Grenoble Alpes, CEA, LITEN, INES, 73375 Le Bourget du Lac, France*

[2] *Institut des Matériaux Poreux de Paris, Ecole Normale Supérieure, ESPCI Paris, CNRS, PSL University, 75005 Paris, France*

Long-term operational stability remains one of the key challenges for the industrialization of perovskite solar cells and perovskite/silicon tandem devices. A major source of instability originates from the high density of defects at the interfaces between the perovskite layer and the adjacent charge transport layers (CTLs). To address this issue, we propose an interfacial passivation strategy based on the engineering of Metal–Organic Framework (MOF) materials to stabilize the perovskite/CTL interfaces. Among various passivation strategies, MOFs have recently emerged as promising materials due to their tunable chemistry, large surface area and their abundant binding sites potentially beneficial for defect healing[1].

We synthetized a chemically and thermally robust MOF based on zirconium clusters[2] through a sustainable approach. The MOF was incorporated into PIN perovskite solar cells based on a $Cs_xFA_{1-x}Pb(I_\gamma Br_{1-\gamma})_3$ absorber with a 1.66 eV bandgap, suitable for tandem applications. The MOF was tested both at the perovskite/hole transport layer (HTL) and perovskite/electron transport layer (ETL) interfaces.

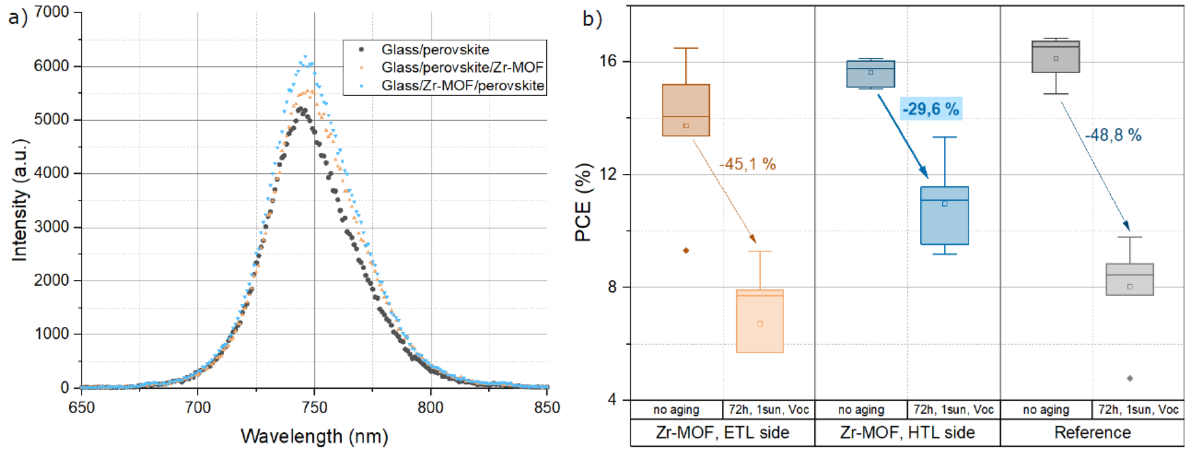

Figure 1: a) PL spectra and b) cells PCE before and after aging, for the different MOF deposition conditions. Percentages refer to the degradation rates between the medians

The integration of the MOF at HTL side led to a significant enhancement in perovskite crystallinity, as evidenced by X-ray diffraction (XRD) and scanning electron microscopy (SEM), with a preferred orientation along the (00l) direction, perpendicular to the substrate. These structural improvements suggest that the MOF can act as a growth scaffold for the perovskite layer. Photoluminescence (PL) and time-resolved PL (TrPL) measurements revealed a 19% increase in PL intensity (*fig. 1.a)*) and longer carrier lifetimes upon MOF passivation. The photovoltaic performances of the passivated devices were largely preserved (PCE ≈ 15.5% vs. 16.5% for control devices), with an improved short-circuit current (J_{sc}). More importantly, under harsh light conditions, i.e. continuous 1 sun illumination at V_{oc} for 72 hours in nitrogen, unencapsulated devices with the MOF exhibited enhanced operational stability, with a degradation rate limited to 29.6%, compared to 48.8% for unpassivated cells (*fig.1.b)*).

This work underscores the potential of MOF-based interfacial engineering to enhance the long-term durability of perovskite solar cells, while offering a chemically tunable platform for further performance and stability improvements.

[1] Ye, Y. & al. (2023b). Metal-Organic Framework Materials in perovskite solar cells: Recent advancements and Perspectives. Small, 19(25). https://doi.org/10.1002/smll.202208119

[2] Rimoldi, M. & al. (2016). Catalytic Zirconium/Hafnium-Based Metal–Organic frameworks. ACS Catalysis, 7(2), 997–1014. https://doi.org/10.1021/acscatal.6b02923