Interface Formation between Metal Halide Perovskites and Oxide Films from Atomic Layer Deposition (POSTER)

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Abstract: Complex interfaces are an inherent characteristic of metal halide perovskite (MHP) based optoelectronic devices, including halide perovskite solar cells (PSC). The interfaces to a large extent determine device functionality and strongly affect device performance stability. The intricacy of these interfaces is owned to the perovskite material itself, which often includes five to six different elemental and molecular components, among them readily reduced metal cations, acidic organoammonium cations, and reactive halide species. Therefore, stabilizing these systems represents an extreme challenge. However, the lifetime of the device does not only depend on the stability of the MHP itself but also on the charge transport layers (CTL), which form a direct interface with the MHP. Among different CTL materials, inorganic metal oxides have demonstrated better stability in comparison to the organic counterpart due to high resilience to heat, light, and the local chemical environment. Recent studies demonstrate that the stability of perovskite solar cells can be improved through deliberately tailoring interface properties and by introducing suitable interfacial layers between the absorber and charge transport layers (CTL) (see figure 1).

This work focuses on designing and analyzing atomic layer deposition (ALD) based functional inorganic CTL on top of perovskite films with and without organic buffer layer. The goal is to establish a fundamental scientific understanding of the chemical interdependencies between the individual molecular building blocks, their impact on physical mechanisms (e.g., charge transport) at the interface. In this study, we investigated the interface between double cation mixed halide perovskite (MHP) thin films ($FA_{0.7}Cs_{0.3}Pb(I_{0.9}Br_{0.1})_3$) and a 5nm thick ALD SnO_x layer using hard X-ray photoelectron spectroscopy (HAXPES). Before ALD deposition, the perovskite film exhibits a homogeneous stoichiometry at the surface and in the sub-surface region. We find that the TDMASn and H_2O_2 precursors used in the oxide deposition process cause mild degradation of the MHP surface resulting in a partial conversion of the MHP film to PbI_2 in line with concomitantly recorded XRD data. Slight differences seen for the oxygen component recorded at 2keV and 6keV excitation energy indicate that the SnO_x film's stoichiometry is different at the surface compared to the interface with the MHP. Furthermore, we investigated using a thin organic buffer layer PCBM on top of the perovskite to mitigate the damage caused by the ALD layer deposition. After ALD-SnO_x deposition, we find that the perovskite stoichiometry remains preserved with the PCBM interlayer as evidenced in the HAXPES data of the I 3d and Pb 4f core-level regions of the buried interface.

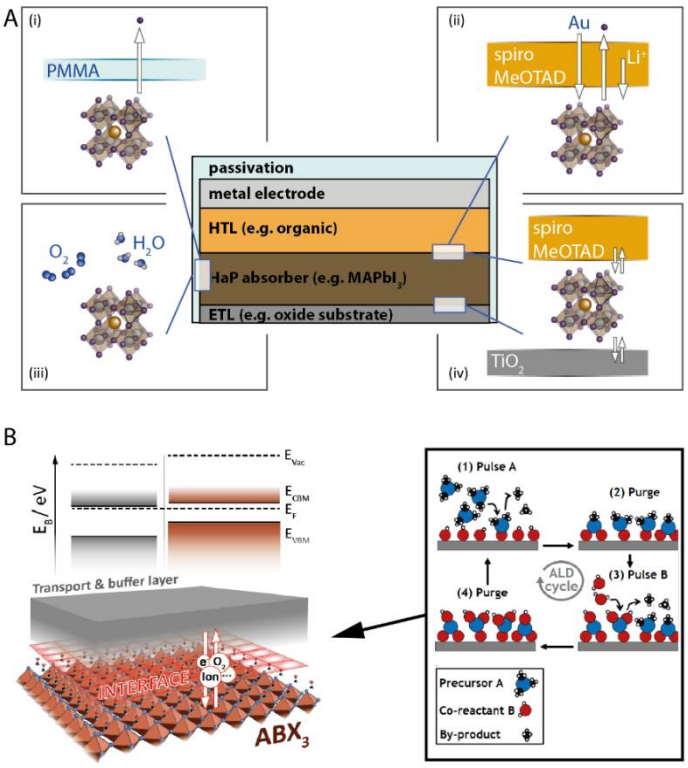

Figure 1 - A) Typical interactions of chemical species in a conventional PSC device layout for potential optimization via interfacial layers: (i) passivation/encapsulation, (ii) environmental gases, (iii) top CTL and electrodes, and (iv) CTL materials layer. B) Target of this proposal is to investigate and tailor the interface between MHP film and buffer/transport layer by using ALD coatings to control chemistry and charge transfer.[2]