FUNDAMENTAL PROPERTIES OF HYBRID PEROVSKITES AND THE ROLE OF ATOMIC LAYER DEPOSITED ALUMINA IN PEROVSKITE SOLAR CELLS

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Although perovskite solar cells (PSCs) have experienced an immense increase in efficiency within a very short time, many of their fundamental aspects are not yet completely understood.
In this work, the main focus is put on addressing the challenges that are related to an understanding of the properties of perovskite material and its interfaces, and how to increase the long-term stability of perovskite solar cells. For this purpose, several laboratory- and synchrotron-based photoelectron spectroscopy (PES) techniques have been applied including X-ray photoelectron spectroscopy (XPS), near-ambient pressure XPS (NAP-XPS), and resonant PES (resPES). Using these techniques, several issues were addressed as described in the following. The contribution of nitrogen to the electronic structure of the methyl ammonium lead triiodide (MAPI) was for the first time experimentally identified, where strong iodine-nitrogen interaction in the valence band (VB) states reflecting a high hybridization of the N2p states into the I5p-derived VB states takes place.[1] A strong influence of the chemistry and morphology of MAPI on the photon flux was detected and the creation of Frenkel pair defects, which can be self-annihilated when the light and voltage are turned off, was postulated.[2] In contrast, water vapor of up to 1 mbar showed a negligible influence on the chemistry and morphology of MAPI.[2] Thermal investigations on MAPI-based and Cs-FAMA-based perovskite have shown that the $[HC(NH_2)_2]^{\pm}$ or $Cs^{\pm}$ are not as much released as $CH_3NH_3^{\pm}$ species from the perovskite upon heating explaining the higher thermal stability of Cs-FAMA-based PSCs.[3] It was also demonstrated that iodine migrates in PSCs under light illumination limiting the PSC performance[4] ; however, this migration can successfully be suppressed by an AlO_x ALD layer.[5] Even an increase in power conversion efficiency over time was found in PSCs containing an atomic layer deposited (ALD) AlO_x layer, which was attributed to a self-healing process induced by the ALD process.[6] A model of the AlO_x/MAPI interface formation was developed where intrinsic defect states of AlO_x play a key role resulting in a covalent bonding at the AlO_x/MAPI interface accompanied by a AlO_x-MAPI derived band that is populated by Al 3s as well as lead, iodine, nitrogen, and oxygen hybridized valence states.[7] It can thus be concluded that both PES and ALD methods are very significant in improving the understanding and stability of PSCs.

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