

# **Interface Design and Characterization of Halide Perovskite Based Semiconductor Devices**

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Hybrid organic inorganic metal halide perovskites (MHPs) denote a family of compound semiconductors, which established a novel class of optoelectronics, most prominently known for the perovskite solar cell. While the power conversion efficiency of these photovoltaic devices saw a steep rise in the past decade, tailoring the interfaces between the MHP film and charge transport layer became the major control lever to enhance performance. The use of photoemission spectroscopy to analyze the chemical and electronic properties of these interfaces has been challenging due to many possible chemical reactions at the buried interfaces.<sup>1,2</sup>

For instance, it has been well documented that the optoelectronic properties of the MHP can be altered by the substrate (or selective contact) underneath,<sup>3</sup> however so far, we do not dispose of any conclusive picture explaining this effect. We hence fabricated a functional lateral heterojunction device, which consists of a substrate with two laterally arranged selective contacts, onto which we deposited MHP films. We then used a series of photoemission measurements along with complementary experiments such as X-ray absorption spectroscopy, Kelvin probe force microscopy, and hyperspectral imaging, to measure how substrate selectivity is affecting the optoelectronic properties at the perovskite surface. We find evidence suggesting that the contact selectivity is inducing a carrier concentration gradient in the perovskite layer across the junction connected to the functionality of the lateral device opening an avenue for fundamental materials studies in operando approaches but also new device architectures including buried cells terminals.<sup>4,5</sup>

Furthermore, I will present synchrotron- and lab-based hard X-ray photoelectron spectroscopy (HAXPES) experiments to address the particular chemistry of MHPs and oxide overlayers grown by atomic layer deposition on top. We find evidence for the formation of new chemical species (PbO, N and halide-containing compounds) and changes in the energy level alignment at the MHP/oxide interface. We also used HAXPES measurements to evaluate lead-free halide perovskite films based on formamidinium tin iodide (FASnI<sub>3</sub>), for which tin fluoride (SnF<sub>2</sub>) is a commonly used additive enabling a retardation of tin oxidation and a reduction of tin vacancies. We targeted films deposited on the organic hole transport layer PEDOT:PSS for which we find the formation of an ultrathin SnS interlayer. This adds a new aspect to the discussion of high-efficiency Sn-based perovskite solar cells which still commonly make use of PEDOT:PSS as HTL material in contrast to Pb-based solar cells.<sup>6</sup>

I will conclude my talk with a general discussion about the use of PES methods for the analysis of MHP layers and in particular the effect of irradiation-induced beam damage via synchrotron and lab-based X-ray sources.<sup>7</sup> By using complementary photoluminescence measurements we are able to investigate beam-induced changes to the optoelectronic properties and track unique physicochemical phenomena such as stimulated self-healing in formamidinium lead bromide (FAPbBr<sub>3</sub>).<sup>8,9</sup>

References:

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