9:30 AM

Webinar:Interface Defect Formation and Ion Migration in Halide Perovskite Semiconductors

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Hybrid organic–inorganic metal halide perovskites (MHPs) have emerged as a versatile class of semiconductors for optoelectronic applications, with perovskite solar cells (PSC) demonstrating remarkable improvements in power conversion efficiency and stability over the past decade. As device performance approaches its theoretical limits, the properties of interfaces between the perovskite and adjacent functional layers have become crucial for minimizing non-radiative recombination and ensuring long-term operation. Ultimately, the formation and evolution of chemically and electronically well-defined interfaces govern efficient charge extraction and device reliability.[1,2]

Photoelectron spectroscopy provides unique insight into the chemical composition and electronic structure of these interfaces but is often complicated by the chemical complexity of buried junctions and the dynamic nature of halide perovskites.[3] In this presentation, I will discuss recent advances using laboratory- and synchrotron-based X-ray photoelectron spectroscopy (XPS), including hard X-ray photoelectron spectroscopy (HAXPES), to investigate the formation of interfaces between MHPs and oxide charge transport layers. Using atomic layer deposited SnO_2 and NiO on mixed-cation mixed-halide perovskite films as model systems, we identify interfacial reactions leading to new chemical species and modifications of the energy level alignment that are directly linked to PSC degradation and reduced photovoltaic performance.[4,5]

Beyond this characterization, I will highlight our recent developments in time-resolved and operando XPS methods that enable the observation of surface voltage dynamics and ion migration under applied electrical bias, respectively. By following changes in the spatial distribution and chemical environment of mobile ionic species in PSCs and lateral perovskite heterostructures, these measurements provide insight into the coupling between electronic structure, interfacial chemistry, and ionic transport during device operation.

Finally, I will discuss broader opportunities and limitations of photoelectron spectroscopy for halide perovskite research, including the influence of X-ray irradiation from both laboratory and synchrotron sources on the material itself.[6] Rather than representing solely a measurement artifact, controlled irradiation can also be exploited to investigate unusual physicochemical phenomena, including stimulated self-healing in formamidinium lead bromide, offering new perspectives on defect dynamics and material resilience.[7]

References

[1] J. Christians, et al. Nature Energy 2018, 3, 68

[2] P. Schulz, D. Cahen, A. Kahn, Chem. Rev. 2019, 119, 3349

[3] S. Béchu, et al. Adv. Energy Mater. 2020, 201904007

[4] N. Mallik, et al. Nano Energy 2024, 126, 109582

[5] N. Mallik, et al. EES Solar 2025, 1, 1004

[6] M. Ralaiarisoa et al. Small Methods 2023, 2300458

[7] V. Milotti, et al. Small Methods 2023, 2300222