

Operando Hard X-ray Photoelectron Spectroscopy Analysis of Halide Transport and Metal Corrosion in Perovskite Solar Cells

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In the past decade, organic-inorganic halide perovskite solar cells (HaPSCs) have made significant progress in power conversion efficiency (PCE nearly 26% [1]) and are a promising low-cost photovoltaic technology. However, their long-term stability and performance are hindered by the instability of their physicochemical and functional properties. Ionic transport has been identified as a critical factor leading to irreversible degradation. Ionic compounds can self-release from the perovskite absorber, inducing defects in the halide perovskite layer. These remaining defects are also sensitive to moisture and oxygen, which accelerate device decomposition. In this regard, identifying and profiling the ions and molecular fragments produced during the lifespan and degradation of HaPSCs is crucial [2]. Here we report an advanced *operando* synchrotron hard X-ray photoelectron spectroscopy (HAXPES) investigation of the dynamic behavior of iodide species in a MAPbI_{3-x}Cl_x (HaP) solar cell under an applied bias [Figure. 1 (left)].

Our study evaluated the performance and stability of stacked Au/Ag/AZO/PCBM/HaP/NiO/ITO/glass structures [3]. The components of the structure, AZO, PCBM, NiO, and ITO represent Al-doped zinc oxide, phenyl-C61-butyric acid methyl ester, nickel oxide, and indium tin oxide, respectively. The experimental core-level analysis showed that the migration of iodide (I⁻) ions from HaP to adjacent electron and hole transport layers required a threshold voltage above the open-circuit voltage (V_{OC}) when an ITO barrier layer was absent between Ag and AZO [Figure. 1 (right top)]. The study found that the diffusion of I⁻ in AZO/PCBM over time is unidirectional and follows a concentration gradient. This unidirectional diffusion of I⁻ leads to its absorption by the Ag layer, which forms a harmful silver iodide (AgI) compound. The deposition of an ITO layer between Ag and AZO as an ion diffusion barrier layer effectively restrained the formation of AgI, thereby improving the stability and performance of HaPSCs [Figure. 1 (right bottom)]. The study provides new insights into different degradation mechanisms and ways to enhance the stability and performance of HaPSCs.

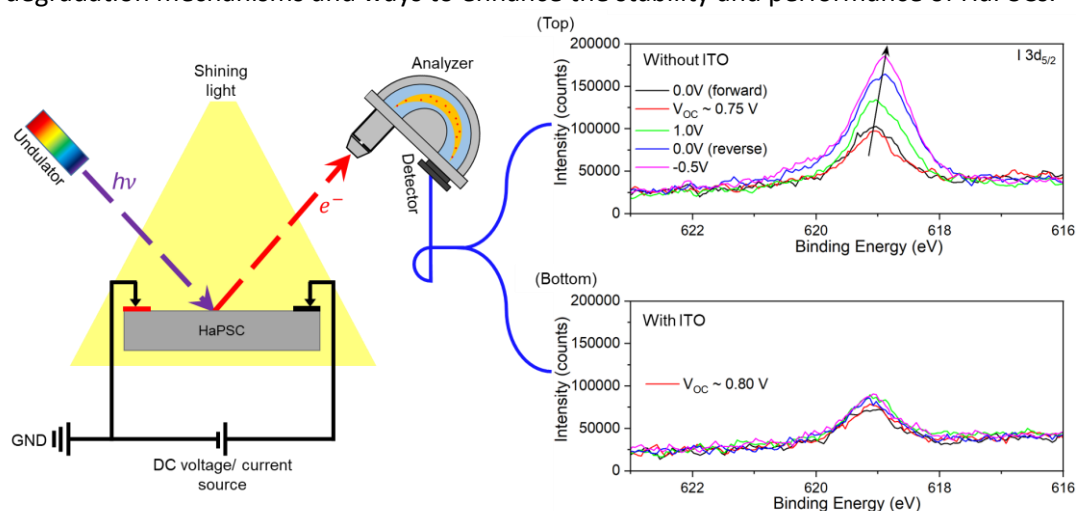


Figure 1: (Left) Simplified operando HAXPES analysis setup under bias voltage based on synchrotron X-rays; (Right) I 3d_{5/2} core level recorded at different bias voltages: (top) without and (bottom) with ITO barrier layer between Ag and AZO. Similar intensity scales and binding energy ranges are used to compare the intensity changes and energy shifts between samples without and with ITO.

1. Best solar cell efficiency chart; <https://www.nrel.gov/pv/cell-efficiency.html> (Accessed March 06, 2023).

2. Gueye et al., ACS Appl. Mater. Interfaces 2021, 13, 42, 50481-50490.

3. Gueye et al., ACS Chem. Mater. 2023, 35, 5, 1948-1960.