

Reversible and irreversible ion migration processes in lead halide perovskites for photovoltaics



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Lead hybrid perovskites are a promising family of photovoltaic absorber materials that have achieved power conversion efficiencies of over 20%. Lead halide perovskites are ionic materials with a low lattice energy which are unusual properties for a photovoltaic material. It has been conjectured that this ionic character may be responsible for the material's defect-tolerant optoelectronic properties that have enabled its success as an efficient photovoltaic material. However, lead halide perovskites are highly susceptible to ion migratory processes which pose a significant challenge to the commercialization of stable devices. In this talk, I will present experimental evidence for a variety of ionic migration processes in perovskite thin films resulting from optical or electrical excitation. We observe from in-situ XRD measurements that bromine-rich ($0.2 < x < 1$) $\text{CH}_3\text{NH}_3\text{Pb}(\text{Br}_x\text{I}_{1-x})_3$ and other mixed-halide perovskites undergo a structural transformation under photoexcitation, segregating into two distinct perovskite phases over the course of minutes. The optical properties are also changed by this transformation resulting in the appearance of intense photoluminescence and absorption features from a lower bandgap phase. The perovskite surprisingly reverts back to its original structure and starting optical spectra when left in the dark. We suggest that photoexcitation induces halide segregation, resulting in iodide-rich domains. These lower bandgap domains act as traps and are likely responsible for the poor open circuit voltages generated by large bandgap, bromine-rich ($0.2 < x < 1$) $\text{CH}_3\text{NH}_3\text{Pb}(\text{Br}_x\text{I}_{1-x})_3$ solar cells. Perovskite solar cells frequently exhibit hysteretic behavior, which is greatly aggravated by the presence of moisture. The influence of electric field and moisture on perovskite films was investigated using a combination of photocurrent, optical, Raman, and Auger mapping techniques on lateral thin-film devices. These studies suggest that irreversible field-induced degradation in air occurs via a hydrated phase, in which the organic cation is loosely bound and can drift in response to an electric field, finally degrading the material to PbI_2 .