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Sychrotron Techniques On Moisture Triggered Crystallization Of Triple-Cation Perovskite To Elucidate Phase Progressive Nucleation

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Synchrotron techniques have been used extensively to characterize the structure and interactions of the perovskite crystals and their complexes with both ex situ/in situ approaches. From the Grazing Incident Wide Angle X-ray Scattering/Small Angle X-ray Scattering (GIWAXS/GISAXS), literature reports the chemical pathways from the plumbate intermediates or meta-stable phase to perovskite crystal identified using in situ X-ray diffraction. However, time evolution of crystallization and phase transition in situ cases usually begins with the prepared solvent to inter-mediated complex film and finally to the perovskite crystal. A comprehensive investigation of perovskites crystallization dynamics and morphology evolution from original precursor solution of CH3NH3PbI3 pristine to solid phase crystals operando and in real time shows perovskite crystal intermediate, comprised of an octahedral [PbI6]4+ centre surrounded by cooperative ions. We present an exciting triple cation film degeneration when probed with humidity by GIWAXS and Mirco-Diffraction synchrotron techniques done at Lawrence Berkeley National Laboratory. High resolution Atomic Force Microscopy (AFM) and Scanning Electron Miscrosopy (SEM) gave polymorphy, crystallinity and molecular interactions with good surface morphology from the maps. On elevated Relative Humidities of about 50%, the films segregate back producing intermediate phases from GISAXS and microdiffraction results. We thus propose optimized film formation protocols for high performing perovskites to lucid crystallization pathways and irreversible films used to develop highly efficient and stable photovoltaic devices.

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