Synchrotron and optical probing of mixed halide perovskites for photovoltaics

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ABSTRACT

The methylammonium lead iodide $CH_3NH_3PbI_3$ ($MAPbI_3$) perovskites have attracted a lot of attention as a possible absorber material for thin film solar cells due to their bandgap energy, high optical absorption coefficients and low-cost solution-processing deposition approaches. $MAPbI_3$ perovskite solar cells have evolved with transformative potential with laboratory efficiencies greater than 20%. Perovskite absorber materials are very inexpensive to synthesize and simple to manufacture, making them an extremely commercially viable option. Perovskites of compositional variations ABX_3 can yield a range of crystal structures, phases and stabilities. The Goldschmidt's Tolerance Factor is a reliable figure of merit or empirical index to forecast the formation of preferred and stable structures and phases with ABX_3 mixed halide perovskite tolerance factors in the range of 0.9 to 1. Here, we probe perovskites of compositional variations ABX_3 with tolerance factors in the range of 0.9 to 1.0, and a large effective ionic radius greater than 200 pm. We report on the structural and optical properties of these perovskites. Photovoltaic (PV) devices were fabricated using these high tolerance factor perovskites. We report we have achieved power conversion efficiencies (PCEs) greater than 21% using the high tolerance factor perovskites investigated. The high tolerance perovskites were also characterized using synchrotron X-ray absorption near edge structure (XANES) spectroscopy at the National Synchrotron Light Source (NSLS) II at Brookhaven National Laboratory (BNL). XANES was used to probe the electronic structure of the high tolerance factor perovskites investigated.

Keywords: Mixed halide perovskites, Goldschmidt's tolerance factor, X-ray absorption spectroscopy, synchrotron radiation