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Intrinsic instability of metal-trihalide perovskite solar cell

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Metal-trihalide perovskite is a new promising third generation active material for solar cell applications. The material is crystallized in a perovskite structure ABX3, where A is an organic cation (e.g. formamidinium), B is the metal cation (lead) and X is the halide anion (iodine). Perovskites exhibit the power conversion efficiency, which is comparable to silicon photovoltaic devices. Perovskite material can be synthesized using low-temperature and low-cost method, combined with the ability to be made flexible, tunable band gap, broad range of absorption spectrum, and high carrier mobility required for solar cells. Although the properties are promising, there are challenges to overcome before perovskite solar cells can be viewed as a competitor to silicon technology. It is commonly assumed that the reaction with water or oxygen in the external environment leads to a poor stability of hybrid halide materials. Its instability appears like a spontaneous phase separation into the formamidinium iodide and lead(II) iodide. Here, we aim to use first-principles calculations to capture energies of the material degradation. Our calculations suggest that the decomposition is exothermic, independent of the water or oxygen in the external environment. It means that the poor chemical stability is intrinsic to metal-trihalide perovskite structure. Now we are working on understanding of the instability mechanism in virtue of electrostatic potential energy of the metal-trihalide perovskite structure. The result will guide the search for materials with improved stability.

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