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Formation and diffusion of metal impurities in perovskite solar cell materials CH3NH3PbI3: implications on the choice of the electrode and the solar cell degradation[1] WENMEI MING, MAO-HUA DU, Oak Ridge National Laboratory — Hybrid organic-inorganic lead halide perovskite CH3NH3PbI3 has emerged as a high efficiency solar absorber material. However, there are rising concerns on the chemical and electrical instabilities of CH3NH3PbI3 and the resulting device degradation. Recently, it was shown both experimentally and theoretically that Au ions can diffuse into the perovskite layer from the electrode causing device degradation even if there is a hole transport layer that separates the two. It is therefore important to understand the effects of the metal electrode on the performance and the stability of the CH3NH3PbI3 solar cell. Although many metal electrodes (e.g., Au, Ag, Cu, Al) have been studied experimentally, the nature of their interaction with CH3NH3PbI3 remains controversial. Here, we report first-principles calculations of a wide range of metal impurities in CH3NH3PbI3. The metal impurities were chosen based on whether their bulk forms have acceptable resistivities and work functions to be used as electrodes in CH3NH3PbI3 solar cells. The goal is to understand the stability and diffusivity of various metal impurities and their effects on carrier transport in CH3NH3PbI3. The implications of our results on the choice of electrodes in CH3NH3PbI3 solar cells are discussed.

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