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First Principles Investigation of Structural Stability and Electronic Band Structure of CH3NH2BiI3 for Lead-free Perovskite Solar Cell Application

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$CH_3NH_3PbI_3$-based perovskite solar cell continues to attract great attention because its power conversion efficiency has been increased rapidly, from 3.8% in 2009 to 22.1% in late 2017. However, the existence of the toxic Pb hindered further large-scale application. Recently, there are several Pb-free candidates that have been proposed. Among all promising candidates, the Bi-based perovskite could be a potential candidate in replacing the Pb-based one since the contribution from Bi 6s (instead of Pb 6s) near valence band maximum (VBM) may share the same characteristic such as the excellent hole transport properties. In addition, more electrons in frontier orbitals (6p) of Bi (compared to that of Pb 6p) are expected to introduce the stronger binding of Bi-I framework, which benefits structural stabilization. In this work, the Pb-free perovskite $CH_3NH_2BiI_3$ was considered and first principles density functional theory (DFT) was used to investigate its structural stability and electronic structures. The $CH_3NH_2BiI_3$ perovskite in orthorhombic structure (which is expected to be the most stable structure at the ground state) was used as an initial crystal structure for structural relaxation. From the results, the relaxed BiI_6 octahedral cage of the orthorhombic $CH_3NH_2BiI_3$ exhibits significant distortion with respect to PbI_6 octahedral cage of $CH_3NH_3PbI_3$. The formation enthalpy per unit formula (ΔH) of $CH_3NH_2BiI_3$ was found to be 0.13 eV lower than the total ΔH of CH_3NH_2 molecule and bulk BiI_3, indicating that $CH_3NH_2BiI_3$ is more stable and may be safe from getting decomposed into CH_3NH_2 and BiI_3 under small external perturbation. In addition, from the chemical potential diagram, it supports the equilibrium growth condition of $CH_3NH_2BiI_3$, i.e. synthesizable, while simultaneously prevents the occurrence of competitive compounds. From band structure calculations, $CH_3NH_2BiI_3$ has the band gap of 1.61 eV and low electron effective mass, which are comparable to those from $CH_3NH_3PbI_3$. However, the VBM was found to be mainly contributed by the electronic states from CH_3NH_2, instead of Bi 6s. It is relatively flat compared to the VBM of $CH_3NH_3PbI_3$, and thus has a larger hole effective mass. Since improvement of structural and electrical properties is usually desirable for development of novel Pb-free perovskite, our theoretical prediction on orthorhombic $CH_3NH_2BiI_3$, (with enhanced structural stability, synthesizability, small band gap, and low electron effective mass) suggests its capability to be another promising candidate in substituting the Pb-based perovskite solar cells.

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