Theoretical Study on Defect Formation Energies and Defect Transition Energies of $(CH_3NH_3)PbI_3$ for Bulk and Surface States

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The organic-inorganic hybrid halide perovskite, $CH_3NH_3PbI_3$, have attracted great attention for its diverse optoelectronic applications, including photodetectors, due to suitable direct band gap with large absorption coefficients. Nevertheless, theoretical studies on trapping states from the defect are not sufficient. Therefore, the defect formation energies and defect transition energies of various kinds of defects, including interstitial impurity, substitution impurity, and vacancy were investigated by density functional theory (DFT) calculations. In this study, we compared those energies in bulk and surface states and found that the defect formation energy was much lower at the surface. Especially, the substitution defect at the surface, MAPb and IPb, showed negative formation energies. In addition, p-type and n-type deep trap levels were calculated in the bulk and surface system, respectively. We expect that deep trap levels at the surface could efficiently increase the dark current via low formation energies. Therefore, the nanoparticle or granular structures of $CH_3NH_3PbI_3$, which have large surface area, could increase the efficiency of the photodetector.