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Less-lead $FAPbI_3$ (100) Surfaces, A theoretical Study

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Hybrid organic-inorganic perovskite solar cells (PSCs) have recently become one of the most efficient materials for photovoltaic applications [1]. Formamidinium lead triiodide ($FAPbI_3$) perovskites possess high light absorption and stability, making them strong candidates for efficient solar cells, yet they suffer from toxicity. The optoelectronic characteristics of environmentally friendly alkaline earth metals substituted $FAPbI_3$ (100) surfaces, in various percentages, with PbI_6 and PbI_5 terminations has been investigated using density functional theory (DFT) as implemented in the Vienna ab initio simulation package [2], (VASP 5.4.4). We have created 14 stable doped structures according to the Goldsmith tolerance factor [3], in the form of $FAPb_{1-x}AE_xI_3$, (AE= Be, Mg, and Ca). Different terminations showed a negligible influence on the optical features, although their effect on the electronic properties is significant. Due to the conduction band (CB) shifting of the PbI_6 termination to the higher energies, an increase of about 0.3 eV in the bandgap of this termination was obtained compared to that of PbI_5, and suitable bandgaps of 1.623 and 1.309 eV were calculated for them, respectively. In doped systems, Mg and Ca substitution made broader bandgaps, while two different decreasing and increasing trends on the bandgap of $FAPb_{0.95}Be_{0.05}I_3$ and $FAPb_{0.96}Be_{0.04}I_3$ structures were observed. Promising optical activity such as appropriate extinction coefficient and light harvesting efficiency for plain and doped (100) surfaces in the visible and UV windows and also the high capacity of all structures to absorb more photons, especially in the near UV region for doped counterparts, altogether, indicate the capability of the (100) surfaces for optoelectronic applications.

Keywords: alkaline earth metals, $FAPbI_3$, perovskites, doping, density functional theory

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