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Tailoring Optoelectronic Properties of All Inorganic Perovskites Through B-site Doping: A DFT Study

Lead halide perovskites have shown great promise as solar absorbers for next-generation photovoltaics, but their toxicity poses significant challenges for practical use. As a result, considerable research has focused on developing environmentally friendly, lead-free alternatives with similar optoelectronic properties, including perovskites based on Sn, Ge, Mo and Bi. In this study, the first-principles calculations based on density functional theory were used to determine the structural, electronic and optical properties of $CsPb1\text{-}xMxBr_3$ ($0 \leq x \ll 1$) perovskite, where M = Bi and Mo. These calculations reveal that low-level doping leads to significant changes in the electronic density of states, introducing localized defect states and bandgap tuning effects, without compromising the host lattice stability. Bi doping induces shallow states near the conduction band, promoting improved charge transport, while Mo doping introduces deeper levels, potentially enhancing light absorption in the visible region. The optical spectra show enhanced absorption coefficients in the solar spectrum, indicating potential improvements in light-harvesting efficiency. These results demonstrate that controlled doping with Bi and Mo in CsPbBr3 provides a promising solution for optimizing all-inorganic perovskites in solar cell applications and paves the way for further experimental exploration of dopant engineering in halide perovskites.

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