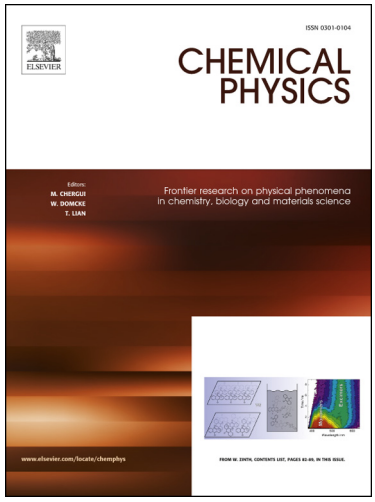

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DFT prediction of band gap in organic-inorganic metal halide perovskites: an exchange-correlation functional benchmark study

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Abstract

We report a comprehensive and systematic study of two halide perovskites by using density functional theory calculations. Two structurally different perovskites have been studied, which are cubic $CH_3NH_3PbI_3$ (**MAPI**) and $HC(NH_2)_2PbI_3$ (**FAPI**). We have used twenty-four exchange-correlation functionals, ranging from three LDA functionals, ten GGA functionals, seven MGGA and four hybrids among others have been tested, in order to determine the accuracy of these methods for the prediction of band gaps. Moreover, we have studied several possibilities to tackle the calculations of perovskites. That is, we have tested Numerical Atomic Orbitals with All Electron Relativistic calculations and compared to Plane Wave framework with pseudopotentials and relativistic corrections. Moreover, we have studied different k-points set, pseudopotentials types, with and without cell optimizations, with and without dispersion corrections and with and without Spin Orbit coupling. The results show that PBE and RPBE exhibit a good compromise between the accuracy of the results and computational demands.

Keywords

DFT methods; Perovskites; Band gap; Exchange-Correlation Functionals; m-GGA