Structural, Electronic and Optical Properties of cubic and orthorhombic $CsPbI_3$ perovskite: DFT Investigation



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Cesium lead Iodide ($CsPbI_3$) perovskite has recently attracted significant attention owing to its rapidly increasing competence when used for solar cell devices. In this study, we make a comprehensive DFT calculation study to determine the structural, electronic, and optical properties of cubic and orthorhombic temperature-dependent phases of $CsPbI_3$ perovskite using the full potential linear augmented plane wave method. For this purpose, different exchange potentials: local density approximation (LDA), Perdew–Burke–Ernzerhof generalized gradient approximation (PBE-GGA), Wu-Cohen generalized gradient approximation (WC-GGA), Engel–Vosko generalized gradient approximation (EV-GGA), Perdew–Burke–Ernzerhof revised for solids (PBEsol), modified Becke–Johnson generalized gradient approximation (mBJ-GGA), new modified Becke–Johnson generalized gradient approximation (nmBJ-GGA), and unmodified Becke–Johnson generalized gradient approximation (umBJ-GGA) were used. Our results on band structure indicate that the cubic and orthorhombic phases have direct energy bandgaps. Among all potentials, bandgaps calculated using the mBJ-GGA method gives the best agreement with experimentally reported values. Additionally, despite the large variations in their lattice constants, the tow phases of $CsPbI_3$ possessed almost similar optical properties. This result indicates a wide temperature range of operation for $CsPbI_3$.

Biography

Hamid Mansoor Ghaithan is a PhD at King Saud University. He is working with perovskite materials simulation using density functional theory.

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