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Structural, Electronic and Optical Properties of cubic and orthorhombic CsPbI3 perovskite: DFT Investigation

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Abstract

Cesium lead Iodide (CsPbI3) 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 CsPbI3 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 CsPbI3 possessed almost similar optical properties. This result indicates a wide temperature range of operation for CsPbI3.

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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