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AB-INITIO study of structural, elastic, electronic and optical properties of ABX3 based perovskites for solar cell application

In this theoretical study, the structural, electronic and optical properties of KBX3 (B = Ge, Sn; X = Cl, I) based perovskites are systematically studied using first principle density functional theory. Self-consistent calculations are performed using plane wave ultra-soft pseudopotential technique and the generalized gradient approximation of Perdew–Burke–Ernzerhof scheme is used to treat the exchange-correlation interactions. The calculated structural parameters are in good accordance with the existing experimental data and theoretical calculations. Elastic constants, Pugh's ratio, bulk modulus, Poisson's ratio and anisotropy factor are studied for the analysis of elastic characteristic. The band structures are calculated and analyzed with respect to variation; (i) as B varies from Ge to Sn and (ii) as X ranges from Cl to I. Furthermore, optical properties of the ABX3 compounds are investigated in details and the analysis reveals that KGeCl3, and KSnCl3 and KSnl3, are promising materials for solar cell applications.

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