$Cs_2AlCuCl_6$: A NEW CLASS OF LEAD-FREE DOUBLE PEROVSKITES WITH PROMISING STRUCTURAL, MECHANICAL, ELECTRONIC AND OPTICAL PROPERTIES

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Abstract

This work presents a comprehensive first-principles study of the structural, mechanical, electronic and optical properties of the novel lead-free double perovskite semiconductor $Cs_2AlCuCl_6$. The full-potential linearised augmented plane wave ($FP-LAPW$) method was employed within the framework of density functional theory

(DFT). We analysed the energetic stability, Goldschmidt tolerance factor (τ) and mechanical properties of this compound. Our findings confirm that $Cs_2AlCuCl_6$ has a perfectly cubic structure within the $Fm-3m$ space group. Furthermore, the mechanical analysis revealed that this material is highly elastic and strong, with high bulk and Young's moduli, highlighting its mechanical robustness. Electronic structure calculations demonstrate that $Cs_2AlCuCl_6$ has direct band gaps of 0.63 eV (GGA) and 1.81 eV (mBJ). Additionally, this compound exhibits significant optical absorption in the visible spectrum, suggesting its potential application in energy conversion technologies. To our knowledge, this is the first study to provide a predictive analysis of $Cs_2AlCuCl_6$, as no previous theoretical or experimental data is available for comparison.