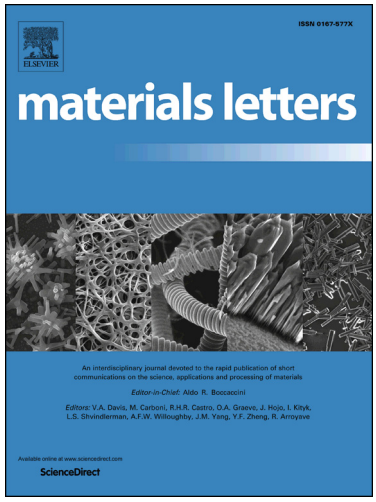

Electronic, Optical and Mechanical Properties of Lead-Free Halide Double Perovskites using First-Principles Density Functional Theory

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Electronic, Optical and Mechanical Properties of Lead-Free Halide Double Perovskites using First-Principles Density Functional Theory

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Abstract

First-principles density functional theory calculations were employed to study the structural, electronic, elastic and optical properties of lead free perovskites Cs_2AgBiX_6 (X = Cl, Br and I) in the cubic phase. Calculations were performed with spin–orbit coupling (SOC) for predicting the accurate band gap and comparison is made with calculations excluding SOC. The calculated band gaps for $Cs_2AgBiCl_6$, $Cs_2AgBiBr_6$ and Cs_2AgBiI_6 are 1.91 eV, 1.42 eV and 0.89 eV respectively and are in good agreement with reported theoretical and experimental results. It is evident from the partial density of state diagrams that the anti-bonding Ag/5*s* and Bi/6*p* states to the halogen 3*p*/4*p* states are involved in the transition from conduction to valence band and this interaction leads to an indirect band gap. Variations in the structural, mechanical, optical and electronic properties of the lead free halide double perovskites Cs_2AgBiX_6 under various exchange correlations are fully investigated. Our studies provide theoretical support for their potential optoelectronic application in solar energy conversion.

Keywords: Halide Double Perovskites, Density Functional Theory, Elastic Properties, Solar cell

1. Introduction

Solar cells based on organolead halide perovskites have seen rapid progress, and is found to be one of the most promising photovoltaic technologies, owing to their solution-processability, low-cost and high efficiencies in the past few years [1, 2, 3, 4].

Power conversion efficiency of organic-inorganic halide perovskites solar cells has reached 22.7% [5]. Significant properties of perovskites like ferroelectricity [6], photoluminescence, superconductivity [7], topological insulators [8] are observed in sensors, solar-cell absorbers, fuel cells (catalytic electrodes) and in optoelectronics. Recent experimental and theoretical results [11, 12, 13, 14, 15] show that halide double perovskites with Ag and Bi possess band gaps which lie in the range of 1.83 eV to 2.19 eV. Very recent computational studies conducted on disordered $Cs_2AgBiBr_6$ system, via controlled doping, show that one can tune the bandgap from 1.93 to 0.44 eV [10].

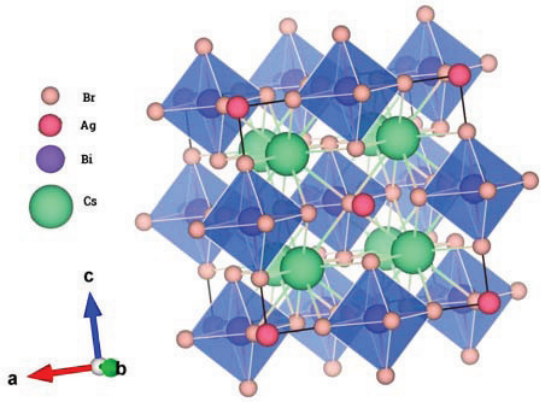

Figure 1: Optimised crystal structure of the halide double perovsite $Cs_2AgBiBr_6$. (Fcc, space group $Fm\bar{3}m$ −225)

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