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Computer based predictions of structural stability and systematic study of magneto-electronic and optical properties of Lead Free Halide Double Perovskites: Cs_2KXCl_6 : X = Co and Ni

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ABSTRACT

In this study, the structural stability, optoelectronic, and magnetic characteristics of lead-free halide double perovskites Cs_2KXCl_6: X = Co and Ni were revealed and understood utilizing a rigorous and systematic investigation employing the density functional theory adopted in WIEN2k simulation software. The given double perovskites are stable in cubic structure having Fm-3 m symmetry, this stability was confirmed by optimized structural, satisfying criteria of mechanical stability and tolerance factor. The half-metallic ferromagnetic feature of materials is caused by unpaired electrons in the crystal field splitted d-orbitals of Co and Ni. The total magnetic moments of these double perovskites were computed, and the calculated results were 4 μB for Cs_2KCoCl_6 and 1 μB for Cs_2KNiCl_6, with the transition metal atoms contributing the most. The fact that these double perovskites exhibit 100% spin polarization at the Fermi level suggests that they might be used in spintronics.

1. Introduction

In electronic science and engineering, spintronics is an emerging technology, as spin degrees of freedom to electrons were used, to develop new materials having novel functionalities. Spintronics is also named magneto-electronics in solid-state devices. In addition to its underlying electronics charge, spintronic makes advantage of the electron's intrinsic spin and related magnetic moment [1]. A large-scale search for novel materials with potential uses in spintronics technology is underway. It can outperform traditional electronic devices in terms of power consumption, processing speed, and non-volatility data capacity [2]. Materials having high spin polarization plays an important role in spintronics. In this field, the materials with 100% polarization at the Fermi level are deserving candidates for half metallicity. In half-metallic materials, the minority spin channel has a bandgap at the Fermi level (E_F), while the majority spin channel overlap with the fermi level and has a metallic character, and the electrons have 100% spin polarization(SP) at the E_F due to the bandgap for one spin channel [3–5]. The magnitude of spin polarization at the Fermi level is defined by the ratio of density of states (DOS) in the spin-up and spin-down orientations, given as $SP = (N_\uparrow - N_\downarrow)/(N_\uparrow + N_\downarrow)$, here $N_\uparrow$ and $N_\downarrow$ represents spin up and spin down occupied states at E_F, respectively [6,7]. The crystal structure, total number of valence electrons, covalent bonding, and significant d-states splitting of electrons, all influence the half-metallic response in materials. Because of 100% spin polarization of half metals, they have a significant role in spin-based electronics and also spin-dependent devices will have an extremely high-efficiency [8]. The spin polarization effect is absent in diamagnetic and paramagnetic materials because the spin-up and down channels have symmetric DOS. On the other hand, the asymmetric DOS of Ferromagnetic materials means that the value of their Spin Polarization is between 0 and 1. Materials with 100% SP at the Fermi level are considered appropriate for spintronic technology.

Half-metals are a type of ferromagnetic material that may be used as both a metal and a semiconductor [9,10]. Using first-principles calculations, de Groot et al. predicted the half-metallic compounds in 1983. They discovered half metallicity in the Heusler alloy for the first time (NiMnSb, PtMnSb) [3]. Later, a variety of materials were studied theoretically and experimentally to detect half-metallic ferromagnetism, including perovskite, double perovskite, transition metal pnictides [11], oxide compounds, and spin-directed materials. The stoichiometric formula for perovskites is ABX_3, where A belong to s or p block element, B from transition or inner-transition elements/part of the s/p block elements, and X is either a halogen element (halide perovskites) [12] or oxygen (oxide perovskites) [13]. The flexibility

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