



DFT investigations on the electronic structure, magnetism, thermodynamic and elastic properties of newly predicted cobalt based antiperovskites: Co_3XN ($\text{X} = \text{Pd}, \text{Pt} \text{ \& \ } \text{Rh}$)

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ABSTRACT

In this report, we have applied the muffin tin orbital method within full-potential linearized augmented plane wave approximation to investigate the intricate details of the electronic structure, elastic properties and magnetism of antiperovskite compounds Co_3XN with $\text{X} = \text{Rh}, \text{Pd}$ and Sn . The detailed analysis of the electronic structure calculations using various chemical bonding indicators suggest the covalent hybridization of the electronic states associated with Co (the high valency transition element) and the X atom (low valency transition element) as the significant interaction liable for the exhibition of the octahedral symmetry by these alloys. The large magnetic moments of Co_3RhN , Co_3PdN and Co_3PtN are observed to be 6.20 μB , 5.20 μB and 6.21 μB , respectively; with a net magnetic moment of around 4.7 μB contributed by Co atoms in each compound. The direct exchange between Co and X atoms and indirect interaction between Co and Co via N atoms is responsible for its ferromagnetic character. The influence of the strain on the overall magnetism and relative atomic moments in the unit cell is also investigated. The anisotropic nature of these alloys and the mechanical properties like ductility increases from $\text{Rh} > \text{Pd} > \text{Pt}$. Also, the Debye temperatures of Co_3RhN , Co_3PdN and Co_3PtN are calculated to be 702 K, 689 K and 606 K, respectively.

Introduction

Among the thousands of members of perovskite family, plethora of materials within the ABO_3 class [1,2] are inquired for their potential applications. Antiperovskites (APV's) are the chemical analogues of simple perovskites where A and O atoms are interchanged by rare-earth or transition-metal ions [3,4]. This class has become an active research field and paved the way to predict some new materials as well as the novel tactics or strategies to explore their physical properties to be applicable in future technologies. The breakthroughs of having large Curie temperatures [5], superconductivity [6], spin glass or topological behavior [7,8], negative thermal expansion [9] and magneto-restrictive effects [10] have intensified their insights for new possibilities. Moreover, without negotiating on other features, the strong ferromagnetic

(FM) order can be induced in such materials, and this recommends the useful comprehensions into the design and manufacturing of spintronic devices or a variety of next-generation device applications [11,12].

Broadly speaking, simple perovskites are having two variants: the normal perovskites and inverse perovskites, which only differ in the stoichiometry and either contain oxygen or other halide atoms. In simple perovskites with ABO_3 -type composition, specifically the atomic positions are A at (0, 0, 0), B at (0.5, 0.5, 0.5) and O at three possibilities in (0.5, 0.5, 0.0) location within Pm-3 m structure [13]; while in M_3XZ type inverse perovskites, the locations are interchanged as X at (0, 0, 0), Z at (0.5, 0.5, 0.5) and M at three possibilities in (0.5, 0.5, 0.0) within the same space group [14]. Here M can be 3d-transition metal or rare-earth, X and Z atoms mostly constitute the 4d or 5d elements or p-group elements. Recently, the magnetic APV's like Mn_3SnC [15] and

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