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Electronic structure, magnetism and elastic properties of Inverse Perovskite Carbide: A first principles study

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ABSTRACT

Antiperovskite materials display many fascinating properties like that of perovskites. We summed up the electronic, magnetic and mechanical properties of Ni_3LiC compound in this work, via density functional theory calculations. The structural optimization via the Birch-Murnaghan approach supply the lattice parameters and ground state energy within the *Fm-3m* space group. Spin resolved band occupation and density of states define its metallic nature with a total ferromagnetic moment of 0.76 μB. The effect of uniform strain is analysed, which shows the increase in magnetic moment with the expansion of the lattice and vice versa. The speculated elastic constants and their different combinations conclude the mechanical strength and stability of this material. The large bulk modulus and B/G ratio claims its ductile and incompressible nature and the Zener's parameter reflects the exhibition of anisotropic properties.

1. Introduction

Perovskite compounds of different classes such as chalcogenide perovskite (AMO_3), double perovskites ($A_2BB'O_6$), Inverse and halide perovskite (ABX_3) have been widely studied from the past few decades [1–4]. Antiperovskites (APVs), mostly being oxygen free materials are the structural analogous of perovskites with remarkable properties. For example the properties include, thermoelectricity in Co_3SnC with a Seebeck coefficient of about 50 μV/K [5] and AXD_3 (A = Ge, Sn, Pb, Al, Zn, Ga; X = N, C; D = Ca, Fe, Co) [6]); superconductivity in Ni_3MgC1 with a critical temperature of 8 K [7], Cr_3GaN and Cr_3RhN [8]; nontrivial topological nature in Cu_3PdN [9] and A_3BX with A =(Sr, La, Ca), B = (Sn, Pb), X=(O,N,C) [10]; spin glass behavior in $GeNCo_3$ [11] and $Mn3Cu_{0.7}Ga_{0.3}N$ [12]; baromagnetic effect in $Mn3Ga_{0.95}N_{0.94}$ [13] and barocaloric effect in Mn_3GaN [14]; magnetostriction in Mn3CuN [15], negative thermal expansion in Mn_3ZnN [16], piezomagnetism in Mn_3AN (A = Rh, Pd, Ag, Co, Ni, Zn, Ga, In, Sn) [17], etc. Still the unexplored treasure of such multireference materials with intriguing properties is being tailored to accommodate some new chemical combinations of elements in the primitive M_3XZ crystal structure.

Recently, Sing *et al* carried out a high throughput DFT investigation on 630 cubic antiperovskites M_3XZ (M = Cr, Mn, Fe, Co, and Ni; Z = C, N; and X is one of the elements from Li to Bi except noble gases and 4f rare-earth metals) and screened 11 novel APV's with stability confirmed from thermal, dynamic and mechanical criteria [18]. Hence, there is a strong motivation to follow-up the experimental verifications on such stable APV compounds for future applications. Among them Ni_3LiC is one of the materials which is being considered in the present study. However, the electronic structure, elastic and magnetic studies on this material are not explored well. Thus, we tried to discuss the effect of strain on the structural, electronic and magnetic properties of Ni_3LiC. This material crystallizes in a *Pm-3m* cubic structure with Li atoms located at the eight corners of a cube, C atom at the body center, and the Ni atoms are located at six face centers of a cube (see Fig. 1). In the methodology section, the theoretical background and the details of calculations methods, exchange correlation potentials, cutoff parameters and convergence criteria are described. Then, the results and discussion part contain the detailed description of the physical properties under the subheadings of structural, electronic, magnetic and elastic properties. Finally, the conclusive remarks about the findings of Ni_3LiC are enlisted in the conclusion section.

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