Physics Letters A 442 (2022) 128178

Contents lists available at ScienceDirect

Physics Letters A

www.elsevier.com/locate/pla

First-principles calculations to investigate structural, electrical, and optical properties of half Heusler alloy LiCrN

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ARTICLE INFO

Article history:
Received 7 March 2022
Received in revised form 19 April 2022
Accepted 26 April 2022
Available online 30 April 2022
Communicated by J.G. Lu

Keywords:
Half Heusler alloy
LiCrN
Half-metallicity
DFT study
Optical properties

ABSTRACT

It is important in spintronics to find high performance materials that can be employ in this field. Based on the density functional theory (DFT), first principles calculations are utilized to inspect the structural, electrical and optical features of half Heusler structure LiCrN. The equilibrium lattice constant is equal to 5.11 Å. The electronic structure results display that the alloy LiCrN shows a half-metallic property. It appears that this structure has semiconductor property with an indirect band gap of 3.65 eV in (PBE-GGA) and 5.06 eV in (HSEO6) in spin down channel and the other spin channel has metallic property. The Cr atom is more effective than the other elements in this material as it carries more valence electrons in outer shell. The spin polarization shows 100% at the Fermi-level. According to Slater–Pauling rule ($Z_t - 8$), the total magnetic moment equals 4 μ_B. Additionally, we study the optical properties as we have semiconductor property in one of spin channels so it can be a candidate in optoelectronic devices. The results appear that this structure is promising in spintronics potential applications.

1. Introduction

The most attractive prospects for spintronics materials are half-metallic ferromagnetic (HMF), which shows metallicity only in a single spin states out of each two and are expected to have a spin polarization (SP) of 100% around the Fermi level (E_F) [1]. The Heusler alloys exhibit metal and semiconductor properties in the spin-up and spin-down channels, respectively. De Groot et al. were the first to recognize half-metallic ferromagnetism as a fact in NiMnSb in 1983 [2]. Until far, various kinds of compounds have been discovered to be HMF, including full-Heusler compounds [3–11], rutile-kind [12], spinel [13], pyrite structure [14], double perovskite and perovskite [15,16], and some diluted magnetic semiconductors [17–20]. Half Heusler alloys with half-metallic properties and high spin polarization at Fermi level consist of LiMnZ (Z = N, P, Si) [21], XCrZ (X = Li, K, Rb, Cs, Z = S, Se) [22], MnVZ (Z = P, As, Sb) [23], NaZrZ (Z = P, As, Sb) [24], RhCrZ (Z = Si, Ge) [25], NiTiX and CoVX (X= Sb and Sn) [26], CoCrZ (Z = Al, Ga) [27], FeVX (X = As, P) [28] and IrCrZ (Z = Ge, As, Sn, Sb) [29]. Because the energy band gap encompasses a large range of frequencies of electromagnetic waves, from in the range infrared to ultraviolet [30–32], optical characteristics of 2D materials have been widely explored [33–38]. Because the combination of electrical and optical properties permits the regulation of electronic current or optical transitions with different degrees of freedom, is important in fundamental physics and applications in electronic–photonic systems.

Magneto-electronics, electro-mechanics, and spintronics are just few of possible applications where these materials could be useful. Depending on the dimensionality and the environment, the transition metals are exceptionally significant because they permit interactions of complex magnetic, resulting in fascinating magnetic, magnetoelectric, piezo-electric features [39–41], and the conversion of non-magnetic materials to magnetic materials [42]. A broad scope of electrical, magnetic, and optical characteristics were discovered in previous studies [43]. The electronic, magnetic and optical properties of the TM are mostly determined by the TM 's' unfilled or filled 'd' bands. Half Heusler alloys are unique from the other Heusler alloys that have high Curie temperature and lattice constants are compatible with semiconductor substrates. Optical applications, magnetic tunnel junctions, power storage, semiconductors, lenses, and medicinal applications have all used these materials [44]. A lot of investigations are carried out on the bulk, interface and surface characteristics of half metallic materials [45–49].

In the current study, we studied new LiCrN compound where the structural, electronic, magnetic, and optical properties of LiCrN by means of first-principles calculations based on density func-

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https://doi.org/10.1016/j.physleta.2022.128178
0375-9601/