Journal of Electron Spectroscopy and Related Phenomena 244 (2020) 146991

Contents lists available at ScienceDirect

Journal of Electron Spectroscopy and Related Phenomena

journal homepage: www.elsevier.com/locate/elspec

First-principles study of half-metallicity bulk rocksalt structure of CsTe and its surfaces

Jabbar M. Khalaf Al-zyadi [a,*], Ahmed Hamad Ati [a], Kai-Lun Yao [b,c]

[a] Department of Physics, College of Education For Pure Sciences, University of Basrah, Basrah 6100, Iraq
[b] School of Physics and Wuhan National High Magnetic Field Center, Huazhong University of Science and Technology, Wuhan 430074, China
[c] International Center of Materials Physics, Chinese Academy of Sciences, Shenyang, 110015, China

ARTICLE INFO

Keywords:
Rocksalt CsTe
Half-metallicity
First-principle study
Formation energy
Surface properties
Density of states

ABSTRACT

We report on the calculation of the structural, electronic, magnetic and half-metal properties of the rocksalt CsTe compound using the first principles method which is based on density functional theory. Although this compound does not possess any transitional metal in its formula, it is found to carry the half-metallic ferromagnetic property at bulk as well as the surfaces. The energy gap is equal to 3.32 eV at the equilibrium lattice constant of 7.7 Å. The formation energy is calculated to be -2.91 eV which reveals that this compound is stable. All the above-mentioned properties with the remarkable features open up the possible employment of the investigated material in several applications related to spintronics.

1. Introduction

Spintronics (spin transport) is a modern field arising from microelectronics and the spintronic devices aim to employ the spin of electrons and the electrons charge to process information [1]. These devices have given more interesting characteristics to spintronic applications including spin valves, nonvolatile magnetic random access memories (MRAM) and magnetic devices [2]. In 1983, de-Groot et al. found the novel class of materials which were called half-metal (HM) ferromagnetic in the half- Heusler ($C1_b$) type in the compounds NiMnSb and PtMnSb according to the first-principles calculations [3]. This class of HM ferromagnetic materials offers a spin channel. One of them is the metallic feature with no gap at a majority or minority spin. The other is the semiconducting or insulating feature with a finite gap at the majority or minority spin in another channel which yields 100 % spin polarization around the Fermi level. Above room temperature, the HM ferromagnetic material offers stability to ferromagnetism [4]. This class becomes important and promising in spintronic devices due to the high spin polarization of this material.

According to the asymmetric electron occupation in the both spin channels, the HM ferromagnet is required to have integral total magnetic moments. Subsequently, many different HM ferromagnetic classes have been predicted theoretically or/and confirmed experimentally [5–11]. The HM ferromagnet has been included in many systems such as full-Heusler alloys ($L2_1$) in Co_2TiSn [5], half-Heusler alloys ($C1_b$) in IrCrZ (Z = Ge, As, Sn and Sb) [6], quaternary alloys in CoFeHfGe [7], perovskite compounds such as $LiBeO_3$ [8], metallic oxides such as CrO_2 [9], and binary compounds such as zinc-blende (ZB) (space group F $\overline{4}$ 3 m, No. 216) such as MnAs [10] and rocksalt (RS) (space group Fm $\overline{3}$ m, No. 225) such as CaSe [11]. All these materials have benefited from the HM ferromagnetic advantage.

Nearly, HM ferromagnet must have a transition metal (3d) in both ZB structures such as CrS [12] and RS such as FeO [13] in all binary compounds. Some binary compounds were reported to be HM ferromagnetic because they do not contain the transition metal (3d) in both ZB and RS structures such as MN (M = Na, K) [14]. The binary compounds must have a high Curie temperature (T_C) which is essential to make spintronic devices [15–17]. Due to the low magnetic moments of the sp half-metallic ferromagnets, they become a favorite base of several spintronic applications [18]. In the recent years, many works have focused on numerous sp magnets such as perfect and glitch bulk solids, nano materials, surfaces and interfaces [19–26]. However, nearly all HM ferromagnets were generally utilized in the form of thin films or multilayers in spintronic devices [27].

In this regard, this study aims to examine the RS CsTe material which does not contain transition metals (3d) in the structure and contains an HM at the bulk [28]. In fact, the surfaces of RS CsTe at (111), (110) and (001) are studied using the first principles calculations. This CsTe

* Corresponding author.
E-mail addresses: Jabbar_alzyadi@yahoo.com, gabbar_alzyadi@yahoo.com (J.M.K. Al-zyadi).

https://doi.org/10.1016/j.elspec.2020.146991
Received 26 April 2020; Received in revised form 18 July 2020; Accepted 15 August 2020
Available online 5 September 2020