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





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ARTICLE INFO	A B S T R A C T			
Keywords: Rocksalt CsTe Half-metallicity First-principle study Formation energy Surface properties Density of states	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 cinternics.			

### 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<sub>b</sub>) 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<sub>1</sub>) in Co<sub>2</sub>TiSn [5], half-Heusler alloys (C1<sub>b</sub>) in IrCrZ (Z = Ge, As, Sn and Sb) [6], quaternary alloys in CoFeHfGe [7], perovskite compounds such as LiBeO<sub>3</sub> [8], metallic oxides such as CrO<sub>2</sub> [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<sub>C</sub>) 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

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Received 26 April 2020; Received in revised form 18 July 2020; Accepted 15 August 2020 Available online 5 September 2020 0368-2048/© 2020 Elsevier B.V. All rights reserved. compound has maintained the half- metallic characteristic in bulk and in all surfaces.

## 2. Computational method

In the current study, all the calculations are made using the first principles full-potential augmented plane wave (FPLAPW) along with the Win2k code [29,30], which are both applied to explore the electronic and magnetic properties of the (111), (110) and (001) surfaces. The generalized gradient approximation (GGA) that was offered by Perdew-Burke-Ernzerhof (PBE) is applied to determine the functional electronic exchange correlation [31,32]. For the Brillouin zone integration, the k-point meshes of  $12 \times 12 \times 1$  for the bulk RS CsTe,  $12 \times 12 \times 1$  for the CsTe in (111), (001) surfaces and  $9 \times 12 \times 1$  for (110) surface are utilized. The maximum value of the angular momentum  $(l_{max})$  is set to be (10). In the interstitial region, the plan cut off  $K_{\text{max}} \times R_{\text{mt}}$  is equal to 8. The radii of muffin tin spheres are set to 2.5 a.u for the atoms Cs and Te. When the separation energy is less than  $10^{-5}\,$ Ry, it means that the calculations of the self-consistency are completed. The electronic configurations (for valence electrons) are being in the form of Cs:  $6 s^1$  and Te:  $5s^2$ ,  $5p^4$ .

### 3. Results and discussion

## 3.1. Relaxation and stability of (111), (110) and (001) surfaces

In order to calculate the properties of (111), (110) and (001) surfaces of the compound RS CsTe, the optimum atomic layers in the slab model for each surface are chosen according to the DOS and the magnetic moments. A slab modal is built, containing thirteen atomic layers which are sufficient to study the electronic and magnetic properties at the surfaces. The equilibrium lattice constant (7.7 Å) of the RS CsTe represents the basis of the construction of the slab model. 15 Å vacuum level above the surfaces is added in order to avoid interactions between adjacent slabs. It is also known that the (111) surface contains one kind of atom, which leads to obtain two types of ends; one of them is Csterminated and another is Te-terminated as indicated in Fig. 1 (b) and (c). For the (110) and (001) surfaces, there is only one type of terminations for each of Cs and Te, since each layer contains both of them in the same layer as illustrated in Fig. 1 (d) and (e). Firstly, four atomic layers at the top of the slab are relaxed and the thickness of the slab relaxes in order to study the surface properties at the equilibrium state for (111), (110) and (100) surfaces by reducing the total energy and atomic force. After relaxation, both ends of Cs/Te slabs for CsTe compound are offered when the atoms of the surface layers move toward the center of the slab, while the atoms at subsurface (1) move toward the vacuum. In addition, the location of atoms at subsurface (2) is much lower than at the surface and subsurface (1). For both Cs- and Te- terminations of the (111) surface, the bond length between the surface and



**Fig. 1.** (a) The crystal structure of bulk RS CsTe, (b) Cs-terminated (111), (c) Te-terminated (111), (d) CsTe-terminated (110) and (e) CsTe-terminated (001) surfaces.

subsurface (1) before relaxation is equal to 3.850 Å. After relaxation, it decreases to 3.603 and 3.813 Å for both Cesium and Tellurium terminations, respectively. The distance between the subsurface (1) and subsurface (2) before relaxation is equivalent to 3.850 Å, while it increases to 3.933 Å for the Cs-termination and then decreases to 3.849 Å for the Te-termination after relaxation. For the (110) and (001) surfaces, the Cs atoms move inward the slab while the Te atoms move outward because of the charge movement from the Cs cation to the Te anion, whereas the bond length for (110) and (001) surfaces is equal to 3.850 Å. After relaxation, the bond lengths for (110) and (001) surfaces are equivalent to 3.850 and 3.871 Å, respectively and the bond lengths between the subsurfaces are 3.851 and 3.862 Å.

In order to compare the stability among (111), (001) and (110) surfaces, the surface energy ( $\sigma_{CSTe}$ ) is also calculated as follows:

$$\sigma_{CsTe} = \frac{1}{A} \left( E_{tot} - \mu_{Cs}^{slab} N_{Cs} - \mu_{Te}^{slab} N_{Te} - TS - PV \right) \tag{1}$$

Where A is the area of the surface,  $E_{tot}$  is the energy relaxed CsTe slab, while  $\mu_{Cs}^{slab}$  and  $\mu_{Te}^{slab}$  are the chemical potentials of the Cs and Te atoms in the slab, respectively. Furthermore, *T*, *S*, *P* and *V* are temperature, entropy, pressure and volume, respectively. All these values are nearly equal to zero and the total potentials of Cs and Te atoms in the slab are in equilibrium with bulk CsTe:

$$\mu_{CsTe}^{bulk} = \mu_{Cs}^{slab} + \mu_{Te}^{slab} \tag{2}$$

By combining Eqs. 1 and 2, one can rewrite Eq. 1 as follows:

$$\sigma_{CsTe} = \frac{1}{A} \left( E_{tot} - \mu_{Cs}^{slab} N_{Cs} - \left( \mu_{CsTe}^{bulk} - \mu_{Cs}^{slab} \right) N_{Te} \right)$$
(2)

The range of  $\mu_{Cs}^{slab}$  is limited by:

$$\Delta H_{for}^{CsTe} + \mu_{CsTe}^{bulk} \le \mu_{Cs}^{slab} \le \mu_{Cs}^{bulk}$$
(4)

$$\mu_{Cs}^{slab} \le \mu_{Cs}^{bulk} , \ \mu_{Te}^{slab} \le \mu_{Te}^{bulk}$$
(5)

Here the formation energy has a similar meaning to the previous work. Therefore:

$$\Delta H_{for}^{CsTe} + \mu_{Cs}^{bulk} = \mu_{CsTe}^{bulk} - \mu_{Te}^{slab}$$
(6)

then

$$\Delta H_{for}^{CsTe} + \mu_{Cs}^{bulk} = \mu_{Cs}^{slab} \tag{7}$$

$$\Delta H_{for}^{CsTe} = \mu_{CsTe}^{bulk} - \mu_{Cs}^{bulk} - \mu_{Te}^{bulk}$$
(8)

By combining Eqs. 1 and 5, one can illustrate that:

$$\Delta H_{for}^{CsTe} \le \mu_{Cs}^{slab} - \mu_{Cs}^{bulk} \le 0 \tag{9}$$

From Eq. 9, the permitted range of Cesium chemical potential is determined. Fig. 2 shows the surface energies of the (001) and (110) surfaces and the Cs- and Te-terminated (111) surfaces of CsTe as a function of the chemical potential  $\mu_{Cs}^{fide} - \mu_{Cs}^{bilk}$ . For the (110) and (001) surfaces, the surface energy is independent of the chemical potential of Cs, while the surface energy of (111) slab has a linear dependence on the Cs chemical potential. The Cs-terminated (111) surface has the lowest surface free energy. So, the Cs-terminated (111) surface is more stable than the (001) and (110) surfaces and the Te-terminated (111) surface.

# 3.2. Electronic structure and magnetic properties of bulk RS CsTe

The RS structure has the Fm  $\overline{3}$  m space group (No. 225), so that its structure has atomic coordinates of Cs which are located at (0, 0, 0) and at (0.5, 0.5, 0.5) for Te, as shown in Fig. 1a. The equilibrium lattice constant (lowest energy) of RS CsTe is 7.7 Å. This constant is employed in our calculations, which is something like the calculated value [28]. The HM gap is defined to be the absolute difference value between the



**Fig. 2.** Surface energies as a function of chemical potentials of  $\mu_{Cs}^{slab} - \mu_{Cs}^{bulk}$ .

top of valence band or the bottom of conduction band and the Fermi level. For this compound, it is equal to 0.22 eV. The half-metallic robust property of the studied compound is an indication of the wide half-metallic gap. The robust property is known to be as a function of lattice deformation, and the spin polarization collapses due to the raising temperature. The cohesion energy ( $E_{coh}^{CSTe}$ ) and the formation energy ( $\Delta H_{for}^{CSTe}$ ) show the thermal stability of the RS CsTe compound which is given in the following formulas:

$$E_{coh}^{CsTe} = (E_{Cs} + E_{Te}) - E_{total}^{CsTe}$$
(10)

$$\Delta H_{for}^{CsTe} = E_{total}^{CsTe} - \left( E_{Cs}^{bulk} + E_{Te}^{bulk} \right) \tag{11}$$

Where  $E_{Cs}$  and  $E_{Te}$  are the isolated atomic energies of Cs and Te atoms, respectively;  $E_{total}^{CsTe}$  is the total energy of bulk RS CsTe, and  $E_{Cs}^{bulk}$  and  $E_{Te}^{bulk}$ are the atomic energies of Cs and Te atoms, respectively. The values of cohesion and formation energies are calculated and found to be equal to 4.85 and -2.91 eV, respectively. The negative sign in the formation energy refers to the stability of CsTe in the equilibrium conditions (energetically stable).

The total density of states (DOS) and the partial density of states (PDOS) of the bulk RS CsTe are calculated and illustrated in Fig. 3. It is demonstrated that the DOS minority spin passes through the Fermi level offering a metal behavior while the DOS majority spin behaves like a semiconductor due to the existence of the energy gap, so the compound has a 100 % spin polarization at Fermi level. The semiconducting energy gap is defined as the absolute value of the energy difference between the lowest energy of majority (minority) spins for the conduction band



Fig. 3. The total and partial density of states of RS CsTe.

(CBM) and highest energy of majority (minority) spins for the valence band (VBM) band. According to the above, the energy gap is estimated to be 3.32 eV. The energy gap is changed according to this relation  $E_0 \propto$  $(1/a_0^2)$ , where E<sub>0</sub> is the energy gap and  $a_0$  is the lattice constant [33]. As demonstrated in Fig. 3, the minority spin of the s band is filled but the p band crosses the Fermi level and also the anti-bonding state is empty. Fig. 4 shows the band structure of bulk RS CsTe at majority and minority spins. From Fig. 4, one can observe that the bands near the Fermi level are mixture of the cationic 6 s state of Cs and anionic 5p state of Te. As a result, the hybridization originates from the mixture between s and p states, which lead to establish bonding and anti-bonding states. At the bonding state, there are four valence electrons so that the s and p bands are filled for the majority spin in band structure, while the anti-bonding is empty. The magnetic moment of RS CsTe is calculated to be 1  $\mu_B$ , where the number of minority spin is  $N\downarrow = 3$ , this value is the same as the theoretical values of previous studies [28]. So, the total magnetic moment is given by the form  $M_t = (N_V - 6) \mu_B$ , where  $M_t$  is the total magnetic moment per formula unit which is defined as the difference between the number of the filled bands for majority and minority spins, as in the form  $M_t = (N \uparrow - N \downarrow) \mu_B$  and  $N_V$  is the sum of electrons at the majority spin and minority spin (the total number of valence electrons). This means that  $N_V = N \uparrow + N \downarrow$  so that the magnetic moment is represented as  $M_t = (N_V - 2N_{\downarrow}) \mu_B$ , a situation that leads to  $M_t =$  $(N_V - 6) \mu_B$ .

As mentioned above, the CsTe compound is energetically stable, so it is a promising nominee for the manufacture of thin films using proper substrates, as shown in Fig. 5. The Rs CsTe has the half-metallic property above and below the lattice constant optimization. The values of CBM and the VBM in the majority-spin direction are utilized to characterize the HM under different lattice constants of the CsTe compound as clear in Fig. 5. Therefore, this compound keeps its HM properties in the values 7.3–8.4 Å region. The HM properties vanish when the VBM and CBM pass the Femi level  $E_F$ .

## 3.3. Electronic structure and magnetic properties of the surfaces

In order to show the HM properties of the RS CsTe compound at the (111), (110) and (001) surfaces, the spin-polarized atomic DOS at surface, subsurface (1) and middle (center) are exhibited along with the band structure calculation of the CsTe slabs as shown in Figs. 6-11. It can be noted that that the (111) surface shows the HM feature due to the semiconducting behavior of the majority spin channel and it also offers the metallic behavior in the minority spin channel (see Figs. 6 and 7). The energy gaps are 1.45 and 3.83 eV of the Cs- and Te-terminated (111) surfaces respectively. This means that the energy gaps decrease by about 2.2 eV for the Cs-terminated (111) surface and increase by about 0.18 eV for the Te-terminated (111) surface. For the (001) surface, (Figs. 8 and 9), both surface atoms of Cs and Te maintain the halfmetallic feature of bulk RS CsTe, i.e., the spin-down electrons are metallic whilst there are energy gaps around the Fermi level of the spinup channels. By comparing Figs. 8 and 9 with Fig. 3, it is observed that both of the gaps of the spin-up channels for the (001) surface atoms of Cs and Te (3.37 and 3.24 eV) are reduced compared to the values of bulk (3.65 and 3.65 eV). From Figs. 10 and 11, one can see that for the Cs and Te atoms of the (110) surface, the minority spin electrons reveal metallic properties, whilst they are found to carry the semiconducting property of majority spin channels. Therefore, the (110) surfaces preserve the half-metallicity, as shown in the bulk CsTe (see Fig. 3). The gap values of spin-up channels are 3.26 and 3.21 eV for the (001) surface atoms of Cs and Te.

Table 1 presents the *l*-decomposed majority and minority spin states within muffin tin spheres and the magnetic moments (MMs) of Cs and Te atoms in the surface, subsurface 1, subsurface 2 and center layer of the slabs for (111), (110) and (001) surfaces. The analogous values of bulk are further computed to compare the difference between the bulk and



Fig. 4. Majority and minority spins band structures of RS CsTe.



Fig. 5. Conduction band minimum and valence band maximum in the spin-up channel as a function of lattice constants of the RS CsTe.



Fig. 6. Density of states of Cs-terminated (111) surface.

surface systems. The MMs of Cs and Te atoms in the bulk RS CsTe are estimated to be 0.021 and 0.497  $\mu_B$ , respectively. The MMs for the surface is investigated with regard to all the atoms in the four terminations



Fig. 7. Density of states of Te-terminated (111) surface.

of the alloy CsTe (111), (110), and (001) surfaces as listed in Table 1. Depending on Table 1, the biggest transformation of the MMs is present for the Te atom in the Te-terminated (111) surface, compared with the MMs of the corresponding atoms in the bulk. Incontrast, the MMs for the atom in the Te at (001) did not change significantly.



Fig. 8. Density of states of Cs atom in the CsTe-terminated (001) surface.



Fig. 9. Density of states of Te atom in the CsTe-terminated (001) surface.



Fig. 10. Density of states of Cs atom in the CsTe-terminated (110) surface.

## 4. Conclusions

In summary, the first-principle calculations are used to investigate the electronic structures, and the magnetic and half-metallic properties of the RS CsTe in bulk and (111), (001) and (001) surfaces. The results show that the compound keeps its half-metallic properties in the bulk and surfaces. This compound is energetically stable in respect of the cohesion energy and formation energy. The stability of surfaces is confirmed by the calculated surface energies. The calculations show that the Cs-terminated (111) surface is more stable than all other surfaces. Moreover, the spin magnetic moment of the Te-terminated (111) surface is shown to be greatly different from the bulk values, while the difference in the spin magnetic moment between the Te atom in the (001) surface and the bulk CsTe is very small.

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



Fig. 11. Density of states of Te atom in the CsTe-terminated (110) surface.

## Table 1

l-decomposed majority and minority-spin electrons within muffin-tin sphere and spin magnetic moments (in unit of  $\mu_{\rm B}$ ) for each atom in the bulk, surface (S), subsurface (Sub) and central (C) layers of the RS CsTe compound.

		-		_	
	Atom	s (maj-/ min-)	p (maj-/ min-)	Total (maj-/ min-)	Μ (μ <sub>B</sub> )
Duille	Cs	0.00/0.00	2 26/2 24	2 16/2 14	0.021
DUIK	CS To	0.90/ 0.90	2.20/2.24	2.07/1.57	0.021
Cator		0.73/0.73	2.25/2.25	2.07/1.37	0.497
(111)	CS (3)	0.90/0.90	2.23/2.23	3.13/ 3.17	0.011
(111)	Te	0.70/0.70	1.04/1.05	1 06 /1 77	0 001
	(Sub1)	0.72/0.72	1.24/1.05	1.96/1.//	0.231
	(Sub1)	0.00/0.00	2.26 /2.25	9.16/9.15	0.015
	(Sub 2)	0.90/0.90	2.20/2.23	3.10/ 3.13	0.015
	(Sub2)	0.00/0.00	0.07/0.04	0 17/0 14	0.025
	CS (Country)	0.90/0.90	2.27/2.24	3.17/3.14	0.025
-	(Cent.)	0 74 /0 74	1 40 /0 00	0.17/0.00	0 700
Te-ter	Te (S)	0.74/0.74	1.43/2.88	2.17/3.62	0.783
(111)	6	0.00 /0.00	0.07/0.04	0.15 (0.1.4	0.000
	Cs	0.90/0.90	2.27/2.24	3.17/3.14	0.033
	(Sub1)				
	Те	0.73/0.73	1.33/0.85	2.06/1.58	0.487
	(Sub2)				
	Te (Cent)	0.73/0.73	1.34/0.84	2.07/1.57	0.500
CsTe-	Cs (S)	0.90/0.90	2.26/2.25	3.16/3.15	0.007
(110)					
	Te (S)	0.73/0.73	1.35/0.79	2.08/1.52	0.564
	Cs	0.90/0.90	2.27/2.24	3.17/3.14	0.032
	(Sub1)				
	Te	0.73/0.73	1.31/0.88	2.04/1.61	0.436
	(Sub1)				
	Cs	0.90/0.90	2.27/2.25	3.17/3.15	0.022
	(Sub2)				
	Te	0.73/0.73	1.34/0.84	2.07/1.57	0.491
	(Sub2)				
	Cs (C)	0.90/0.90	2.27/2.25	3.17/3.15	0.025
	Te (C)	0.73/0.73	1.34/0.84	2.07/1.57	0.498
CsTe-	Cs (S)	0.90/0.90	2.26/2.25	3.16/3.15	0.012
(001)					
	Te (S)	0.73/0.73	1.34/0.60	2.07/1.33	0.507
	Cs	0.90/0.90	2.27/2.25	3.17/3.15	0.027
	(Sub1)				
	Те	0.73/0.73	1.34/0.84	2.07/1.57	0.517
	(Sub1)				
	Cs	0.90/0.90	2.27/2.26	3.17/3.16	0.019
	(Sub2)				
	Te	0.73/0.73	1.33/0.80	2.06/1.53	0 474
	(Sub2)	21/0/01/0	1.00, 0.00		0.17 1
	(Sub2)	0.90/0.90	2.27/2.26	3 17/3 16	0.023
	Te (C)	0.73/0.73	1.34/0.80	2.07/1.53	0.499
	10(0)			, 1.00	0

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#### J.M.K. Al-zyadi et al.

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

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