



Origin of *p*-type half-metallic ferromagnetism in carbon-doped BeS: First-principles characterization

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ABSTRACT

Ab-Initio calculations are used to investigate the electronic and magnetic properties of carbon-doped at Be (C@Be) and S (C@S) sites in BeS semiconductor. Structural stability of both (C@Be and C@S) doped systems is taken into account by calculating the formation energies. We found that C@Be doped system maintains its non-magnetic insulating behaviour with smaller band gap of 0.6 eV as compared to bulk. On the other hand, when C-doped at S-site (C@S), a half-metallic ferromagnetic state induced which can be explained on the basis of electronegativity difference between dopant atom and replaced cations. The C 2*p* orbitals are mainly responsible for the metallicity and magnetism with stable moment of 1.06 μ_B /C atom. Interestingly, the magnetic ground state *i.e.*, ferromagnetic (FM) or anti-ferromagnetic (AFM) depends on the distance between C-atoms. A most stable-ferromagnetizing ordering is evident when the distance between two C atoms is very small ≈ 3.46 Å, due to strong C-C coupling with high magnetic transition temperature of $T_c = 814$ K. However, it is noticed that long range ferromagnetic clustering are not favourable. Our calculations demand experimental investigations of electronic and magnetic properties in C-doped BeS.

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1. Introduction

Fully spin-polarized (half-metallic ferromagnetic (HMF)) materials have been attracted great scientific and technologically interest as they display remarkable revolution in field of spintronics for next-generation high speed [1,2], large storage [3], and low power consumption microelectronic devices [4,5]. In this respect, diluted magnetic semiconductors (DMS) which are combination of magnetic and semiconductor materials have been attracted much attention due to their potential applications in opto-electronics as optical limiters [6,7]. Basically, DMS obtained by doping 3*d* transition metals such as Mn, Cr, Mg, Ca, Ti, and Cu [8–11] in non-magnetic insulators. A number of room temperature FM DMS have been reported by transition metal doping such as Mn-doped SnO₂ [12], Al, Mn, V, Cr, Fe, Co, and Ni-doped TiO₂ [13–15], Ni, Co, V, Cr, and Ti-doped In₂O₃ [16–18], Fe, Mn, Ga, Mn, and As-doped ZnO/GaN [19,20], and Cr-doped AlN and ZnTe [21,22]. Due to high curie temperature ($T_c = 300$ K) [20,22] among the HMF materials, Cr-doped II-VI DMS have been extensively studies [23] which

exhibit an exceptional range of functional electronic properties such as blue lasers [24], fluorescent displays in light emitting diodes [25], transparent conducting oxides [26], and intermediate band solar cells [27].

Interestingly, room-temperature ferromagnetism in chalcogenides [28] and II-VI/III-V semiconductors such as ZnO, SrO, MgO, TiO₂ [29–33] is found by doping non-magnetic light elements like nitrogen and carbon atoms. Fan [10] and Pan et al., [34] figured out that C doping at S site (C@S) induced a stable *p*-type half metallic structure in ZnS and CdS, respectively. Moreover, it is theoretically investigated by Yang et al., [35] that magnetism can be induced only when electronegativity of dopant is less than the replaced atom. They found magnetic moment in ZnO/ZnS by C doping at O/S sites because electronegativity of C is less than that of O/S. In contrast, when C-doped at Se/Te sites in ZnSe/ZnTe, systems exhibit non-magnetic insulating nature because electronegativity of C is larger than that of Se/Te.

In this work, we investigate the electronic and magnetic properties of carbon doped BeS semiconductor by replacing C-at both Be (C@Be) and S (C@S) sites. First, the stability of doped compounds (C@Be and C@S-BeS) is analyzed by calculating their formation energies. Then, magnetic solutions are analyzed by comparing the total energy solutions of FM and AFM ordering and also study the

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effect of C-doping at different position of S-sites to probe the stable magnetic ground state.

2. Computational methods

Present calculations performed using full-potential linearized augmented plane wave (FP-LAPW) method within the framework of density functional theory as implemented in the WIEN2K code [36]. Local spin density approximation (LSDA) is used as the exchange correlation potential. A $2 \times 2 \times 1$ supercell is taken into account having 32 total atoms which contains 16 atoms of Be and S each. For the wave function expansion inside the atomic spheres, a maximum value of $l_{max} = 10$ is chosen and the plane-wave cutoff is set to $R_{mt} \times K_{max} = 7$ with $G_{max} = 12$. The muffin-tin sphere radius is chosen as 1.6, 2.0, and 1.7 a.u. for Be, S, and C, respectively. Moreover, a $5 \times 2 \times 2$ of k -mesh generates 12 points in reduce brillouin zone which is found to be well converged for both bulk as well as doped systems and the forces minimized upto 5 Ry/a.u. Specifically, we have used a dens k -meshes of $7 \times 3 \times 3$ and $9 \times 4 \times 4$ to check the energy convergence and found that difference in total energy is up to 25 meV, which has no big influence on our main conclusion. Along with fully optimization of the atomic positions by relaxing the atomic forces up to 2 Ry/a.u. is taken into account for each calculation as discussed in these works [37–39] that structural relaxation show prominent effect on the physical properties of the materials. For doped systems, one Be and S atoms separately replaced by one C-atom with doping concentration of only 6.25%, which can be easily achieved in the experiment. The magnetic ground state along with curie temperature (T_C) is figured out from the total energy solutions of FM and AFM as $\Delta E = E_{fm} - E_{afm}$ with respect to distance (d (Å)) between two carbon atoms.

3. Results and discussion

3.1. Bulk BeS

Bulk beryllium sulphide (BeS) belongs to the family of II-VI semiconductor with space group $F\bar{4}3m$ (No. 216) having covalent bonding [40] among the Be and S atoms. The experimental band gap of BeS is 5.5 eV [41] with theoretical predicted in-direct gap of 3.7 eV [42]. The underestimation of energy gap is due to a well known problem of exchange–correlation potential. The calculated spin polarized total and partial DOS of bulk BeS with experimental lattice constant of 4.87 Å [43] are shown in Fig. 1, which confirms the non-magnetic and insulating behaviour of BeS with band gap of 3.5 eV. Because, the majority and minority DOS have the same occupation number and net magnetic moment is zero. The total DOS are mainly composed of S atoms near E_F with minor contribution of Be atoms. From partial DOS of Be and S atoms (Fig. 1(a) and (b)), one can clearly see that in the valence band near E_F S 3p states are mainly responsible in the total DOS, with a very small contribution of Be 2s states. In conduction band, states at 4 eV to 5 eV mainly comes from Be/S 2p/3p orbitals. The calculated spin-polarized band structures are also plotted in Fig. 1, which confirms the DOS. The indirect band gaps $\Gamma - X$ and $\Gamma - Z$ have almost the same value of 3.5 eV for both majority and minority bands.

3.2. Doped systems

To analyze the structure stability of doped systems, we calculated formation energies (E_f) of C@Be and C@S doped models from the following equation,

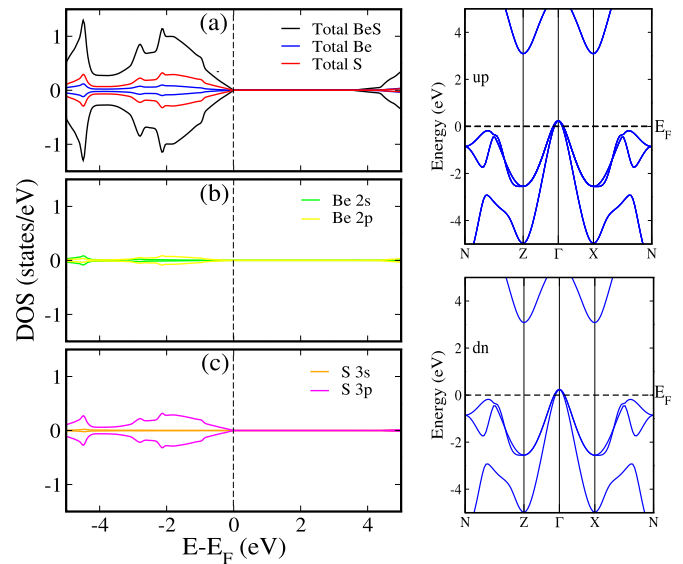


Fig. 1. Calculated spin polarized (FM configuration) total DOS of (a) bulk BeS, Be, and S atoms and partial DOS of (b)/(c) Be/S atom along with band structures. The Fermi level (E_f) is represented by vertical dashed line in each DOS.

$$E_f = E_{doped} - E_{undoped} - \mu_c + \mu_{Be/S}, \quad (1)$$

where $E_{doped}/E_{undoped}$ is the total energy of doped/undoped systems, where as μ_c and $\mu_{Be/S}$ refers to the chemical potentials of C and Be/S atoms, respectively. Our calculated E_f for C@Be/C@S doped-system is 3.50 eV/2.44 eV, respectively, which shows that C@S doped model energetically more favourable to form as compared to C@Be doped structure.

First, we study the physical properties of C@Be doped system and optimized bond lengths of Be–S, Be–C, and S–C are 2.10 Å, 3.46 Å, and 4.05 Å, respectively. The calculated spin-polarized total, partial S/C DOS atom in Fig. 2(a) and (b)/(c), respectively. From Fig. 2(a), one can clearly see that doped system keeps its non-magnetic and semiconducting behaviour as found in the case of bulk BeS but gap

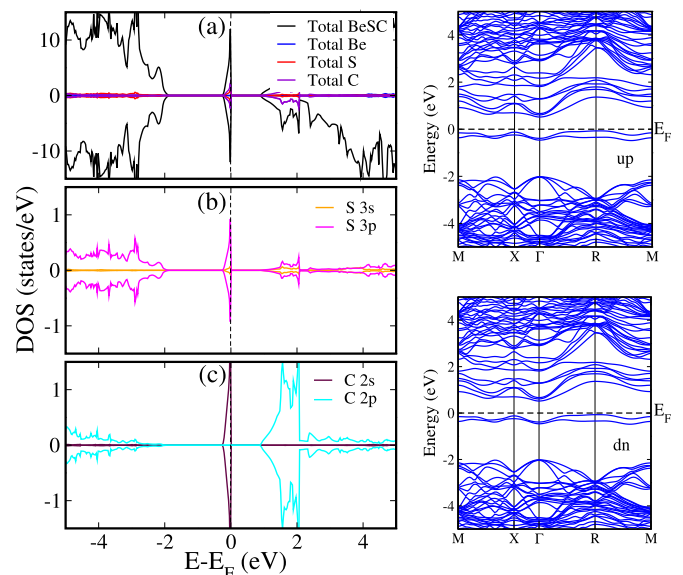


Fig. 2. Calculated FM spin polarized (a) TDOS of BeS, Be, S, and C, (b) PDOS of S, and (c) C atoms along with spin-polarized band structures in C@Be doped system.

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