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Effects of Chromium (Cr) doping on Structural, Electronic and Magnetic Properties of Barium Selenide Compound: A Theoretical Investigation

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The structural, electronics, and magnetic properties of $Ba_{1-x}Cr_xSe$ compound at doping concentrations, x=0.06, 0.12, and 0.25 were investigated using full potential linearized augmented plane wave (FP-LAPW) method based on density functional theory (DFT).The Wu-Cohen generalized-gradient approximation (WC-GGA) exchange correlation potentials were used to compute structural properties, while the electronic and magnetic properties were explored using the WC-GGA coupled with modified Becke-Johnson (mBJ) scheme. Our findings show that $Ba_{1-x}Cr_xSe$ are half-metallic ferromagnets (HMFs) having 100% spin polarization at Fermi level (E_F). For investigated compounds, the half-metallic gap gets narrow out as doping concentration rises from 6% to 25%.All compounds are confirmed to be ferromagnetic since the Cr atom is able to induce an integral total magnetic moment of ~ 4.0 μ_B. By creating new states at E_F as a result of fractional replacement of Cr at Ba site, half-metallicity and magnetism get developed, which makes them potentially relevant for spintronic applications.

Keywords: $Ba_{1-x}Cr_xSe$ compound; Electronic properties; Magnetic properties; DFT

1 Introduction

The modern branch of study known as spintronics (spin-based electronics) aims to enhance the data storage and processing capabilities of spin-based devices. It is favoured over conventional electronics because of its many benefits, including non-volatility, faster data processing, higher transistor densities, and lower power consumption, among others. For magnetic materials to be employed in spintronic devices, they must have spin polarisation at Fermi level (E_F), a wide half-metallic gap, and a high Curie temperature[1]. In recent decade, transition metal (TM) doped II-VI and III-V magnetic semiconductors[2-8] have attracted momentous interests of research groups due to their excellent ferromagnetic properties. These magnetic semiconductors can be categorized as right HMFs having 100% spin-polarization at E_F. Of them, BaSe, a member of the II-VI family, is a technologically significant material with a variety of uses in micro-electronics, light-emitting diodes, and laser diodes *etc*.[9]. Impurities in host BaSe semiconductor drastically alter the ground state aspects of the compound. With the help of the full-potential linearized augmented plane wave method (FP-LAPW), Bahloul *et al.*[6] recently analysed $Ba_{1-x}Cr_xSe$ (x=0.25,0.50 and 0.75) alloys and discovered that Cr-d and Se-p states play a vital responsibility to determine electronic properties of these alloys, which further support their half-metallic ferromagnetic (HMF) behaviour. In last few years, the density functional theory (DFT) calculations have been performed to calculate half-metallicity in a variety of TM substituted II-VI semiconductors such as Ti doped BeS[4], Ti substituted MgSe[5], Cr doped BaTe[7], Cr doped BaS[8] *etc.*

II-VI chalcogenides, specifically the calcium[9-10] and barium chalcogenides[6-8], have been the subject of extensive research in recent years. Under normal conditions, these compounds crystallise as a closed-shell ionic system with a rock-salt structure type (B1). In the present work, we have investigated the electronic and magnetic properties of $Ba_{1-x}Cr_xSe$ compoundatdoping concentrations, x=0.06, 0.12, and 0.25 with the aim that the compounds in the existing collection exhibit half-metallicity, which might be an ultimate material for spintronic devices.

2 Methods of Calculation

The highly precise all electron FP-LAPW method as implemented in WIEN2k[11] code were employed to

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*Corresponding authors: (E-mail: hardevdft@gmail.com) predict ground state properties of $Ba_{1-x}Cr_xSe$ at x =0.06, 0.125, and 0.25. The semi local exchange-correlation potential *i.e.* modified Becke-Johnson potentials (TB-mBJ) coupled with generalized gradient approximation (GGA) were used to explore the electronic and magnetic properties[12]. The convergence parameter $R_{MT}K_{Max}= 7$ was used to control the size of basis set, where K_{Max} is size of greatest K vector of plane wave and R_{MT} are average radii of muffin-tin spheres of Cr, Ba and Se atoms. The convergence criteria for charge and energy were set to be 10^{-4} Ry and 10^{-2} e, respectively. To define the separation between valance and core states, -6 Ry cut off energy was preferred.

BaSe exit in rock-salt structure having space group Fm-3m, such that Ba atom is located at (0, 0, 0) and Se atom at (0.5, 0.5, 0.5) positions. For $Ba_{1-x}Cr_xSe$, the (2×2×1), (2×1×1) and (1×1×1) super cells, having 32, 16 and 8 atoms, respectively were constructed and one Ba site was substituted by Cr impurity.

3 Results and Discussion

To explore ground state properties of $Ba_{1-x}Cr_xSe$ at x=0.06, 0.12, and 0.25, the lattice parameters have been optimized in the neighborhood of experimental lattice parameter of the pristine BaSe[13] (Table-1).

Table1 — Calculated lattice constant (a), Formation energy (E_{form})and Half-Metallic Gap (E_{HM}), for of $Ba_{1-x}Cr_xSe$ (x =0.06, 0.125, and 0.25)

Compounds	a(Å)	E_{form}(eV)	E_{HM} (eV)
$Ba_{0.94}Cr_{0.06}Se$	6.49	-29.37	0.89
$Ba_{0.88}Cr_{0.12}Se$	6.43	-59.34	0.87
$Ba_{0.75}Cr_{0.25}Se$	6.34	-129.70	0.59

Further to check the structural stability of the compounds, the formation energy of the resultant compounds has been calculated using the following expression:

$$E_{for}= E_{cell}- E^0_{base} - xE^0_{dopant} + xE^0_{Ba} \qquad ...(1)$$

where E_{cell}, E^0_{base}, $E^0_{dopant}$and E^0_{Ba} are the total energy of Cr-doped BaSe, host BaSe, dopant Cr and Ba, respectively, and *x* represents concentration of dopant.

Moreover, the calculated formation energies are founds to be negative as listed in Table-1, shows stability of these compounds.

The total density of states (TDOS) of $Ba_{1-x}Cr_xSe$ (x =0.06, 0.125, and 0.25) shows unequal distribution of DOS at E_F (Fig-1) for both spin-up and spin-down channels. The electronic and magnetic properties of present materials have been distorted significantly after Cr-doping and the resultant compounds reveals both metallic and semiconducting performance in spin-up and spin-down channels, respectively. Because of this marvellous feature, these compounds exhibit half metallic ferromagnetism and thus highly effective for spin injection.

The calculated HM gap (E_{HM}) for all the resultant compounds in spin-down channel are listed in Table-1 and therefore these compounds are responsible to exploit the effectiveness of spintronic devices. Half-Metallic Gap (E_{HM}) is a crucial distinguishing property and helpful for understanding the half-metallicity. It can be the minimum value either of $E_F-E_v^{top}$ or $E_c^{bot}-E_F$, where, E_v^{top} and E_c^{bot} denote the energy corresponding to valence band (VB) maxima and conduction band (CB) minima, respectively[3].

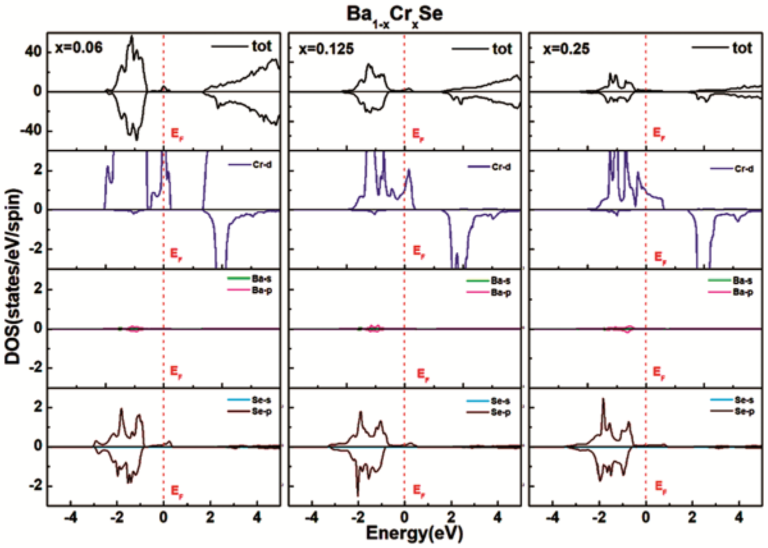

Fig. 1 — Total (TDOS) and partial density of states (PDOS) for $Ba_{1-x}Cr_xSe$ compounds at x=0.06, 0.125, and 0.25.

Table 2 — Total and atom resolved spin magnetic moment (M) of $Ba_{1-x}Cr_xSe$ (x=0.06, 0.12 and 0.25)

Compounds	$M_{tot}(\mu_B)$	$M_{Ba}(\mu_B)$	$M_{Cr}(\mu_B)$	$M_{Se}(\mu_B)$	$M_{int}(\mu_B)$
$Ba_{0.94}Cr_{0.06}Se$	4.00	0.00	4.00	-0.14	0.29
$Ba_{0.88}Cr_{0.12}Se$	4.00	-0.00	3.98	-0.13	0.29
$Ba_{0.75}Cr_{0.25}Se$	4.00	0.00	3.98	-0.09	0.28

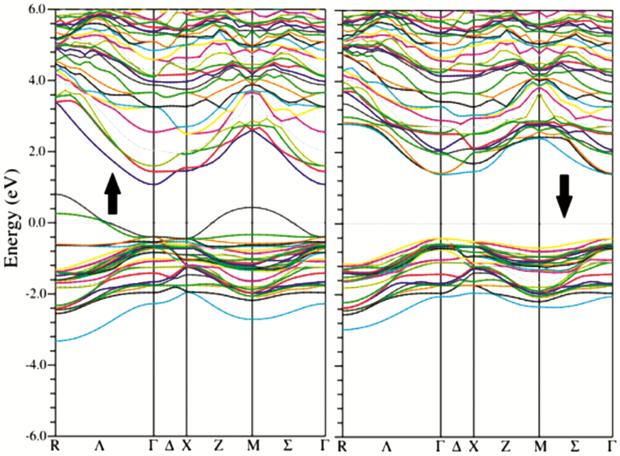

Fig. 2 — Spin resolved band structure for $Ba_{1-x}Cr_xSe$ compounds at x= 0.125.

In order to assess the contribution of different atoms toward half metallicity, the partial density of states (PDOS) (Fig. 1) of $Ba_{1-x}Cr_xSe$ compounds has also been studied. It can be seen that, the E_{HM} in spin-down channel is caused by strong p-d hybridization between Cr-d and Se-p states, while Ba-s, Ba-p, and Se-s states have a negligible impact on both spin channels.

The total and individual atom magnetic moments of $Ba_{1-x}Cr_xSe$ compounds have been calculated (Table 2), which shows that the involvement of Ba and Se atoms is minimal compared to that of 3d-states of Cr to the overall magnetic moment. Additionally, the HM behaviour of these materials is supported by the integer value derived for their total magnetic moments.

In order to figure out the temperament of bands at and near the E_F, the band structures of $Ba_{0.88}Cr_{0.12}Se$ (as a reference compound) have been examined in the irreducible Brillouin zone with high symmetry points as shown in Fig. 2. The band structures of all other compounds are generic in nature. The bands due to Se-p and Cr-dstates separated in energy range -2.65eV to -0.75eV in valance band (VB) with minimal contribution of Se-s, Ba-s and Ba-p in both spin states. Bands around E_F are often caused by Cr-d states, having very little contribution from Se-p states in spin-up channel, whereas in spin-down channel, these states are shifted towards CB. In spin-down channel, the deficiency of bands at/above E_F, reveals its semiconducting behaviour. The HMFs in these compounds is primarily determined by the hybridization of Cr-d and Se-p states, which can be explained by the Zener's p-d exchange model[14–15] and double exchange mechanism[16]. The resulting compounds may be seen as useful spintronic materials because of possessing high valued HM gap.

4 Conclusion

Half-metallic ferromagnetic response for $Ba_{1-x}Cr_xSe$ compound at doping concentrations, x=0.06, 0.12, and 0.25 have been analysed by first-principles calculations. The electronic and magnetic properties are explored using modified Becke-Johenson (mBJ) exchange potential coupled with GGA correlation. The resultant compounds are true half-metallic with a considerable value of E_{HM}. The fundamental reason behind half-metallic performance of these materials is hybridization between Cr-d and Se-p states. The total magnetic moment of the compounds is4.00 μ_B, which is mainly contributed by the Cr-d states. The possibilities for using the materials in spintronic are revealed by our predicted results, which would encourage experimentalists to develop this kind of materials.

References

1 Fecher G H, Kandpal H C, Wurmehl S, Felser C & Scho¨nhense G, *J Appl Phys*, 99 (2006) J106.
2 Saini H S, Singh M, Reshak A H & Kashyap M K, *J Magn Magn Mater*, 331 (2013) 1.
3 Saini H S, Kashyap M K, Kumar M, Thakur J, Singh M, Reshak A H & Saini G S S, *J Alloys Compd*, (2015) 649184.
4 Saini H S, Singh M, Reshak A H & Kashyap M K, *Comp Mat Sci,* 74 (2013) 114.
5 Poonam H, Saini S, Thakur J, Pundir A K, Singh M & Kashyap M K, *AIP Conf Proc*, 2093 (2019) 020001.
6 Bahloul H, Mokaddem A, Doumi B, Berber M & Boudali A, *J Supercond Nov Magn*, 32 (2019) 2185.
7 Berriah K, Doumi B, Mokaddem A, Elkeurti M, Sayede A, Tadjer A & Araújo J P, *J Comp Elec*, 17 (2018) 909.
8 Mehra P, Saini H S, Sinhmar S, Thakur J & Kashyap M K, *Vacuum*, 182 (2020) 109760.
9 Murtaza G, Khenata R, Safeer A, Alahmed Z & Omran S B, *Comp Mater Sci*, 9143 (2014).
10 Mishra M, Sharma G, Kothari R, Vijay Y & Sharma B, *Comp Mater Sci*, 51340 (2012).
11 Blaha P, Schwarz K, Madsen G K H, Kvasnicka D, Luitz J, Laskowski R, Tran F & Marks L D, WIEN2k, An Augmented Plane Wave + Local Orbitals Program for Calculating Crystal Properties (Karlheinz Schwarz, Techn. Universität Wien, Austria), 2018. ISBN 3-9501031-1-2.
12 Wu Z & Cohen R E, *Phys Rev*, 73 (2006) 235116.
13 Grzybowski T A & Ruoff A L, *Phys Rev*, 27 (1983) 6502.
14 Dietl T, Ohno H & Matsukura F, *J Cibert D. Ferrand Sci,* 287 (2000) 1019.
15 Dietl T, *Semicond Sci Technol*, 17 (2002) 377.
16 Sato K, Dederichs P H & Yoshida H K, *J Phys Soc Jpn*, 76 (2007) 024717.