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# Ferromagnetism in $d^0$ Binary Compounds MC (M = Be, Mg, Ca, Sr, Ba and Ra): A Modified Becke Johnson Potential Study

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We have performed the FP-LAPW calculation based on the density functional theory (DFT) to study the electronic and magnetic properties of binary compounds MC (M = Be, Mg, Ca, Sr, Ba and Ra). The density of states (DOS) and band structures were studied to understand the electronic properties. We have employed an orbital independent semilocal exchange potential called modified Becke Johnson (mBJ) which includes a large proportion of electrons residing in the interstitial regions. Thus the information obtained from mBJ is more accurate as compared to conventional DFTs (GGA/LDA) as their potential is electron orbital dependent. Among the systems under our investigation CaC, SrC, BaC and RaC has given the 100% spin polarization at Fermi energy ( $E_F$ ) within GGA whereas mBJ open a gap for all the systems. The total magnetic moment was found to be  $2.00 \mu_B$  which is an integer value as expected for the HMF systems. The large half metallic gaps and location of  $E_F$  was found to be robust with respect to lattice constants in RaC and BeC.

**KEYWORDS:** DFT, GGA, mBJ, Half-Metal, Ferromagnetism.

## 1. INTRODUCTION

Half-metal ferromagnets (HMFs) have received a lot of theoretical and experimental attention because of their promising applications in spintronics, nonvolatile memories, optical switches, magneto-optical devices.<sup>1-3</sup> Spintronic is the study of two fundamental components of materials i.e., magnetic and electronic properties. The effect of electrons' spin and charge in magnetic semiconductors are utilized for developing spin based semiconducting devices. Basically Spintronic deals with the magneto-electronics, which was born with the discovery of the half-metallic ferromagnets in 1983 in NiMnSb.<sup>4</sup> In HMF compounds one of the spin channel presents a gap at the Fermi level, while the other has a metallic character, leading to 100% carrier spin polarization at the Fermi level ( $E_F$ ).<sup>5</sup> This exceptional property leads to an idea that such an electronic devices can be built where not only the charge but also the spin of the electron spin can play a vital role in transferring the signal and thus it is free of ohmic

energy dissipation. Now, the researchers have realised the importance of HMF as an energy material for future technological applications.<sup>6</sup> Theoretically many systems have been studied so far and found to be HMFs e.g., ferromagnetic oxides such as  $\text{CrO}_2$ <sup>7</sup> and  $\text{Fe}_3\text{O}_4$ ,<sup>8</sup> some Perovskite compounds  $\text{Sr}_2\text{FeMoO}_6$ ,  $\text{Ca}_2\text{FeMoO}_6$ ,<sup>9</sup> Heusler alloys like  $\text{Co}_2\text{MnAl}$ ,<sup>10</sup>  $\text{Co}_2\text{CrSi}$ ,<sup>11</sup>  $\text{Co}_2\text{FeGe}$  (LSDA + U),<sup>12</sup>  $\text{Co}_2\text{VAl}$ ,<sup>13</sup>  $\text{Co}_2\text{MnGe/Sn}$ ,<sup>14</sup>  $\text{Co}_2\text{CrAl}$ ,  $\text{Co}_2\text{CrGa}$ ,<sup>15</sup>  $\text{Co}_2\text{CrAs}$ <sup>16</sup> etc. at their ground state. Other than the transition metal based compounds as mentioned above, the HMFs are also found in some binary compounds. The binary ferromagnets are of particular interest due to their structural stability, high Curie temperature low, magnetic moment, wide band gap and ideal materials for fabricating all spin based semiconductor devices.<sup>17,18</sup> In early 1970s the discovery of ferromagnetism in the Eu-based binary semiconductor ( $T_C < 50^\circ \text{K}$ ) have attracted more research interest in this field. After that the major attention was given to study the electronic and magnetic properties of binary magnetic semiconductors. Among the binary compounds a new type of HMF has been reported, called  $d^0$  binary systems with all its constituents non-magnetic.<sup>19</sup> The magnetic properties of these materials are not exclusively related to the presence of magnetic ions but can be strongly determined

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by the hybridization of  $sp$ -states.<sup>20,21</sup> Kusakabe et al. studied the Ca-pnictides (CaP, CaAs, CaSb) and predicted to be HMFs.<sup>22</sup> Sieberer et al.<sup>23</sup> and Volnianska et al.<sup>24</sup> found HMFs in many II–V compounds and explained the spin polarization of  $p$ -states of anions. Some of the alkali earth metal based binary compounds (MgC, CaC, SrC, BaC) are also predicted to be a better candidate for HMFs.<sup>25</sup> Galanakis<sup>28</sup> proposed the description about the formation of magnetic moments  $M_i = (8 - Z_i)$  (where  $M_i$  is the total magnetization and  $Z_i$  is the total number of valence electrons) in non-transition metal based binary compounds. The calculation of the electronic structure plays an important role in determining the magnetic properties for HMFs. In this article we have revisited the electronic structure (DOS and band structure) of MC (M = Be, Mg, Ca, Sr, Ba and Ra) which was investigated by traditional DFTs like GGA/LDA.<sup>25,26</sup> The disadvantage of traditional DFT<sup>29</sup> is due to the lack of their mix bonding, where large portion of electrons resides in the interstitial region. These electrons are not accounted for the calculation as the potential is orbital dependent. Thus the result of electronic structures may not be accurated as expected. Here we have used a latest and an accurate orbital independent exchange semilocal potential which is obtained by modifying Becke and Johnson exchange potential called mBJ.<sup>30,31</sup> The mBJ exchange potential

is reported to be a widely used tool and more effective in determining the accurate ground state electronic structures.<sup>32</sup> Currently in semiconductor BeX (X = S, Se, Te),<sup>33</sup> double perovskites  $(Ba/Sr)_2$  FeReO<sub>6</sub>,<sup>34</sup> full-Heusler alloy Co<sub>2</sub>VSb,<sup>35</sup> X-Phosphides/Nitrides (X = B, Al, Ga, In),<sup>36,37</sup> zinc blende transition metal,<sup>38</sup> topological half-Heusler (THH),<sup>39</sup> etc. the mBJ has worked more successfully.

## 2. COMPUTATIONAL DETAILS AND CRYSTAL STRUCTURE

A computational code (WIEN2K)<sup>40</sup> based on FP-LAPW method has been applied for calculations of structural, electrical and magnetic properties. Non-spherical contributions to the charge density and potential within the Muffin Tin (MT) spheres were considered up to  $l_{\max} = 10$  (the highest value of angular momentum functions). The cut-off parameter was  $R_{\text{MT}} \times K_{\max} = 7$  where  $K_{\max}$  is the maximum value of the reciprocal lattice vector in the plane wave expansion and  $R_{\text{MT}}$  is the smallest atomic sphere radius of all atomic spheres.<sup>41</sup> In the interstitial region the charge density and the potential were expanded as a Fourier series with wave vectors up to  $G_{\max} = 12 \text{ a.u.}^{-1}$ . The number of  $k$ -points used in the irreducible part of the brillouin zone is 286. The crystal structure of non-transition metal based

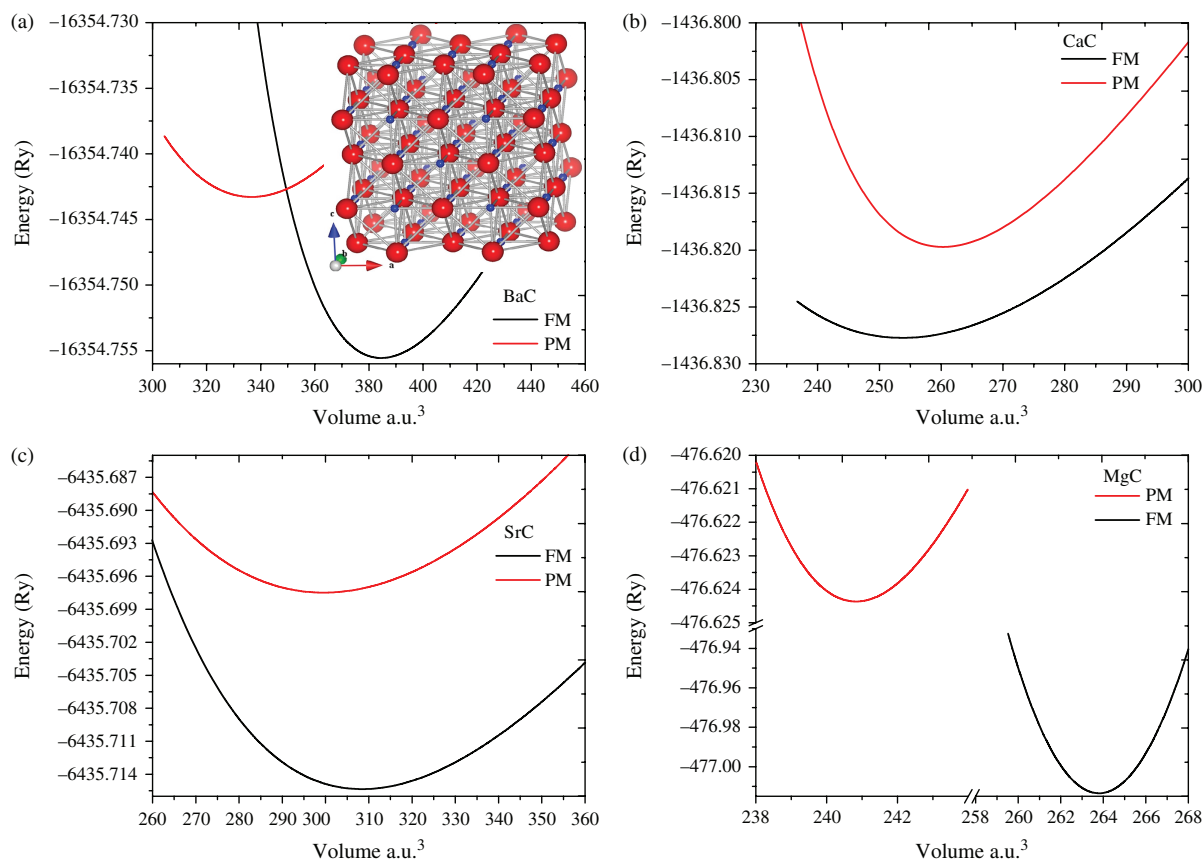


Fig. 1. Volume optimization of MC in Ferromagnetic (FM) and Paramagnetic (PM) configurations.

**Table I.** Lattice constant, Bulk modulus and Equilibrium energy ( $E_0$ ) within PM and FM configurations.

MC	Lattice constant Å			Bulk modulus		$E_0$ (Ry)	
	Prev. <sup>24</sup>	FM	PM	FM	PM	FM	PM
MgC	5.09	5.04	5.387	707.934	3316.336	-476.640	-476.6245
CaC	5.75	5.32	5.279	69.439	116.905	-1436.826	-1436.820
SrC	6.15	5.71	5.621	59.794	42.850	-6435.714	-6435.694
BaC	6.49	6.02	5.843	7.459	37.508	-16354.757	-16354.743

binary compound with chemical formula MC (M = Be, Mg, Ca, Sr, Ba and Ra) consists of fcc sublattices with atoms at M-red (0, 0, 0) and C-blue (1/2, 1/2, 1/2) having space group  $Fm\bar{3}m$  is shown in Figure 1(a).

### 3. RESULTS AND DISCUSSION

Systematic calculations of the electronic and magnetic properties of binary compounds MC were carried out in this work. The calculated results of the electronic structures were compared to study the effect of the different kinds of atoms and valence electrons on the magnetic properties and in particular the band gap. The structural optimization was performed for both the ferromagnetic (FM) and paramagnetic (PM) configurations. A series of total energy calculations as a function of volume can be fitted to Murnaghan's equation of states (Eq. (1))<sup>42</sup> and the volume versus energy curve is shown in Figure 1.

The detail values of the optimized Lattice parameters, bulk moduli and equilibrium energies for both FM and PM configurations are presented in Table I. The optimized lattice parameters were slightly lower than the previous results. The percentage changes in the lattice constants with respect to previous results<sup>25</sup> are 0.98%, 7.52%, 7.15%, and 7.24% for MgC, CaC, SrC and BaC respectively. In all the cases the structure within ferromagnetic (FM) configuration is the most stable with lowest energy (ground state energy) as shown in Figure 1.

$$E(V) = E_0 + \left[ \frac{(V_0/V)^{B_0}}{B_0 - 1} + 1 \right] - \frac{BV_0}{B_0 - 1} \quad (1)$$

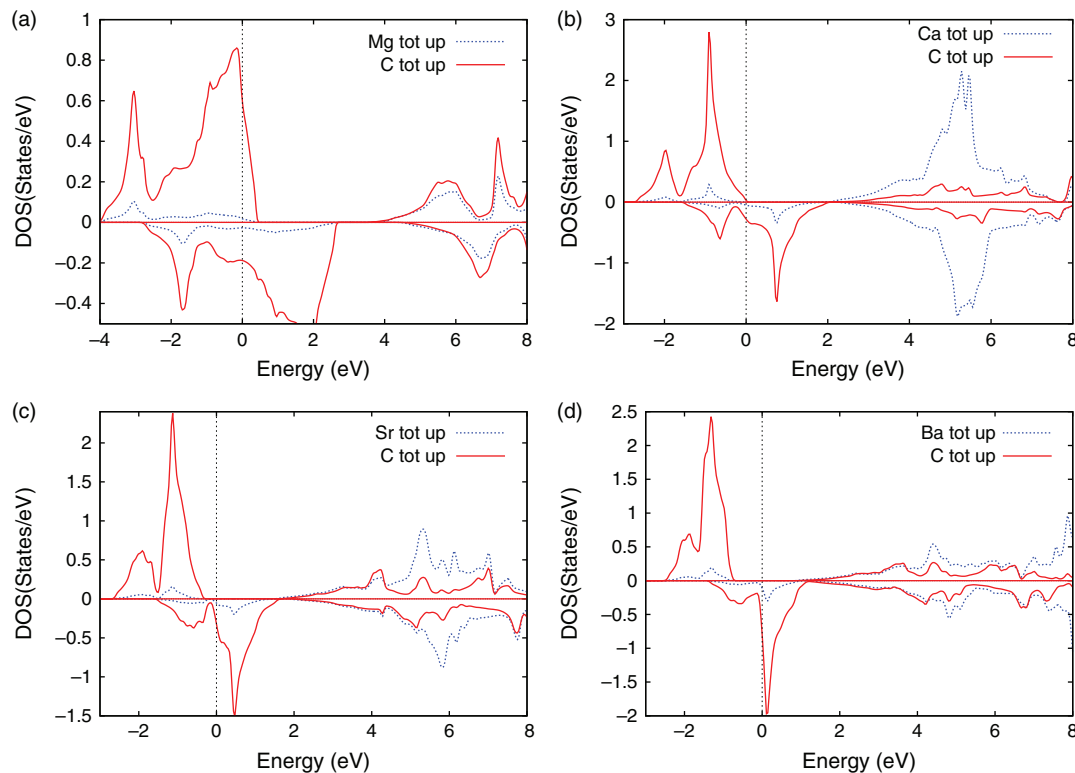
where  $E_0$  is the minimum energy at  $T = 0$  K,  $B$  is the bulk modulus at the equilibrium volume and  $B_0$  is pressure derivative of the bulk modulus at the equilibrium volume.

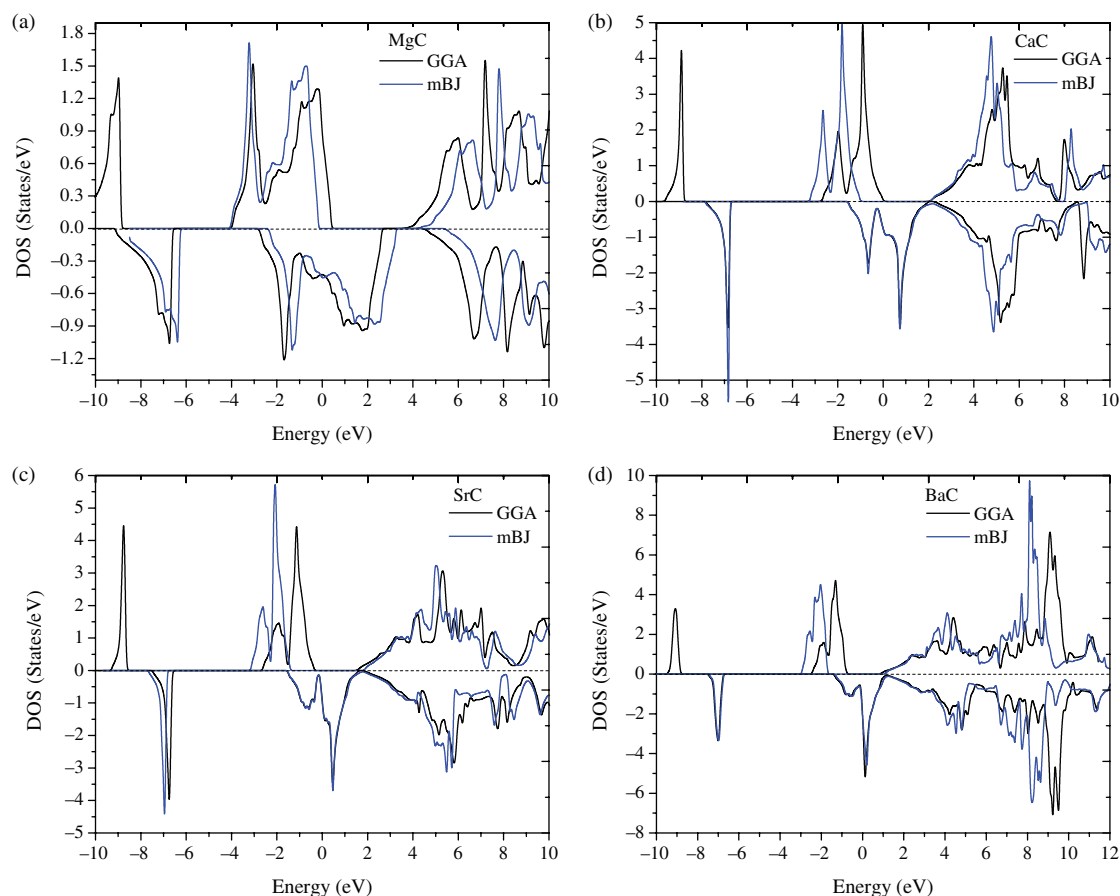
#### 3.1. Electronic and Magnetic Properties

The electron spin polarization ( $P$ ) at Fermi energy ( $E_F$ ) of a material is defined by Eq. (2).<sup>43</sup>

$$P = \frac{\rho \uparrow (E_F) - \rho \downarrow (E_F)}{\rho \uparrow (E_F) + \rho \downarrow (E_F)} \quad (2)$$

where  $\rho \uparrow (E_F)$  and  $\rho \downarrow (E_F)$  are the spin dependent density of states at the  $E_F$ . The  $\uparrow$  and  $\downarrow$  assigns the majority and the minority states respectively.  $P$  vanishes for paramagnetic or anti-ferromagnetic materials

**Fig. 2.** Partial DOS of (a) MgC, (b) CaC, (c) SrC and (d) BaC.



**Fig. 3.** Total DOS of (a) MgC, (b) CaC, (c) SrC and (d) BaC (GGA-Black and mBJ-Blue).

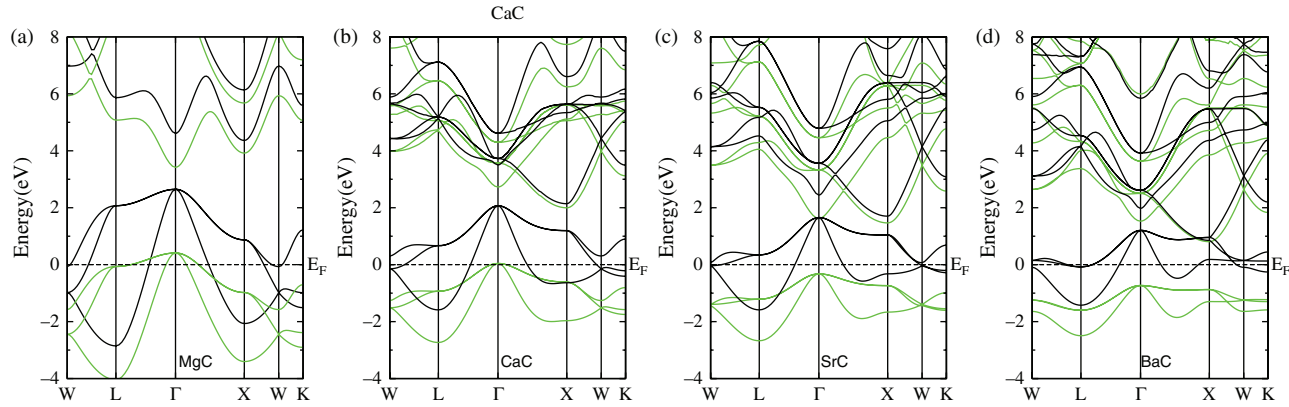
even below the magnetic transition temperature. The HMF has a finite value in ferromagnetic materials below Curie temperature.<sup>44</sup> The electrons at  $E_F$  are fully spin polarized ( $P = 100\%$ ) when the DOS at one of the channels is equal to zero. Here, we have observed dispersed DOS around  $E_F$  in the spin down channel. The reason for this large value of DOS in spin down is due to the passing of  $E_F$  through the strongly localized C- $p$  states whereas the contribution of M- $p$  states is very small in both the spin channels as illustrated in Figures 2(a-d). The dispersed DOS for SrC and BaC are 2.10 states/eV and 3.10 states/eV respectively in their minority channels whereas the DOS at majority channel is nil, which gives 100% spin polarization at  $E_F$  (Figs. 3(c-d)). The calculation within GGA predict CaC, SrC and BaC are to be a HMF with 100% spin polarization at  $E_F$  whereas MgC gives 36%, a metallic behaviour (Table II). According to our results, the compound MgC is purely metallic as it shows extended DOS at  $E_F$ ,  $\rho \uparrow(E_F) = 1.3$  states/eV and  $\rho \downarrow(E_F) = 0.60$  states/eV within GGA (see Table II). Whereas with the implementation of mBJ potential the band gap in the spin up channel has been increased for all the systems (Fig. 3). The compound MgC which was found to be metallic within GGA has now been changed to half-metal with wide

opening of band gap at  $E_F$  in its spin up channel, see Figure 3(a).

The binary compound under investigation does not contain transition metals thus the mechanism of the ferromagnetism is different from the concept of double exchange and  $p$ - $d$  exchange or  $d$ - $d$  exchange splitting in determining the magnetic moment. Here the pivotal role has been played by the spin polarization of the  $p$ -states of C atoms. Even the formation of spin gap is found to be at the spin up instead of spin down channel as in the case of 3d metal based compounds. As explained by Galanakis  $d^0$ -ferromagnets are made up of  $sp$  hybridization, in spin down the  $s$  and  $p$  orbitals of the two  $sp$  atoms hybridize creating bonding and anti bonding hybrids. The bonding

**Table II.** Energy gap ( $E_g$ ) and Spin polarization calculated within GGA/mBJ.

MC	Energy gap (eV)			Spin polarization		
	Prev. <sup>25/26</sup>	$E_g$ (GGA)	$E_g$ (mBJ)	$\rho \uparrow(E_F)$	$\rho \downarrow(E_F)$	$P\%$
MgC	—	—	4.00	1.30	0.60	36
CaC	0.83/0.81	1.80	3.40	0.20	1.80	100
SrC	0.81/0.72	1.60	3.20	0.00	2.10	100
BaC	0.61/0.54	1.10	2.20	0.00	3.10	100

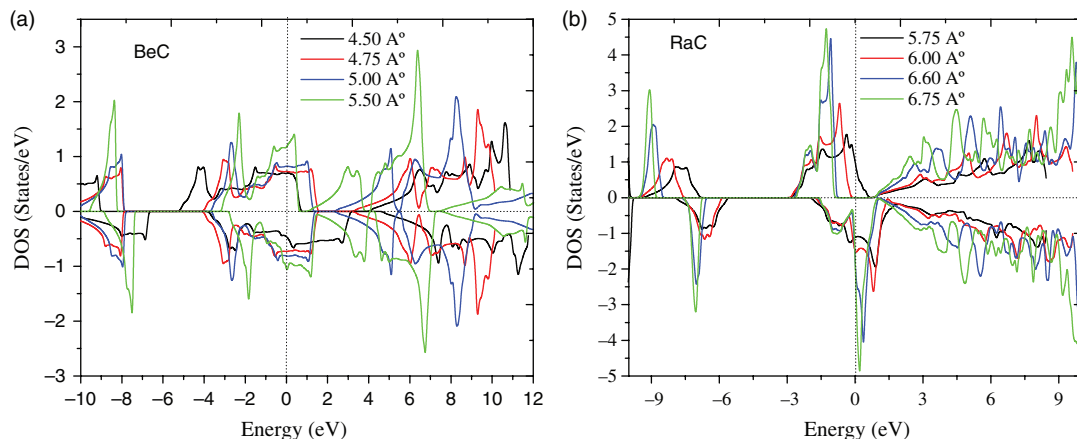


**Fig. 4.** Band structures and total DOS of (a) MgC, (b) CaC, (c) SrC and (d) BaC (Spin Up-green and Spin Down-black).

$sp$  states are occupied while the anti-bonding ones are empty leading to a total of 4 occupied spin down bands. In the spin-up band the bonding  $s$  state is occupied and the Fermi level crosses the bonding  $p$ -states since it has less than 8 valence electrons in the unit cell.<sup>45</sup> The band gap is defined as the difference between the lowest energy along X symmetry in conduction band and the highest energy along  $\Gamma$  symmetry in valence band thus it is an indirect band gap.<sup>46</sup> For CaC, SrC and BaC the minority channel is metallic whereas majority channel is insulating with indirect energy gaps 1.80/3.40 eV, 1.60/3.20 eV and 1.10/2.20 eV respectively within GGA/mBJ as shown in Figures 4(b–c). The calculated energy gap has over-estimated the previous results of CaC (0.83 eV), SrC (0.81 eV) and BaC (0.61 eV)<sup>25</sup> (Table II). We have also studied the electronic and magnetic properties of RaC and BeC by varying the lattice constants arbitrarily (Fig. 5). The properties of RaC were found to be similar with that of SrC and BaC but the properties of BeC has showed metallic character, see Figure 5(a). As shown in Figure 5(b), RaC is purely metallic for  $a = 5.75 \text{ \AA}$  and the corresponding magnetic moment is  $1.890 \mu_B$  which seems

to be deviated from the rule of 8,  $M_t = (8 - Z_t)$ .<sup>28</sup> As we have increases the lattice constant the energy band gap appears to be prominent as a result of exchange splitting of the C- $p$  states at the Fermi level. At  $a = 6.75 \text{ \AA}$  we have calculated the maximum band gap for RaC which is around 2.70 eV and the corresponding magnetic moment is an exact integer value  $2.00 \mu_B$  (Table III). The magnetic moment stabilizes to  $\sim 2.00 \mu_B$  with the increase in lattice constants from  $6.50 \text{ \AA}$  –  $7.50 \text{ \AA}$  (Fig. 6). In case of BeC the magnetic moment is negligibly small and gives negative value below  $a = 4.50 \text{ \AA}$  which indicates that this compound is a feeble anti-ferromagnet. The explanation of BeC is similar to that of MgC for the lattice constant at and above  $a = 5.00 \text{ \AA}$  within GGA as both of them are metallic in fcc structure and no gaps at the Fermi level. We have noticed that the increase in lattice constant increases the magnetic moments thus retain the ferromagnetic character as shown in Figure 6 for BeC (Table III).

All the information regarding the partial, total and the previously calculated magnetic moments are summarized in Table IV. The calculated total magnetic moment is close to an integer value in case of CaC as expected for the

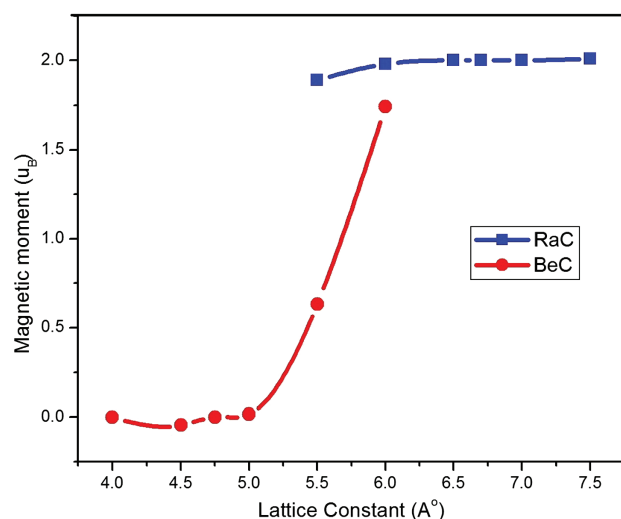


**Fig. 5.** Variation of DOS with change in lattice constants of (a) BeC and (b) RaC.

**Table III.** Variation of magnetic moments (MM) and Energy gap ( $E_g$ ) with lattice constants ( $a$ ) of RaC and BeC.

$a$ (Å)	RaC		$a$ (Å)	BeC
	$E_g$ (eV)	MM ( $\mu_B$ )		MM ( $\mu_B$ )
5.75	0.00	1.890	4.00	-0.045
6.00	0.70	1.980	4.50	-0.001
6.50	1.60	2.000	4.75	0.000
6.70	2.00	2.000	5.00	0.015
7.00	1.90	2.000	5.50	0.633
7.50	1.70	2.010	6.00	1.744

half-metallic systems (Table IV). In most cases the calculated magnetic moments are in good agreement with the previous results<sup>25</sup> except for MgC which has a huge deviation of almost 45% within GGA but mBJ agrees well. In all cases C sites contribute much more to the total magnetic moment as compare to X sites. There are six valence electrons in MC for example BaC(Ca:6s<sup>2</sup> and C:2s<sup>2</sup>2p<sup>2</sup>); C-s states occupies the low energy below -5 eV and C-p states are predominant in the Fermi level (Fig. 2(d)). Though the contribution of M atoms to the total magnetic moment is small but it results in the hybridization of C-p and M-s states. As shown in Figure 2 the two sharp peaks in spin up and spin down channels represent the exchange splitting of C-p states around Fermi level. As a result of exchange splitting of C-s and C-p states the partial magnetic moment of C atom is more as compared to M. For a binary compound to be a HMF, it has to obey the rule of 8,  $M_t = 8 - Z_t$ .<sup>28</sup> For example BaC (Ca:6s<sup>2</sup> and C:2s<sup>2</sup>2p<sup>2</sup>); the total number of valence electrons is 2+2+2=6, then  $M_t = 8 - 6 = 2.00 \mu_B$ . In our results we have found the total magnetic moment is 2.00  $\mu_B$  for BaC thus we can predict this compound a HMF with integer value of magnetic moment. Similar explanation may follows for other MC compounds as well.

**Fig. 6.** Variation of magnetic moments with lattice constants.**Table IV.** Total and partial magnetic moments ( $\mu_B$ ) of MC (M = Mg, Ca, Sr, Ba).

MC	Prev. <sup>25/26</sup>			Calculated		
	M	C	Total	M	C	Total (GGA/mBJ)
MgC	0.09	1.23	1.72/1.64	0.045	0.766	0.95/2.00
CaC	0.15	1.52	2.00/2.00	0.154	1.539	1.99/2.00
SrC	0.12	1.61	2.00/2.00	0.106	1.549	2.00/2.00
BaC	0.12	1.56	2.00/2.00	0.120	1.492	2.00/2.00

## 4. CONCLUSION

HMFs are a special type of materials due to its 100% spin polarization at  $E_F$  and wide application in the field of spintronics. In this work, we have investigated the electronic and magnetic properties of non-transition metal based binary compound MC (M = Be, Mg, Ca, Sr, Ba and Ra). We employed the most recommended semilocal exchange potential called mBJ to calculate the accurate ground state electronic structures. We have found that MgC, CaC, SrC and BaC are half metal at FM configuration within mBJ. The calculated total magnetic moment was found to be 2.00  $\mu_B$  per formula unit which governs the Slater-Pauling rule,  $M_t = 8 - Z_t$ . The electronic structures of RaC and BeC are robust to lattice constants, RaC exhibits half-metallicity for higher value of lattice constants while BeC is metallic in all cases. Among all these compounds MgC gives the largest mBJ gap of about 4.00 eV in its majority spin. The HMFs with low magnetic moment are of great interest as they can be a promising candidate for the spintronic applications.

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