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First-Principles Study of Electronic Properties and Robust Half Metallicity of Mixed $Sr_{1-x}Ca_xBeO_3$ (x = 0.25) Perovskite

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Abstract – The electronic and magnetic properties of pristine and Ca-doped $SrBeO_3$ have been investigated using full potential linearized augmented plane wave (FPLAPW) method based on density functional theory (DFT). The generalized gradient approximation (GGA) has been used to treat exchange and correlation potentials. Our results reveal that pristine $SrBeO_3$ and mixed $Sr_{1-x}Ca_xBeO_3$ (x = 0.25) perovskites have 100% spin polarization at Fermi level which ensure the robust half metallicity even after Ca-doping in $SrBeO_3$ perovskite. The magnetic moment of ~ 2.0 μ_B has been obtained for both which is consequence of hybridization of alkaline earth metals (Ca and Sr) p-states and O-p states. Due to the robust half metallicity and significant magnetism, the mixed $Sr_{1-x}Ca_xBeO_3$ (x = 0.25) perovskite may also be useful in spintronic devices.

Keywords – DFT; FPLAPW; Half Metallicity; Spintronics

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I. INTRODUCTION

Half-metallic compounds are characterized by the coexistence of metallic behavior of one spin electrons and the insulating/semiconducting behavior of other. The electronic density of states of such compounds is 100% spin polarized at Fermi level (E_F) and in these compounds, the metallic single spin charge carriers dominate the conductivity. After the remarkable discovery of HM ferromagnetism in NiMnSb by de Groot et al. [1], the research in this field has made significant developments. The HM character can also be confirmed very well experimentally these days [2-4].

ABO_3 perovskite oxides exhibit a broad spectrum of physical properties such as piezoelectricity, semiconductivity, ferroelectricity, superconductivity, metallic conductivity, paramagnetism, ferromagnetism, half metallicity etc. [5] and these properties can be controlled by several ways such as by changing ion size, electronic configuration and preparative conditions. Metallic $SrRuO_3$ has attracted much interest of researchers due to its unusual high Curie temperature (T_c = 160 K) which is unique among 4d/5d transition metal oxides [6,7].

In the past, RTFM was reported in various kinds of perovskites e.g. $BaTiO_3$ [8], double perovskites Sr_2FeMoO_6 [9] and doped perovskites $Bi_{0.5}Na_{0.5}TiO_3$ [10] etc. A-site substituted $Sr_{1-x}Ca_xRuO_3$ was found metallic, but it suffers a substantial lattice contraction and a gradual loss of FM [11,12] due to the lowering of the DOS at E_F. Mahmood et al. [13] investigated the Half-metallic ferromagnetism and optical behaviors of $XBeO_3$ (X=Mg, Ca, Sr and Ba) perovskites. They showed thermodynamically stability, half metallicity and room temperature (RT) ferromagnetism of all compounds by computing their Curie temperatures and spin polarizations [13].

After reviewing the literature, we planned to check whether the half metallicity and magnetism get retained by $SrBeO_3$ after Ca-doping at Sr-site or not using density functional theory (DFT) approach [14,15].

II. THEORETICAL APPROACH

We performed electronic structure calculations of pristine $SrBeO_3$ and mixed $Sr_{1-x}Ca_xBeO_3$ (x = 0.25) using the all-electron full-potential linearized augmented plane-wave (FPLAPW) method [16] based on DFT as implemented in WIEN2k package [17]. The exchange and correlation effects were taken into account by Generalized Gradient Approximation (GGA) within Perdew--Burke--Ernzerhof parameterization [18]. The radii of the Muffin-tin sphere (R_{MT}) for various atoms were taken in such a way to ensure nearly touching spheres and thus to avoid the charge leakage. The plane wave cut-off parameters were decided by $R_{MT}k_{max}$ = 7 (where k_{max} is the largest wave vector

of the basis set). The Fourier expansion of potential in the interstitial region was expanded up to G_{max} =12 a.u.$^{-1}$ and the maximum value of partial waves inside the atomic sphere was l_{max} = 10. The k-space integration was carried out using the modified tetrahedron method [19] and the self-consistency was obtained with 10×10×10 k-mesh in the Brillouin zone (IBZ) for both compounds. The calculations were based on the supercell approach for mixed perovskite where one Sr atom at (0,0,0) in the (2×2×2) supercell of SrBeO3 was replaced by Ca-atom to obtain $Sr_{0.75}Ca_{0.25}BeO_3$ as depicted in Fig. 1

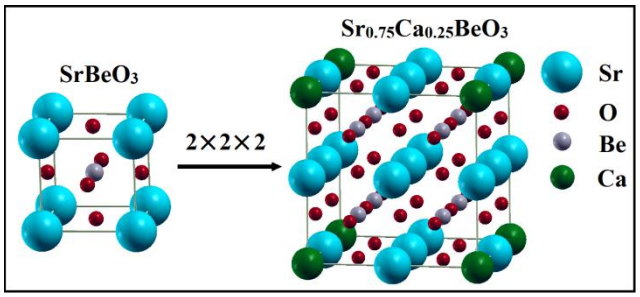

Fig. 1: Schematic for simulating $Sr_{0.75}Ca_{0.25}BeO_3$ via substituting one Sr atom by Ca in (2×2×2) supercell of $SrBeO_3$.

III. RESULTS AND DISCUSSION

The most of the ABO_3 type perovskites have as an ideal cubic structure within pm3m (221) space group, similar to that of the mineral perovskite ($CaTiO_3$), which consists of a corner sharing BO_6 octahedral where A and B cations are coordinated by 6 and 12 O-anions, respectively. To start with, we considered the lattice parameter of $SrBeO_3$ (3.67 Å) as calculated by Mahmood et al. [13] and performed the structural optimization for $SrBeO_3$ and $Sr_{0.75}Ca_{0.25}BeO_3$. We have obtained a lattice parameters of 3.674/3.663 Å for $SrBeO_3$/$Sr_{0.75}Ca_{0.25}BeO_3$. With the optimized parameters, the final calculations of density of states (DOS) were performed.

Before analyzing the mixed perovskite, it is important to study the nature of DOS and contributions of various atoms in it for pristine $SrBeO_3$ compound. For this, we have examined total and partial DOS of $SrBeO_3$ in Fig. 2. It is clear that the total DOS is highly spin polarized with 100% spin polarization at E_F. A suitable band gap in majority spin channel was observed for it. After observing Sr-p, Be-p and O-p states, we found strong exchange splitting near the E_F for majority spin channel. On the other hand, these states cross the E_F in minority spin channel. Therefore, $SrBeO_3$ is half metallic in nature.

The calculated bandstructure and total DOS for the mixed $Sr_{1-x}Ca_xBeO_3$ (x = 0.25) perovskite is shown in Fig. 3. The total DOS of mixed compounds is exactly similar to that of pristine case. Therefore, the origin of half metallicity and magnetism is expected to be same for both compounds. 100% spin polarization at E_F governs the mixed compound as half metallic also. The bandstructure also confirms the band gap in majority spin channel of mixed $Sr_{1-x}Ca_xBeO_3$ (x = 0.25) perovskite.

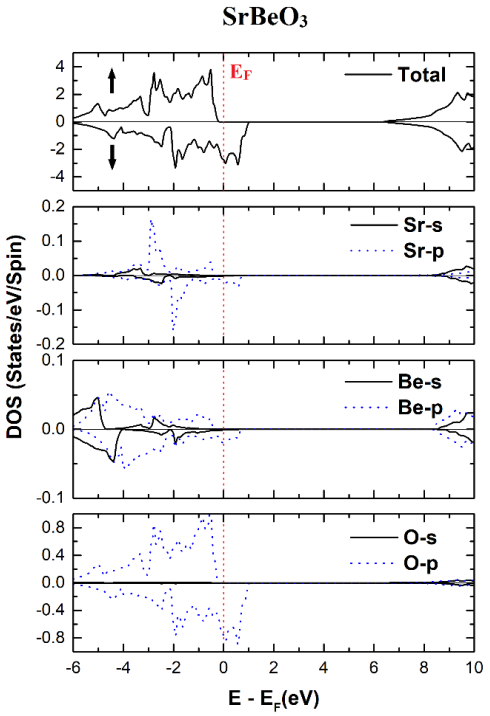

Fig 2: Total and atom resolved DOS of $SrBeO_3$. E_F is set at 0 eV

Further, the existence of HM gap (a minimal gap for spin excitation) instead of band gap in one spin channel is a striking feature of the HM compounds. This gap is of unique importance for creating a hole and an electron and is defined as the minimum value out of (E_F-E_{top}) and (E_{bot}-E_F) where E_{top}/E_{bot} represents the energy corresponding to top of valence band (VB)/ bottom of conduction band (CB). A true HM ferromagnet is governed by a non zero HM gap [20]. We observed a HM gap for $SrBeO_3$/$Sr_{0.75}Ca_{0.25}BeO_3$ as 0.22/0.18 eV. A small decrease in this gap is expected for mixed compound as the atomic radius of Ca is somewhat larger than Sr.

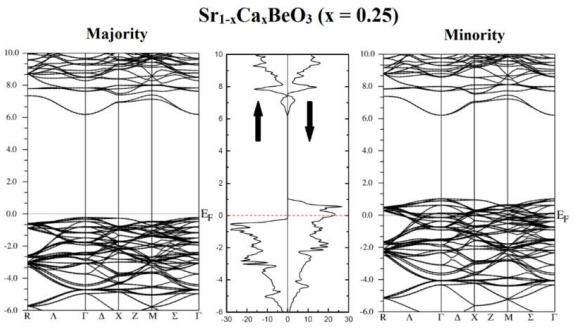

Fig 3: Band structure and total DOS of mixed $Sr_{0.75}Ca_{0.25}BeO_3$ perovskite compound

Finally, total and partial magnetic moments for both compounds were calculated, and it was observed that the main contributor in total magnetic moment (2.0 μ_B for both) is O-atom. Be-moment aligns antiparallel to the moments of all other atoms. Integer value of magnetic moment also confirms 100% half metallicity for both compounds.

IV. CONCLUSIONS

In the present work, we predicted the electronic and magnetic properties of $SrBeO_3$ and mixed $Sr_{1-x}Ca_xBeO_3$ (x = 0.25) perovskites using DFT approach. It was found that both compounds are half metallic ferromagnets with 100% spin polarization at Fermi level. The magnetism in these materials results essentially due to hybridization of Ca/Sr-p states and O-p states. The total magnetic moments for both compounds come out to be integer values (2 μ_B), which confirm the ferromagnetic character. Due to the interesting half-metallic properties and sufficient magnetism, mixed $Sr_{1-x}Ca_xBeO_3$ (x = 0.25) perovskite may be a potential candidate for spintronic applications.

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