

Magneto-electronic studies of the inverse-perovskite (Eu₃O)In



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ABSTRACT

Ferromagnetic metallic inverse-perovskite (Eu₃O)In is studied using hybrid functional theory (HF) in the frame work DFT. The calculated structural parameters and geometries of the material are calculated by different exchange correlation potentials and found that HF results are closed to the experiments. Electronic charge density explains the bond nature and polarization. The spin polarized electronic band profiles and density of states reveal the metallic nature of the compound. The Eu f-state splitting show that the valance bands are dominated mainly by f-[a₂], f-[x(T₁)], f-[y(T₁)] and f-[z(T₁)] states. The ground state magnetic phase of the compound is optimized. The optimum energy and magnetic susceptibility confirm the ferromagnetic nature of the compound. On the basis of different properties presented it is predicted that this compound is magnetoresistive material.

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1. Introduction

Ferromagnetic materials have attracted great attention because of their excellent properties and promising applications in storage information industry. The information is stored in the form of bits which are read by magnetic read heads [1]. The current read heads in hard drives are giant magnetoresistive (GMR) type based on multilayer thin film technology [2–4]. The basic physics behind the drop of the resistivity in GMR is the presence of a magnetic field, results in electronic phase separation between ferromagnetic metallic lyres sandwiched anti-ferromagnetic metal. Recently, improved material synthesis techniques in the quest to develop high temperature superconductors and other efficient materials lead researchers to perovskites. In these materials, the application of a magnetic field causes the resistivity to drop by several orders of magnitude, which would be ideal for storage device applications.

(A₃X)E is the general formula of inverse perovskites, where A is the alkaline-earths or rare-earth elements, X=H, B, C, N and O, and E is the p-group elements [5–7]. For the first time the inverse perovskites were misinterpreted as the binary compounds or the modifications of incorrect compounds A₃E. In the last century for (X=C) a large number of rare-earth metal inverse perovskites compounds (R₃C)E were reported [6]. These carbide compounds are expected to be brittle and electrically conductor [6,8]. Nitrides with metallic behavior with E=Al, Ga, In, Tl, Sn and Pb were also

reported with trivalent rare-earth metals [7]. Europium carbide and corresponding alkaline-earth metal carbides are apparently not existed [6]. Ram and Kanchana [9] recently studied La₃InZ (Z=N, O) inverse perovskites and reported different properties of the compounds.

The f-block element europium (Eu) usually appears in divalent Eu²⁺ (4f⁷) or trivalent Eu³⁺ (4f⁶) states in the compounds [10], the fluctuation between these states may occur very frequently, results an intermediate valence state situation. These different electronic configurations of Eu atoms are localized at different crystallographic sites (inhomogeneous mixed-valence situation) and occurrence of the element with different electronic valence states distributed on the same crystallographic sites (homogeneous mixed-valence situation) is almost rare.

The inverse perovskite (Eu₃O)In was prepared from pressed powder pellets of Eu–In melt beads of appropriate composition of Eu₂O₃ [6]. The structural analysis of (Eu₃O)In by X-ray diffraction shows its existence in cubic phase with space group *Pm* $\bar{3}$ *m* having lattice constant 5.128 Å. On the basis of absolute value of electrical resistivity it was reported that (Eu₃O)In that the electrical resistivity of the compound is much larger but the compound still behave like metal. The compound is also investigated by the X-ray absorption spectroscopy (XAS), Eu²⁺ (4f⁷) state of Eu is reported in the compound and there is no indication for Eu³⁺ (4f⁶) present [6], whereas in some compounds like EuFe₂As₂ Eu exist in two oxidation states Eu²⁺ (4f⁷) and Eu³⁺ (4f⁶) [11]. The magnetic susceptibility measurement of (Eu₃O)In compound shows ferromagnetic order at 185 K. The presence of conduction electrons in In compound show large ferromagnetic interaction between

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europium atoms at higher temperature and the effective magnetic moment Eu ($\mu_{\text{eff}} = 7.94 \mu_B$) is reported [6].

In this article we study the structural, electronic and magnetic properties of the inverse-perovskite $(\text{Eu}_3\text{O})\text{In}$ using GGA, GGA+ U , GGA-PBE-sol, hybrid functional (HF) and HF B3PW91 within the frame work of DFT. The aim of the present work is to explore the electronic structure and magnetic properties of the compound for possible advance technological applications. Electronic properties of the compound are investigated on the basis of spin polarized electronic band structure, total and partial densities of states. The stable magnetic phase of the compound is evaluated by the minimization of the magnetic energy in different magnetic phases and by magnetic susceptibility curve utilizing the BoltzTrap Package [12].

2. Computational details

In the present work Kohn–Sham equations [13] are solved to calculate the physical properties of the inverse perovskite $(\text{Eu}_3\text{O})\text{In}$ in frame work of DFT using WIEN2k software [14]. The structural, electronic and magnetic properties of the compound are calculated by GGA [15], GGA+ U [16,17], HF PBE-sol and HF B3PW91 [18] exchange correlation potentials. For GGA+ U calculations it is assumed that the density matrix is diagonal and U is the same for all Coulomb onsite interactions ($U_{ij} = U$) and J is also the same for all exchange interactions ($J_{ij} = J$). There are several methods to incorporate the U -term [16,17] but here we used the method developed by Anisimov et al. [19], self-interaction correction (SIC) as implemented in the WIEN2k package. For full potential method we use an “effective” $U_{\text{eff}} = U - J$ by setting $J = 0$. After examining several values of Hubbard potential in order to adjust the $\text{Eu-}4f$ orbitals level in the density of the final value used is $U_{\text{eff}} = U - J = 7.0 \text{ eV}$ for U .

HF is effective tool to explain the correlated electron system. In lanthanides B3PW91 is effective potential to treat these systems [18]. Similarly for the HF calculations exact exchange α is set 0.75 eV in order to get better result. The core electrons are treated fully relativistically and the valence electrons are treated semi-relativistically. In order to ensure that no electron leakage is taking place semi-core states are included so that accurate results can be achieved; 286 k -points are used and $R_{\text{MT}}K_{\text{max}} = 8.00$ determines the plane wave basis functions.

3. Results and discussion

3.1. Structural properties

For the investigation of the ground state structural properties of the inverse perovskite $(\text{Eu}_3\text{O})\text{In}$ energy per unit cell of the compound is optimized and structural parameters are evaluated using the fitted Birch–Murnaghan equation of state [20] like our previous works [21,22]. In rare-earth inverse perovskite $(\text{Eu}_3\text{O})\text{In}$; Eu is located at (0.5, 0.5, 0), (0.5, 0, 0.5) (0, 0.5, 0.5), oxygen at (0.5, 0.5, 0.5) and In is at (0, 0, 0) sites with space group $Pm\bar{3}m$ (no. 221). The optimization curve for the compound by different potentials like GGA, GGA+ U , HF-PBESol and HF-B3PW91 are presented in Fig. 1. The evaluated structural parameters like lattice constant, volume, bulk modulus and ground state energy are listed in Table 1. It can be seen from the table that the lattice parameter of $(\text{Eu}_3\text{O})\text{In}$ by GGA is 4.94 Å, which is 3.5% less than the experimental reported result [6], this is due to the fact that GGA cannot treat f -orbital of Eu properly, by applying GGA+ U and HF-PBE-sol the lattice constant of the compound is 5.09 Å, 0.58% underestimated, while by HF-B3PW91 the calculated lattice is 0.15% less

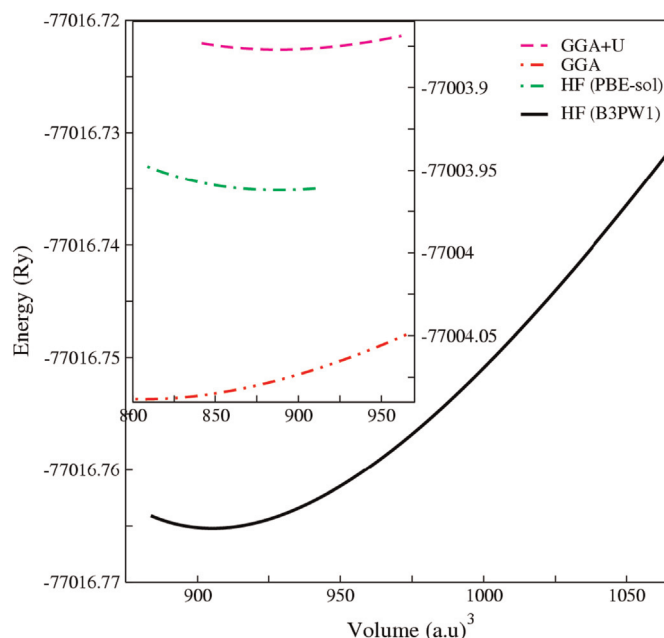


Fig. 1. Optimization plot of $(\text{Eu}_3\text{O})\text{In}$, energy versus volume by GGA, GGA+ U , HF-PBESol and HF-B3PW91.

than the experimental reported value. The comparison of all these results shows that HF-B3PW91 treat accurately the 4 f -state of Eu in $(\text{Eu}_3\text{O})\text{In}$. Hence HF-B3PW91 is more effective to study $(\text{Eu}_3\text{O})\text{In}$ and localized the 4 f -state of Eu.

The structural geometries are also investigated by these potentials and are listed in Table 1. The bond lengths between different atoms are compared with the experimental reported values [6], and found that our calculated bond lengths are under estimated up to 0.15% by HF-B3PW91. The bonds lengths between Eu–O, Eu–In and In–O are 2.56 Å, 3.6204 Å and 4.4341 Å respectively. This shows the reliability of the work that HF-B3PW91 properly treats f -state, while GGA, GGA+ U , HF PBE-sol underestimate the structural parameters.

Electron charge density has a unique importance to understand the chemical bonding nature and charge transfer between the ions of the material when its constituent atoms combine to form a compound. The two dimensional (2-D) electron charge density for (100) and (110) planes are presented in Fig. 2(a–d). The bonding nature between different atoms for both spins is dominantly ionic and the charge leakage is rare between the atoms hence covalent behavior is very small. The distribution of the electronic charge density in (100) plane is spherical around In atoms as shown in Fig. 2(a) and (c) and very small charge density in the region between the In atoms and Eu atoms indicate that the bond between In and Eu is ionic. In spin down case polarization take place and the dumbbell shape of Eu and O represent the covalent character, shown in Fig. 2(d) (110) plans in which the ionic character is down and converting toward covalence bond.

3.2. Electronic properties

Physics of the strongly correlated electrons system is one of the most challenging tasks of present-days for both theoretician and experimentalist. A wide variety of interesting phenomena can be attributed to the electronic correlations like metal–insulator transitions, the giant and colossal magnetoresistivity, superconductivity and heavy-fermions behavior. Self-consistent field (SCF) calculations are performed to study the spin-polarized electronic nature of the compound $(\text{Eu}_3\text{O})\text{In}$. The calculated spin-polarized band structure for the compound by GGA, GGA+ U , HF

Table 1
Calculated and experimental lattice constant (a_0), bulk modulus (B), ground state energy (E_0) volume (V_0), bond lengths and magnetic moments of Eu of (Eu₃O)In.

Parameters	GGA PBE-sol	GGA + <i>U</i> PBE-sol	HF PBE-sol	HF B3PW91	Experimental [a]
a_0 (Å)	4.94	5.09	5.09	5.12	5.128
B (GPa)	55.64	54.00	51.00	56.63	–
E_0 (Ry)	– 77004.11	– 77003.88	– 77003.96	– 77016.77	–
V_0 (Å) ³	120.52	131.55	131.57	134.07	134.84
Bond lengths					
$d_{\text{Eu-O}}$ (Å)	2.4250	2.5077	2.5077	2.5600	2.5600
$d_{\text{Eu-In}}$ (Å)	3.4595	3.6013	3.6013	3.6204	3.6260
$d_{\text{In-O}}$ (Å)	4.2002	4.3402	4.3402	4.4341	–
Magnetic moment					
Eu (μ_B) × 3	6.75	6.95	6.97	7.13	7.57

Ref. a: [6].

PBE-sol and HF B3PW91 is plotted in Fig. 3. In case of spin up band the f-state of Eu occurs at the Fermi level is due to the delocalization because GGA cannot treat f-state properly. To overcome this problem and to localize the f-state electrons we use GGA + *U*, HF PBE-sol and HF B3PW91. It can be seen from the figure that HF B3PW91 localized the f-state properly. In spin up state Fermi level is covered by orbitals make the compound metallic. While in case of spin down polarization take place and the f-bands jumps into the conduction band again the Fermi level is covered by orbitals. Hence the compound is metallic in nature for both spin states. Our results are consistent with experimental data [6]. As concern to the oxidation state of europium it was reported by XAS data [6] that europium exist in the form of Eu²⁺ (4f⁷) and there is no indication for Eu³⁺ (4f⁶) present, whereas in some rare-earth tellurides, samarium mononictdes [23,24], samarium monochalcogenides [23], EuFe₂As₂ etc. [11] the lanthanides exist in mixed oxidation states. To study the ground state valance configuration of those system self-interaction corrected local-spin density approximation (SIC-LSD) were utilized [25].

To get a clear look into different states in the band structure the total density of states of the compound are plotted in Fig. 4(a). The contribution to the total density of states (DOSs) of the compound (Eu₃O)In varies in the same way as the contribution of compound to the band structure. The partial density of states for the compounds is presented in Fig. 4(b). The core states are mainly due Eu-p states which hybridized with a small a small contribution of O-p state. The other contribution to the core states is indium d-state. In the spin down state this contribution shifts towards higher energy level in the band structure. The bottom of the valence band of the material is dominated by O-p state with a small contribution of Eu-p and Eu-d states. The top of the valence is contributed by overlapped In-p, O-p and Eu-f states; this contribution to density of state cross over the Fermi level which indicates the metallic nature of the compound. The conduction band is mainly dominated by Eu-d state with relatively small contribution from the Eu-p, In-p and In-d states.

For the detailed description of the electronic band structure we calculate the 4f-state splitting of Eu in the compound as shown in

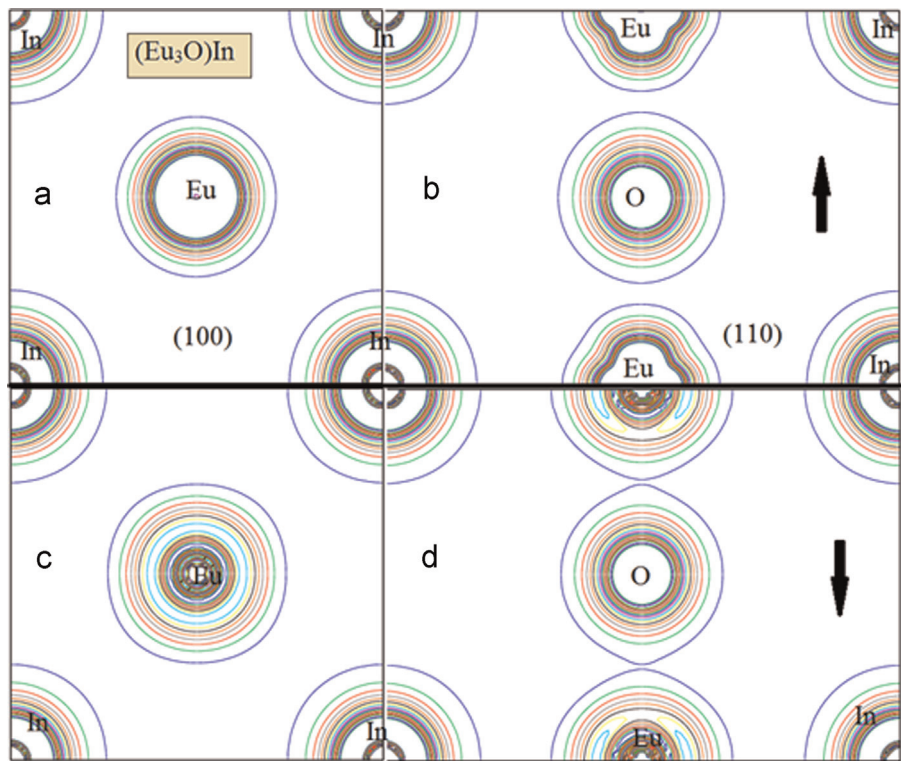


Fig. 2. Two dimensional electronic charge density of (100) and (111) plans of (Eu₃O)In.

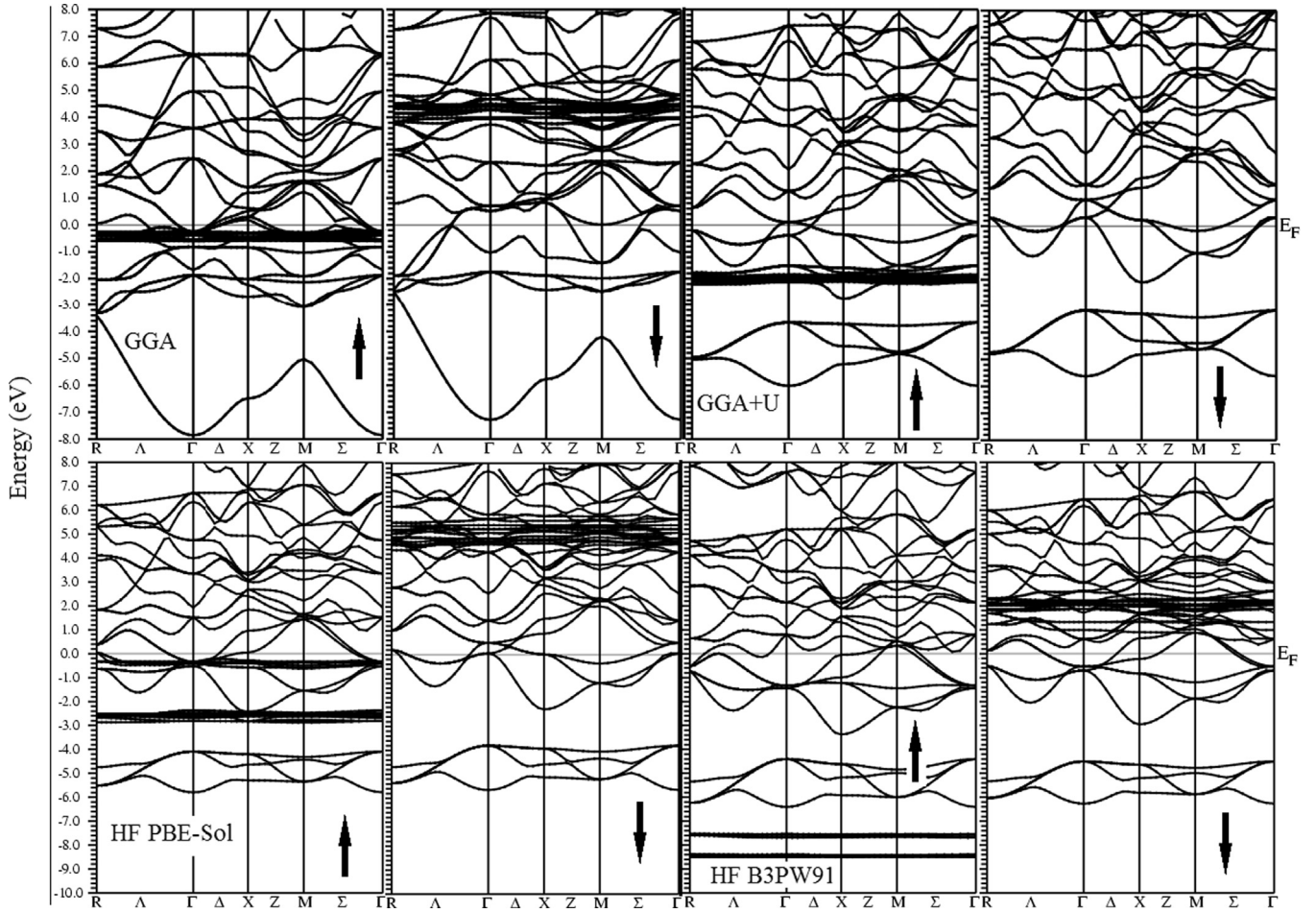


Fig. 3. Spin-polarized electronic band structures of $(\text{Eu}_3\text{O})\text{In}$ by GGA, GGA+U, HF-PBEsol and HF-B3PW91.

Fig. 5. It can be clear from figure that 4f-DOS, that the valance states are dominated mainly by $f\text{--}[(a_2)]$, $f\text{--}[x(T_1)]$, $f\text{--}[y(T_1)]$ and $f\text{--}[z(T_1)]$ states, while $f\text{--}[\kappa_2(T_2)]$, $f\text{--}[\eta_2(T_2)]$ and $f\text{--}[\zeta_2(T_2)]$ states contributed in the conduction bands.

3.3. Magnetic properties

To study the ground state magnetic properties of the compound we optimized the double cell for ferromagnetic and anti-ferromagnetic phases. Ferromagnetic and anti-ferromagnetic optimizations are performed for the material to know the stable magnetic phase. The calculated energy difference ($E_{\text{FM}} - E_{\text{AFM}}$) per unit cell of ferromagnetic (E_{FM}) and anti-ferromagnetic (E_{AFM}) phases is -1.0317 Ry. The stable magnetic of the compound is ferromagnetic in which the material lower its ground state energy as compared to the other phases, and found in agreement with the experiment [6].

Magnetism in perovskites is due to the indirect exchange interactions of partially filled shell via conducting electrons. There are two types of indirect exchange interaction one is double exchange while the other one is super exchange. In most of the cases double exchange favor ferromagnetic interaction, while super exchange anti-ferromagnetic interactions [26,27]. The magnetic interaction between two magnetic ions Eu^{2+} double exchange ($\text{Eu}^{2+} - \text{O}^{2-} - \text{Eu}^{3+}$) favor ferromagnetic; while super exchange ($\text{Eu}^{3+} - \text{O}^{2-} - \text{Eu}^{3+}$) is anti-ferromagnetic.

The local and total magnetic moments of $(\text{Eu}_3\text{O})\text{In}$ are calculated by GGA, GGA+U, HF-PBEsol and HF-B3PW91. The magnetic moment of $(\text{Eu}_3\text{O})\text{In}$ is the contribution of Eu, O, In and interstitial

sites. The magnetic effect of Eu, O and In occur inside muffin-tin sphere while the interstitial magnetic moments arises from the atomic sites in a crystal is outside muffin-tin sphere. The major contribution of the magnetic moment comes from Eu due to the partially filled 4f-state, while some contribution comes from O, In and interstitial sites. The calculated magnetic moment of Eu per unit cell of $(\text{Eu}_3\text{O})\text{In}$ by different exchange correlation potentials GGA, GGA+U, HF-PBEsol and HF-B3PW91 are $6.75 \mu_B$, $6.95 \mu_B$, $6.97 \mu_B$ and $7.13 \mu_B$ respectively. The comparison with experimental reported value ($7.57 \mu_B$) [6] shows that the results of HF-B3PW91 are consistent. The difference in the theoretical and experimental values is due to the well-known limitations of DFT, because of electrons exchange correlation. The oxygen magnetic moment is negative ($-0.7755 \mu_B$) which indicates that it is aligned in opposite direction. The contribution from In site is $0.0850 \mu_B$ while from the interstitial sites is $0.5639 \mu_B$, resulting net magnetic moment of $21.2634 \mu_B$ per unit cell. The non-integer value of the total magnetic moment confirms the metallic nature of the compound. Hence $(\text{Eu}_3\text{O})\text{In}$ is a ferromagnetic metal.

BoltzTrap code [12] is utilized to calculate the magnetic susceptibility (χ) of the compound in order to confirm the magnetic order of the compound. Magnetic susceptibility and inverse of magnetic susceptibility plotted against temperature in Fig. 6 in which χ is scaled ($10^{-3} \text{ emu mol}^{-1}$) and temperature in Kelvin. Magnetic susceptibility explains the magnetic order of a material and inversely related to temperature [27,28]. It can be seen from the figure that susceptibility decreases with the increase of temperature. The substantial decrease occurs in susceptibility at 170 K, our calculated plot of χ^{-1} with temperature follow the same trend

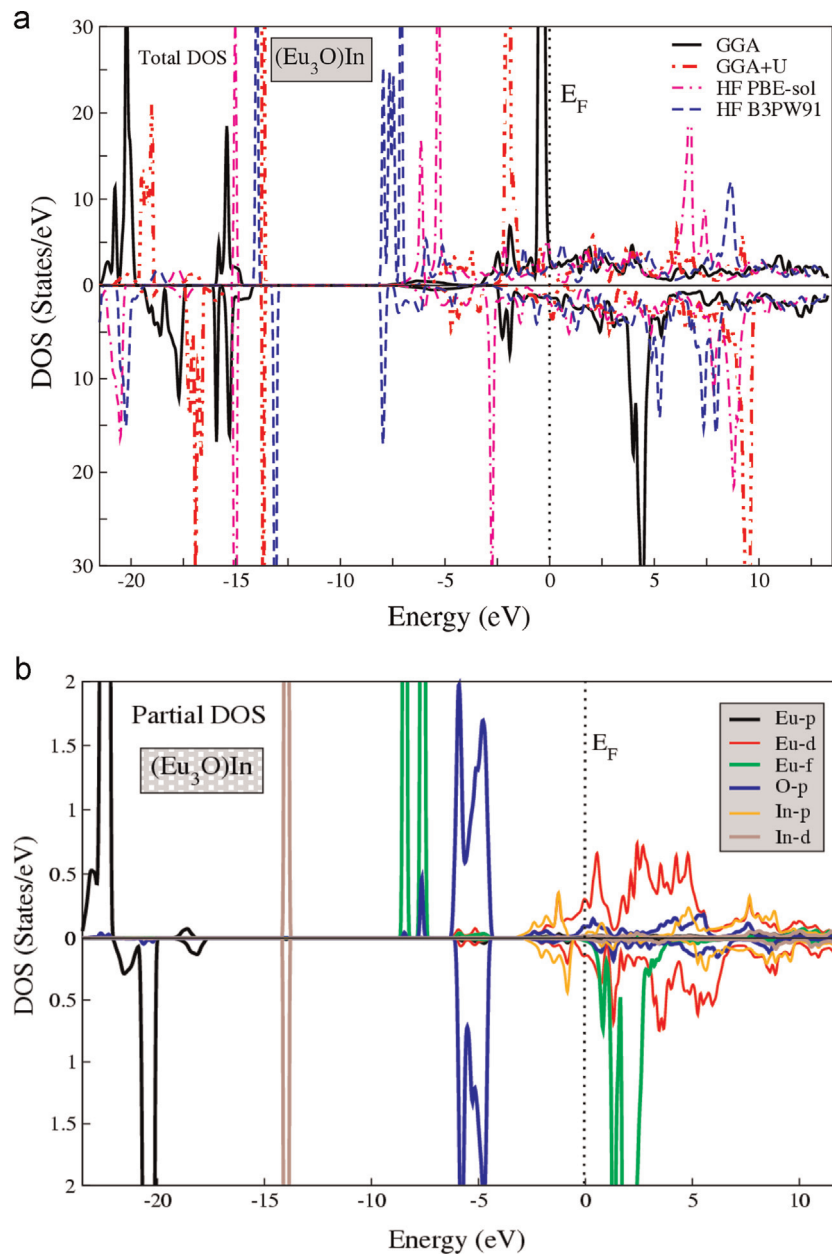


Fig. 4. Spin-polarized total and partial density of states of $(\text{Eu}_3\text{O})\text{In}$ by GGA, GGA+U, HF-PBESol and HF-B3PW91.

as reported in Ref. [6]. The saturation in magnetic susceptibility probably occurs beyond a temperature 50 K. The magnitude of the magnetic susceptibilities of the compound is at temperature 50 K is $9.88 \times 10^{-3} \text{ emu mol}^{-1}$. Hence it can be concluded that magnetic susceptibility justifying the ferromagnetic nature of the material.

Ferromagnetic and anti-ferromagnetic metals perovskite oxides are magnetoresistive [29,30], weak magnetoresistance is present almost in all compounds [31]. Magnetoresistance is the change in the electrical resistance of a material by external magnetic field and are uses in storage devices [32,33]. As $(\text{Eu}_3\text{O})\text{In}$ compound is experimentally metal heaving high electrical resistance, on the bases of ferromagnetic phase with metallic high resistive nature it is expected that Eu_3OIn is magnetoresistive material.

Similarly specific heat at constant pressure (C_p) is calculated for the material at temperature range 0 up to 400 K. Heat capacity produces a degree change in temperature of a substance by absorbing heat and an extensive property, proportional to the size of

the system. Materials with high value of specific heat are used as good coolant agents in different industries. In the present work a plot for the material is sketched in between molar specific heat at constant pressure C_p ($\text{J mol}^{-1} \text{ K}^{-1}$) and temperature T (K) in Fig. 7. The increase in temperature increases the ability of molar heat capacity of a substance. It can be seen from the figure that C_p is constant from 0 K to 300 K and then increases exponentially. This trend goes on further in the same way justifying the Debye theory of specific heat [28]. The abrupt increase above 300–400 K and finally a stage reaches where phase transition occurs.

4. Conclusions

In summary structural, electronic nature and magnetic properties of the cubic inverse-perovskites $(\text{Eu}_3\text{O})\text{In}$ is studied using the all electron spin-polarized density functional theory (DFT). The structural parameters and geometries of the material are studied

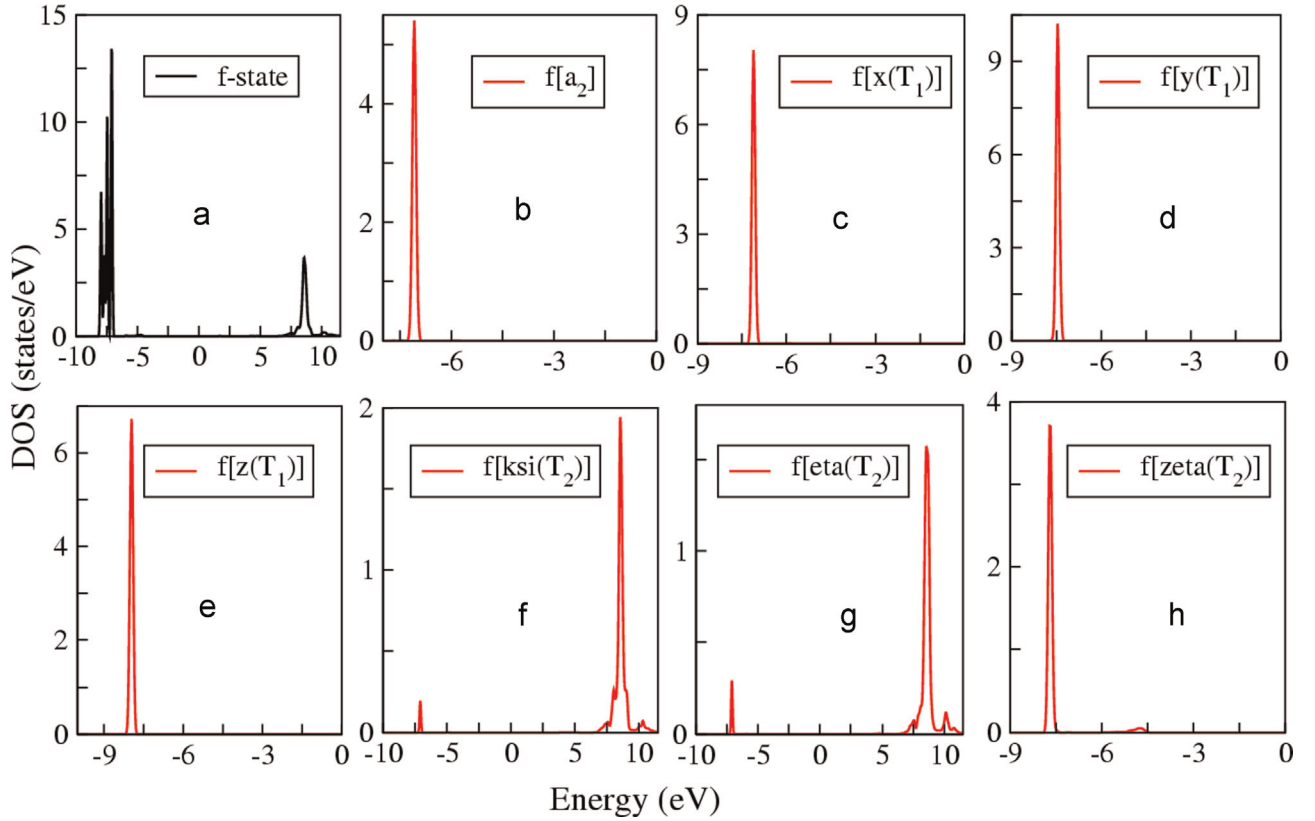


Fig. 5. (a) f-State DOS and splitting of f-states (b) $f[a_2]$, (c) $f[x(T_1)]$, (d) $f[y(T_1)]$, (e) $f[z(T_1)]$, (f) $f[\kappa(T_2)]$, (g) $f[\eta(T_2)]$ and (h) $f[\zeta(T_2)]$ of Eu in $(Eu_3O)In$.

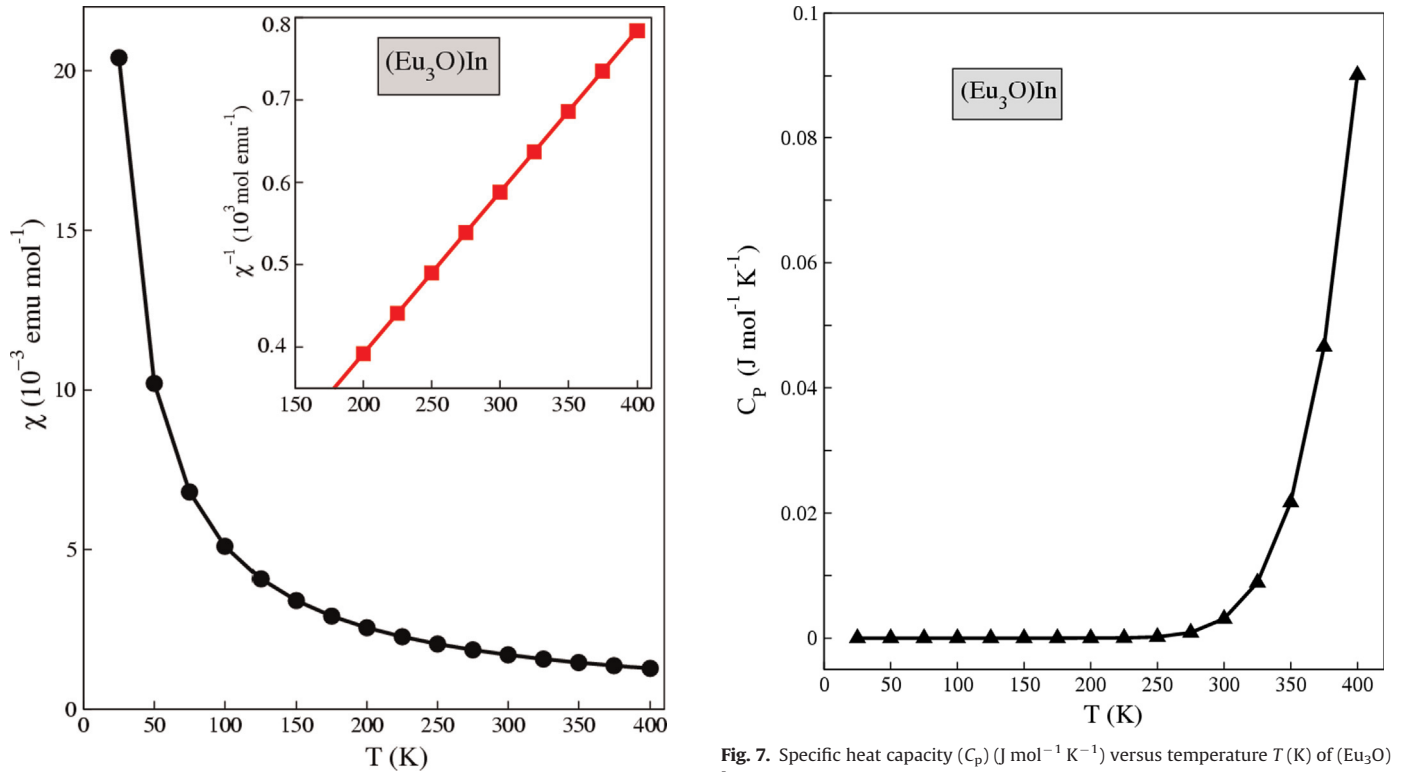


Fig. 6. Magnetic susceptibility (χ) and inverse of magnetic susceptibility (χ^{-1}) plots against temperature of $(Eu_3O)In$.

Fig. 7. Specific heat capacity (C_p) ($J mol^{-1} K^{-1}$) versus temperature T (K) of $(Eu_3O)In$.

by different potentials which show that the results of HF-B3PW91 are in agreement with the experiments. The electronic band structures and density of states reveal that the compound is

metallic in nature. The density of states of Eu-f state splitting of the material show that the valance states are dominated mainly by $f[a_2]$, $f[x(T_1)]$, $f[y(T_1)]$ and $f[z(T_1)]$ states. The optimum energy and magnetic susceptibility calculated by BoltzTrap code show that $(Eu_3O)In$ is ferromagnetic. On the basis of different physical

properties presented in this article it is predicted that the material is magnetoresistive.

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