

First principle studies of electronic and magnetic properties of Lanthanide-Gold (RAu) binary intermetallics



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ARTICLE INFO

Article history:

Received 14 July 2016

Accepted 22 August 2016

Available online 23 August 2016

Keywords:

Lanthanide-Gold intermetallics

Electronic band profiles

Magnetic properties

Chemical bonding, cohesive energies

Ab-initio calculations

ABSTRACT

In this article we explore the electronic and magnetic properties of RAu intermetallics (R=Ce, Pr, Nd, Sm, Gd, Tb, Dy, Ho, Er, Tm, Yb and Lu) for the first time. These properties are calculated by using GGA, GGA+U and hybrid density functional theory (HF) approaches. Our calculations show that HF provides superior results, consistent to the experimentally reported data. The chemical bonding between rare-earth and gold atoms within these compounds are explained on the basis of spin dependent electronic clouds in different planes, which shows predominantly ionic and metallic nature between Au and R atoms. The Cohesive energies of RAu compounds show direct relation with the melting points. Spin-dependent electronic band structure demonstrates that all these compounds are metallic in nature. The magnetic studies show that HoAu and LuAu are stable in non-magnetic structure, PrAu is stable in ferromagnetic phase and CeAu, NdAu, SmAu, GdAu, TbAu, DyAu, ErAu, TmAu, YbAu are anti-ferromagnetic materials.

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1. Introduction

Noble metals (Cu, Ag, Au) based compounds are attractive for material scientists for their high oxidation and corrosion resistance, high stability, good strength, ductile and magnetic nature, very high melting points, good conductance and wide-range applications in high-temperature structural materials [1]. Generally the intermetallics with B2 or CsCl structure that contains one transition and a simple metal atom exhibit diverse physical phenomena. They are best for the systematic study of magnetic properties, electronic structure, cohesive properties, charge transfer and chemical bonding [2]. This class of compounds is antiferromagnetic [3] and metallic in nature with no band gap. The binary alloys of gold with the rare-earth elements are characterized by the cubic CsCl-type crystal structure B2 with space group Pm3m (No. 221), having the Wyckoff positions: R atom at (0,0,0) and Au atom at (0.5,0.5,0.5) [4–6] except CeAu [5] which has CrB type crystal structure [7,8]. However experiments also show the cubic CsCl-type structure for CeAu compound [9]. Lanthanides in these compounds are trivalent [7,10,11] except Yb which is

divalent [12]. Therefore, some of the physical properties of Yb such as the metallic radius, electronegativity etc are quite different than those of the normal trivalent rare-earth metals.

The compounds of lanthanides is the first group of atoms containing f-orbital [13]. One of the interesting subgroups of lanthanide compounds is the noble metals (Cu, Ag and Au) based stable lanthanides. Among this group the most stable compounds are those of Au with the rare-earth elements [14]. The bond stabilities are in the order of $R_{Au} \gg R_{Cu} > R_{Ag}$ (R=Ce, Pr, Nd, Sm, Gd, Tb, Dy, Ho, Er, Tm, Yb and Lu) [15].

Ionic as well as metallic bonds are present between gold and lanthanide atoms [7,16,17]. Electron transfer from the rare-earth metal to gold occurs as the electronegativity difference of these atoms are favorable for ionic bond formation [18]. The ionic and metallic bonding in these intermetallics can be confirmed from the fact that these compounds have high melting points [16,19–21] high dissociation energies [7,16,22] and high bond energies [23]. The stable nature of these compounds is due to the large electronegativity difference (> 1.13) and equiatomic stoichiometry of gold and lanthanides [10,15,19]. There exists a correlation between the stability trend and the relative melting behavior of these compounds [17]. Their melting points increase steadily as a function of atomic number from 1372 °C for CeAu to 1780 °C for LuAu respectively, with the exception of YbAu whose melting point is

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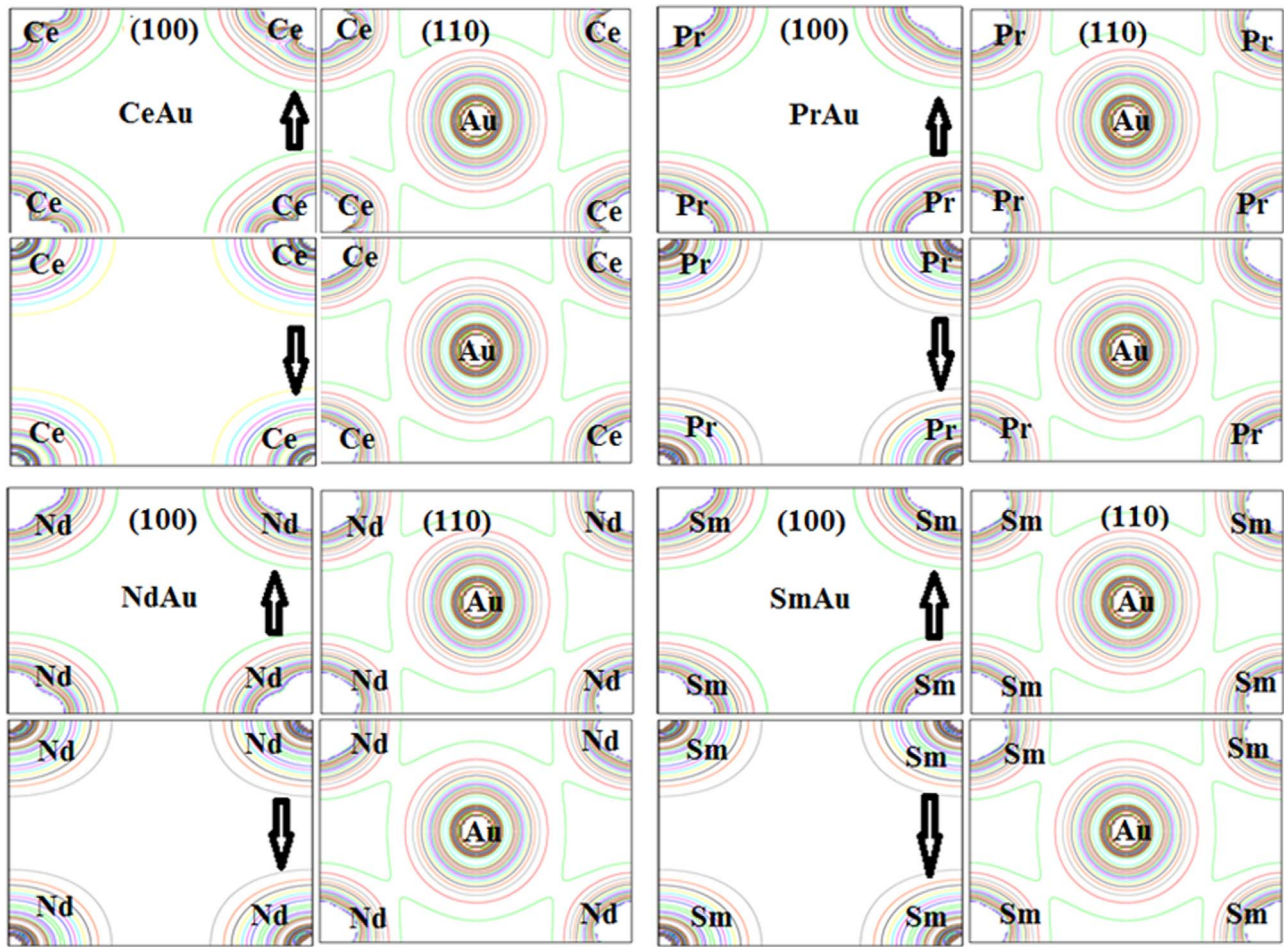


Fig. 1. Spin polarized electronic charge density of RAu compounds (R=Ce, Pr, Nd, Sm, Gd, Tb, Dy, Ho, Er, Tm, Yb and Lu) in (100) and (110) planes.

Table 1

Cohesive energies, total ground state energies and ground state energies of free atoms of R(R=Ce, Pr, Nd, Sm, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu) and Au atoms.

Compound	E_{Coh} (Ry)	E_{total} (Ry)	E_{R} (Ry)	E_{Au} (Ry)
CeAu	−18.449	−55.809	−17,717	−38,074
PrAu	−18.524	−56,564	−18,471	−38,074
NdAu	−18.579	−57,338	−19,246	−38,074
SmAu	−18.800	−58,948	−20,855	−38,074
GdAu	−18.900	−60,638	−22,545	−38,074
TbAu	−19.156	−61,515	−23,422	−38,074
DyAu	−19.674	−62,414	−24,320	−38,074
HoAu	−20.130	−63,334	−25,240	−38,074
ErAu	−20.335	−64,277	−26,182	−38,074
TmAu	−20.400	−65,241	−27,147	−38,074
YbAu	−18.051	−66,226	−28,134	−38,074
LuAu	−20.990	−67,239	−29,144	−38,074

1292 °C [6]. The low melting point of YbAu is attributed to the divalency of Yb in YbAu [24].

The RAu compounds were synthesized by reacting the reactants in a sealed boron nitride container at 1372K temperature [25]. The reactions were highly exothermic and the heat evolved was used to sustain the reaction [17,23] and stable compounds were formed [26]. The CsCl structure for these compounds was confirmed by X-ray diffraction [26,27].

Although these compounds are very important due to their interesting physical properties, but even then limited experimental as well as theoretical studies are reported on them, that make their applications limited. To the best of our knowledge no

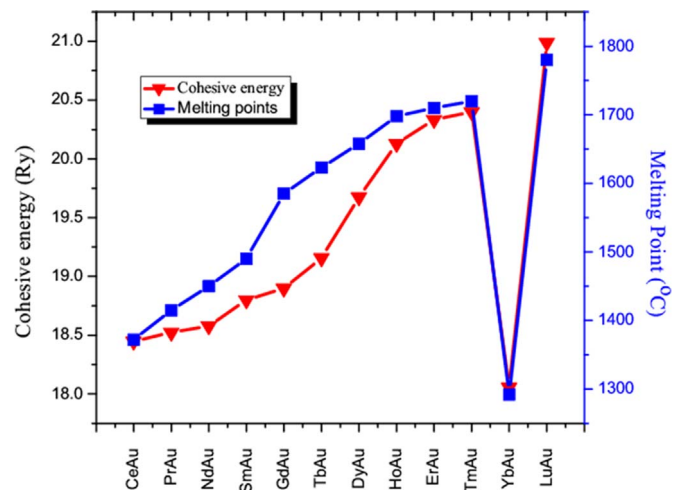


Fig. 2. Cohesive energy (Ry) and melting points (°C) of RAu(R=Ce, Pr, Nd, Sm, Gd, Tb, Dy, Ho, Er, Tm, Yb and Lu) intermetallics.

experimental or theoretical work has been reported on the electronic structure of these compounds, and similarly almost no theoretical work is available on the magnetic properties of these compounds. In this paper we explore the electronic structure and magnetic properties of these compounds, using the full potential linearized augmented plane waves (FP-LAPW) method within the framework of density functional theory.

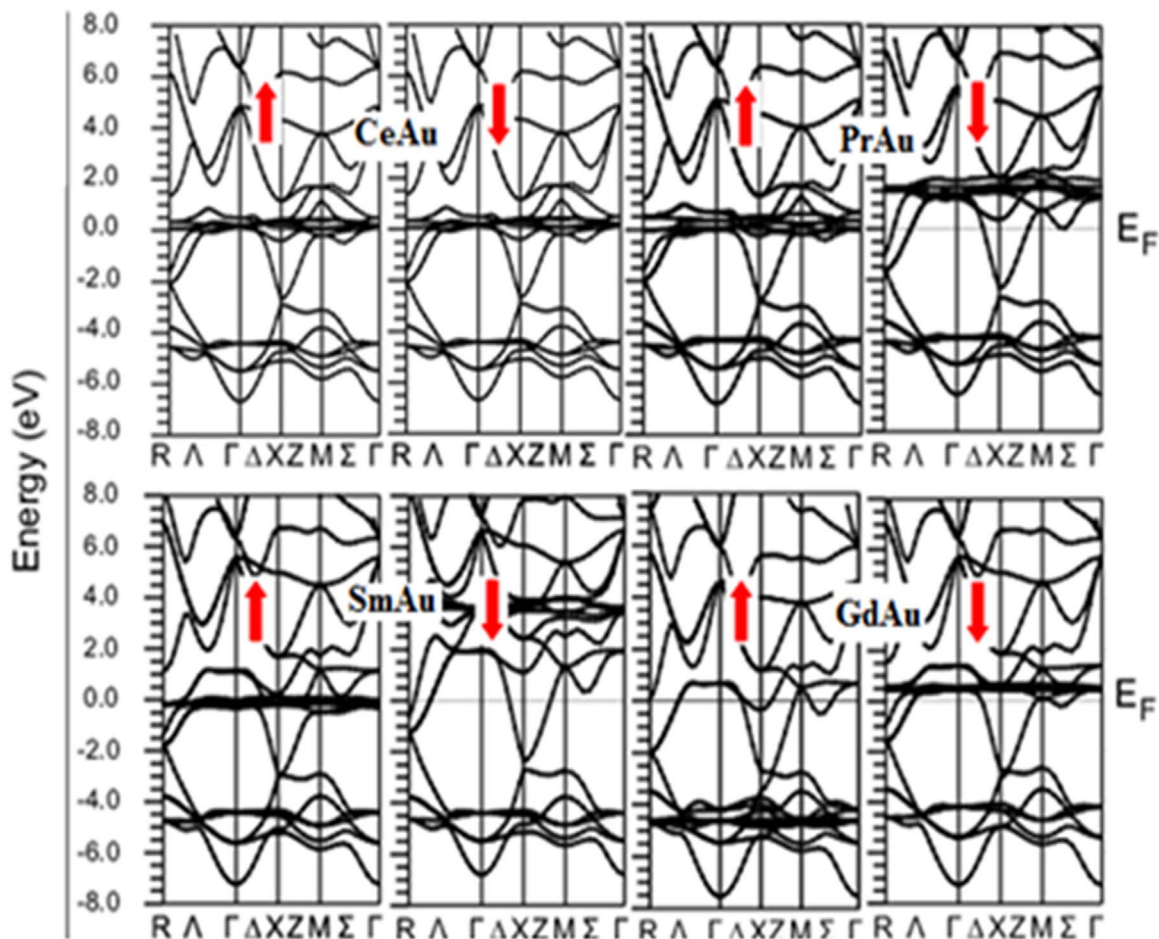


Fig. 3. Spin polarized band structures of RAu (R=Ce, Pr, Nd, Sm, Gd, Tb, Dy, Ho, Er, Tm, Yb and Lu) intermetallics.

2. Computational details

Electronic and magnetic properties of RAu (R=Ce, Pr, Nd, Sm, Gd, Tb, Dy, Ho, Er, Tm, Yb and Lu), compounds are explored with the full potential linearized augmented plane waves (FP-LAPW) method with the GGA, [28,29] GGA+*U* [30–32] and HF exchange correlation functional [33] to solve the Kohn–Sham equations [34]. Details of the FP-LAPW method and WIEN2k package used in the present calculations were discussed previously [35]. For accurate and converged results by GGA+*U* an approximated correction value of Hubbard potential (*U*) for the self-interaction correction (SIC) was chosen after investigating and testing several values of *U* in order to adjust the R-4f orbitals level in the density of states. For all calculations 1000 k-points and RMT-*K*_{max}=8.00 basis functions are used.

3. Results and discussions

3.1. Chemical bonding

Charge distribution around the atom determines the nature of chemical bonding and we calculated the electronic charge density for RAu (R=Ce, Pr, Nd, Sm, Gd, Tb, Dy, Ho, Er, Tm, Yb and Lu) compounds. The Contour-plots of charge density for RAu compounds are shown in Fig. 1. It is obvious from the plots that there is not much bonding charge that may link the R and Au atoms covalently. The charge density distribution is spherically symmetric about each atom that shows that these compounds have strong ionic character. This can be confirmed from the

electronegativity difference of the two atoms, R and Au, which is in the range of 1.42–1.37, suggesting more ionic character. The Fig. 1 also indicates that the gold atom lies at the center and eight R atoms are positioned at the corners of the cube. The spin dependent plots also show that some metallic character between R and Au atoms. Hence, the overall bonding in these compounds is predominantly ionic and metallic.

3.2. Cohesive energy

Cohesive energy is the energy required to decompose a crystal into its constituent atoms that shows that greater the amount of cohesive energy of a compound greater will be its stability [36]. The cohesive energies (*E*_{coh}) of the bimetallic compounds (RAu) are calculated by using the equation [37],

$$E_{\text{coh}} = E_{\text{total}} - (E_{\text{R}} + E_{\text{Au}})$$

where *E*_{coh} is the cohesive energy of the crystal, *E*_{total} is the total energy of the crystal while *E*_R and *E*_{Au} are the ground state energies of the free atoms of the lanthanide and gold, respectively, calculated by GGA. As we move from CeAu to LuAu the lattice constant of these compounds decreases which means increase in the rigidity of a crystal. Consequently cohesive energy will increase and this trend is clearly seen in Table 1.

High melting point means high cohesive energy [38] and the melting points of RAu compounds increase from CeAu to LuAu except YbAu which has the lowest melting point because of its divalency. In divalent state, the ionic radius is comparatively greater than the trivalent state. Therefore, the charge is low and

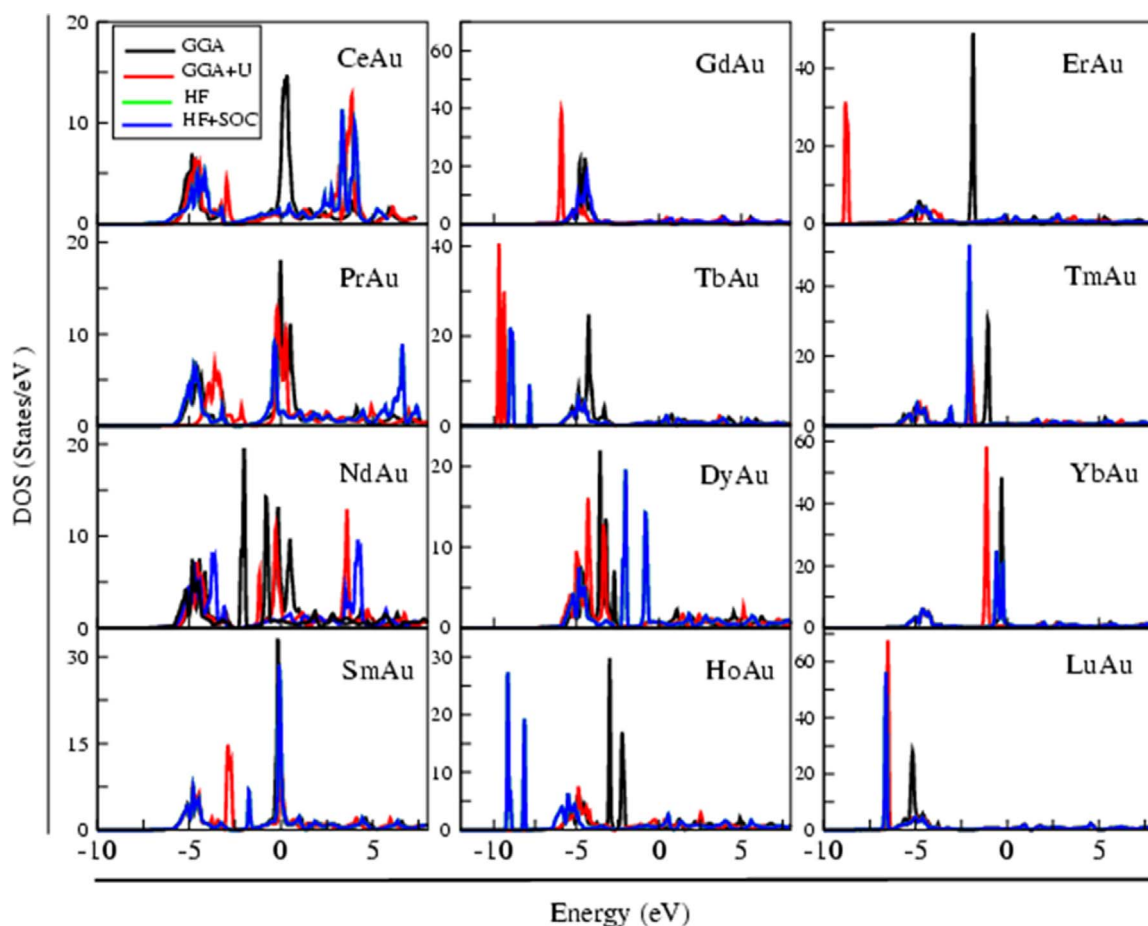


Fig. 4. Total density of states of RAu compounds ($R=\text{Ce, Pr, Nd, Sm, Gd, Tb, Dy, Ho, Er, Tm, Yb and Lu}$), by GGA, GGA+ U , HF and HF+SOC potentials.

attraction is lesser which results low melting point, least ionic character and smaller cohesive energy. The cohesive energies of these compounds increases in the same fashion as presented in Fig. 2.

3.3. Electronic properties

The study of band structure is very significant for understanding the electronic nature of a material and its possible technological applications. Bandgap of a compound is defined as the energy differences between the top of valence band and the bottom of conduction band. The computed band structure along the high symmetry directions Γ , Δ , H, N, Σ , $\diamond$ and P in the Brillouin zone for spin-up and spin-down channels for RAu ($R=\text{Ce, Pr, Nd, Sm, Gd, Tb, Dy, Ho, Er, Tm, Yb and Lu}$) have been shown in Fig. 3. No bandgap is observed in both spin up and spin down band structures for these compounds, hence all of them are metals. The results of their electronic behavior in terms of energy bands, total density of states (TDOS) and partial density of states (PDOS) are shown in Figs. 4 and 5, respectively. In case of spin-up as well as spin-down configurations, the valance and conduction bands overlap significantly at Fermi level, indicating metallic behavior. The charge density and band structure of four representative compounds are shown in Figs. 1 and 3, respectively and rest of the compounds are similar to them. The effects of four different potentials GGA, GGA+ U , HF and HF+SOC on the total density of states are given in Fig. 4. It is clear from the figure that GGA+ U have greater effect on the localization of the density of states as they has d and f orbitals, while the HF+SOC has caused splitting of orbitals. The HF alone has no effect on the compounds under study.

The main energy bands of RAu ($R=\text{Ce, Pr, Nd, Sm, Gd, Tb, Dy, Ho, Er, Tm, Yb and Lu}$) compounds are located at two energy ranges between -20 eV to -19 eV and -8 eV to 6 eV . The low lying energy bands between -20 eV and -19 eV are Au-p and R-p and are separated from the bands that participate in the conduction process. The group of bands between -5 eV and 0 eV just below the Fermi level is mainly due to 5d states of Au and part of 4f of R atom. The 4f of R atoms lying around the Fermi level. The conduction bands above the Fermi level are largely due to the R-4f state, which hybridizes with the Au-5d orbital.

It is evident that the low lying bands for these compounds are due to the Au-p and R-p orbitals. The energy bands around the Fermi level for these compounds between -6.5 and 6 eV are mainly dominated by the hybridized states of Au-d, R-f and R-d. Some of the R-f, Au-d and R-d cross the Fermi level this means that these compounds have typical metallic character.

3.4. Magnetic properties

To explore the ground state magnetic order of RAu compounds ($R=\text{Ce, Pr, Nd, Sm, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu}$), we optimized the double cell of each compound ferromagnetically, anti-ferromagnetically and nonmagnetically like our previous works [37,39,40]. The energy difference, for RAu compounds per unit cell is given in Table 2, which shows that CeAu, NdAu, GdAu, TbAu, DyAu, ErAu, TmAu and YbAu are stable in the anti-ferromagnetic, PrAu is in ferromagnetic and HoAu and LuAu in nonmagnetic states. All the computed results are in conformity with the available experimental results [3] as shown in Table 2. To investigate the origin of magnetism in the compounds under investigation

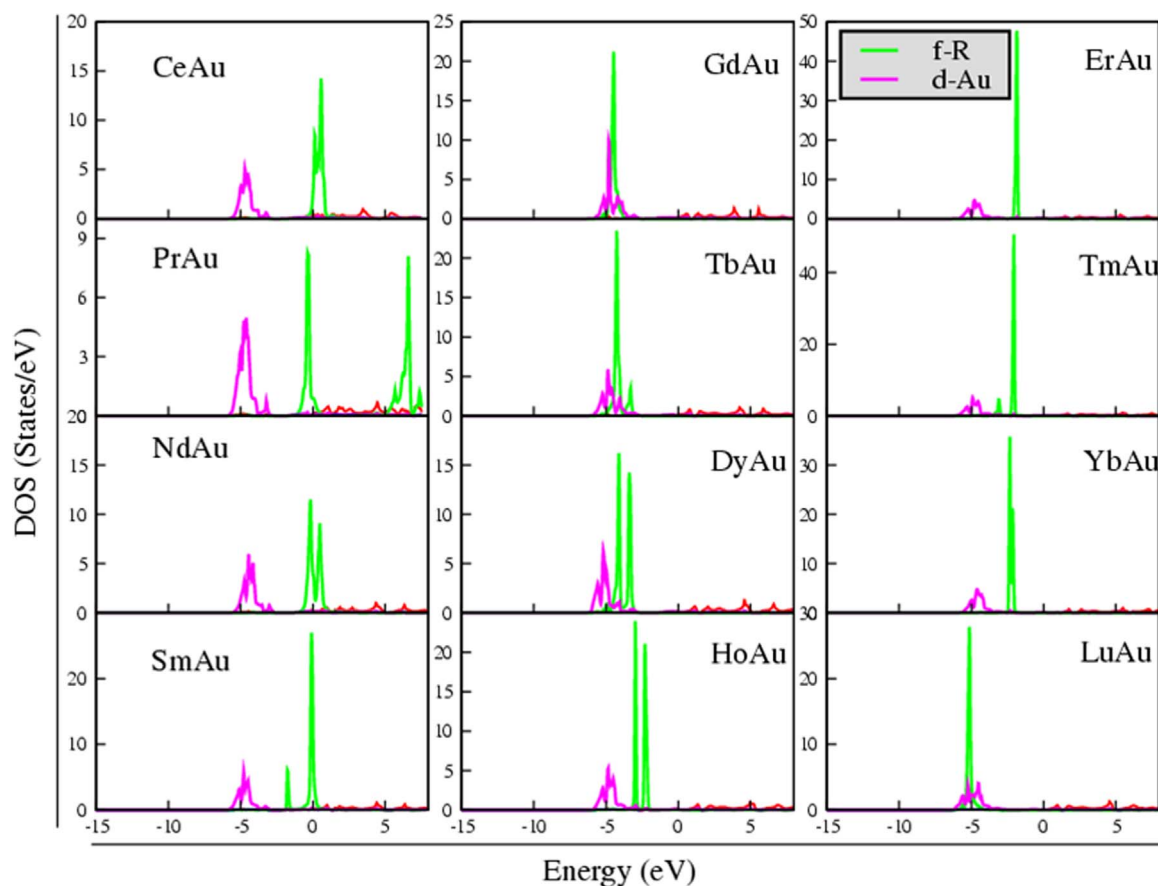


Fig. 5. Partial density of state of RAu (R = Ce, Pr, Nd, Sm, Gd, Tb, Dy, Ho, Er, Tm, Yb and Lu) intermetallics.

Table 2

Stable ground state energies per unit cell calculated for RAu(R=Ce, Pr, Nd, Sm, Gd, Tb, Dy, Ho, Er, Tm, Yb and Lu) intermetallics.

Compound	E_{Para} (Ry)	E_{FM} (Ry)	E_{AFM} (Ry)	Expt.	Present work
CeAu	−55,809.429208	−55,806.430843	−55,809.4308	–	AFM
PrAu	−56,564.050659	−56,564.106317	−56,564.0509	–	FM
NdAu	−57,338.368179	−57,338.492453	−57,356.0517	–	AFM
SmAu	−58,947.224525	−58,947.574402	−58,961.4513	–	AFM
GdAu	−60,657.027263	−60,638.830690	−60639.1927	AFM [3,45]	AFM
TbAu	−61,515.356380	−61,515.755411	−61518.0633	AFM [3,46]	AFM
DyAu	−62,413.873565	−62,414.147566	−62,414.6129	AFM [3,45]	AFM
HoAu	−63,334.330012	−63,334.310010	−63317.4075	PM [3]	NM
ErAu	−64,276.534961	−64,276.533794	−64276.5352	AFM [3,46]	AFM
TmAu	−65,241.123356	−65,241.142392	−65,241.1442	AFM [3,46]	AFM
YbAu	−66,228.501665	−66,228.501460	−66228.5017	AFM [3,47]	AFM
LuAu	−67,238.771436	−67,238.769915	−67238.7706	–	NM

spin polarized single cell calculations are performed by using GGA PBEsol, GGA+U, HF (B3LYP) and HF potentials within the framework of DFT. The calculated effective magnetic moments are presented in Table 3. It is clear from Table 3 that the HF (B3PW91) results are closer to the experimental results than other potentials used. This shows that HF (B3PW91) is effective for calculating magnetic properties of these compounds. This is because these compounds are strongly correlated and hence need extra potential like “U” to treat correlation effect in these compounds.

The Magnetic moments of GdAu, TbAu, HoAu, ErAu, DyAu, TmAu and YbAu are given in Table 3, our results are in closer agreement with the experimental results [3]. The difference in the calculated results is due to the electron exchange-correlation effect. DFT generally underestimates the electronic bandgap.

All the similar compounds of coinage metals should have the same magnetic moments [41] as obvious from the case of TmCu,

TmAg and TmAu whose experimental magnetic moments are 7.56, 7.15 and 7.32 μ_B respectively. That shows that our theoretically determined magnetic moment of TmAu (3.92 μ_B) is comparatively more acceptable than the calculated values 1.34652 μ_B and 1.3 μ_B for TmCu and TmAg respectively reported by Chand *et al* [42].

The total magnetic moment of binary intermetallics is the contribution of two metals and their interstitial regions. In this case Au atom and the interstitial regions have negligible magnetic moments. Therefore, the net spin magnetic moment is due to the 4f-state electrons of the rare earth atoms. In brief the incomplete 4f sub shell of rare earths is the origin of the magnetic moments [43]. This can be verified by the fact that as we move from left to right in the period, the number of unpaired electrons increases up to Gd and then decreases. Thus the magnetic moment increases up to GdAu and then decreases till the LuAu become nonmagnetic [44].

Table 3

Calculated and experimental effective / total magnetic moments of RAu (R=Ce, Pr, Nd, Sm, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu) intermetallics by GGA PBE-sol, GGA+U, HF-B3LYP and HF-B3PW91 in unit of μ_B .

Compound	GGA PBE-sol	GGA+U (U)	HF-B3LYP (α)	HF-B3PW91 (α)	Expt [3,48]
CeAu	1.95	2.94 (4 eV)	2.94 (0.35)	2.96 (0.35)	–
PrAu	2.26	2.30 (4 eV)	2.40 (0.55)	2.58 (0.55)	–
NdAu	3.53	3.67 (4 eV)	3.8 (0.35)	3.9 (0.35)	–
SmAu	5.80	6.18 (5 eV)	6.20 (0.60)	6.21 (0.60)	–
GdAu	7.10	7.27 (6 eV)	7.28 (0.95)	7.30 (0.95)	7.29
TbAu	5.90	7.8 (7 eV)	7.82 (0.92)	7.93 (0.92)	9.54
DyAu	4.80	5.2 (5 eV)	6.32 (0.90)	7.2 (0.90)	10.22
HoAu	3.70	4.0 (5 eV)	4.12 (0.80)	8.4 (0.80)	10.50
ErAu	2.50	2.8 (8 eV)	3.7 (0.65)	5.0 (0.65)	9.42
TmAu	1.20	2.0 (8 eV)	3.4 (0.25)	3.92 (0.25)	7.32
YbAu	0.015	0.81 (7 eV)	1.8 (0.65)	2.6 (0.65)	0.81
LuAu	0.0009	0.0009 (3 eV)	0.00094 (0.35)	0.0011 (0.35)	–

4. Conclusion

In summary this work reports the investigation of electronic and magnetic properties of RAu intermetallics (R=Ce, Pr, Nd, Sm, Gd, Tb, Dy, Ho, Er, Tm, Yb and Lu) which are studied for the first time using GGA, GGA+U and HF based on DFT. Our results of magnetic properties show that the results of HF are much consistent with the available experimental data as compared to GGA and GGA+U. The chemical bonding are explained on the basis of electronic charge densities. The bond between R and Au are ionic and metallic in nature. Cohesive energies show that the stability of RAu compounds increases as we move from CeAu to LuAu with the exception of YbAu which has the least stability due to its divalent nature. The band structures show that all these compounds are metallic in nature. The calculated magnetic phase stability of the compounds under consideration are well consistent with the available experimental results.

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