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Electron correlation and spin-orbit coupling effects in scandium intermetallic compounds ScTM (TM = Co, Rh, Ir, Ni, Pd, Pt, Cu, Ag and Au)

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Spin-polarized density functional calculations are performed to study the correlation and spin-orbit coupling (SOC) effects in scandium intermetallic compounds viz. ScTM (TM = Co, Rh, Ir, Ni, Pd, Pt, Cu, Ag and Au) using FP-LAPW + lo method. The LDA, LDA + U and LDA + U + SOC exchange-correlation functionals are used to calculate the structural parameters and we found that the LDA + U results are consistent with the experiments. The electronic properties reveal that these compounds are metallic in nature. Correlations effects are determined using the U/W ratio and we found that ScCo, ScIr, ScPd, ScPt, ScCu and ScAg are highly correlated compounds, whereas ScRh, ScNi and ScAu are intermediately correlated compounds. Furthermore, stable magnetic phase for each compound is optimized, which reveals that ScCo, ScRh, ScPd, ScPt and ScCu are stable in ferromagnetic phase, ScIr, ScNi and ScAu are anti-ferromagnetic, whereas ScAg is a nonmagnetic material.

Keywords: Intermetallic compounds; CsCl-type structure; correlations effects; spin-orbit coupling; *ab initio* calculations.

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1. Introduction

The electron–electron correlation effect (EECE) and spin-orbit coupling (SOC) have attracted great attention in materials physics due to their important roles in defining many fascinating properties like unconventional superconductivity[1–3] conductor–insulator transitions in Mott-insulators,[4] transport properties,[5] half-metallicity, spin-charge separation, etc.[6] SOC is important in strongly correlated systems and is observed in some transition metal (TM)-based compounds. Although they are interesting and play crucial roles in understanding the physics and chemistry of materials, they are complex to be completely realized for various materials and thereby the main objective of this paper is to discuss them in detail.

SOC effect is usually considered in the condensed matter phenomenon as a weak relativistic correction to the Schrödinger equation (SE), however, nowadays it is attracting enormous attention due to its capability to justify the observed phenomenon[7–10] as some TMs confirm that this effect is more than just a minor correction to the SE. This effect causes nontrivial topological order in TM-based compounds due to the large SOC effect, especially in the 4*d*- and 5*d*-TM compounds.[11–14] Unlike earlier beliefs, it is a well-established fact of modern condensed matter physics that this effect plays a key role and hence modifies and/or controls some significant properties of the 4*d*- and 5*d*-TM compounds.

Like SOC, EECE is a fascinating effect in TM compounds and on the basis of this effect, materials are categorized; as strongly correlated electron systems, intermediately correlated and weakly correlated systems. The parameter that categorizes materials is the U/W values, where U is the Hubbard potential and W is the bandwidth. We represent this ratio by C_e. The C_e value is larger than 1 for the strongly correlated electron systems, it is approximately equal to 1 for intermediately correlated systems and it is less than 1 for weakly correlated electron systems.[15]

It is generally observed that the EECE decreases and the SOC effect increases as one moves from top to bottom in a TM column in the periodic table. As mentioned above, these two effects are critical in TM compounds for understanding their physics and chemistry. Therefore, the understanding of these effects is quite necessary for the applications of these compounds in various emerging technologies. In this paper, we systematically investigate the EECE as well as SOC effects for TM compounds from left to right or from top to bottom in the periodic table in intermetallic ScTM compounds.

The ScTM (TM = Co, Rh, Ir, Ni, Pd, Pt, Cu, Ag and Au) family of compounds crystallizes in the cubic CsCl-type structure having the Space Group No. 221 (Pm-$3m$) with the lattice constants ranging from 3.160 Å to 3.416 Å.[16] Scandium is considered as the first TM and also a member of the rare-earth family, but it does not have any unpaired $4f$ electrons. Various experimental and theoretical studies on the physical properties of scandium-based compounds, e.g., structural, electronic, thermodynamic and mechanical properties, have been reported in literature.[17–24] This comprehensive study provides a clear picture of the EECE and SOC effects

with the variation in the TM element in these compounds. Furthermore, the structural, electronic and magnetic properties of the compounds under study are also calculated and discussed in detail.

2. Computational Details

Spin-polarized density functional calculations are performed within the frame work of the full-potential linearized augmented plane waves plus local orbitals (FP-LAPW + lo) technique[25] to investigate the structural, electronic and magnetic properties of ScTM (TM = Co, Rh, Ir, Ni, Pd, Pt, Cu, Ag and Au) materials. The theoretical investigations are carried out by LDA,[26] LDA+U and LDA+U+SOC[15] functionals. The muffin-tin radii are considered in such a manner that no charge leakage can occur. The basis set is expanded in terms of plane waves up to $R_{\mathrm{MT}}K_{\max} = 7$, where R_{MT} is the smallest atomic radius and $K_{\max}$ is the maximum value of k-vector.

Furthermore, the maximum angular momentum, $l_{\max}$, is set to 10. However, in the interstitial region, maximum value of charge density is considered as $G_{\max} = 12$. A k-mesh of 3000 k-points is considered in the Brillouin zone having the grid size of $14 \times 14 \times 14$ using the Monkhorst–Pack mesh.[27] The orientation of spins in the spin-orbit coupling calculations is considered to be along the [100] direction.

3. Results and Discussion

3.1. *Structural properties*

The structural optimizations are performed using experimental lattice constants[16] by LDA, LDA+U and LDA+U+SOC for ScTM (TM = Co, Rh, Ir, Ni, Pd, Pt, Cu, Ag and Au) compounds. Hubbard U parameter is optimized for each compound by comparing the calculated lattice constants with the experimental ones. The obtained optimized U values are found to be 3, 2, 4, 1, 3, 9, 6, 8 and 1 eV for the TM atoms in ScCo, ScRh, ScIr, ScNi, ScPd, ScPt, ScCu, ScAg and ScAu compounds, respectively. In addition to the above optimization for obtaining suitable U values for the TM atoms in the materials under focus, the U value is also optimized to be 2 eV for the d-state of Sc atom in all of these compounds.

The calculated values of the lattice constants for these compound along with their ground state properties like volume (V_0), bulk modulus (B) and energy (E_0) by LDA, LDA + U and LDA + U + SOC are presented in Table 1. The results show that the computed lattice constants of ScTM compounds by LDA + U are close to the experimental values reported in Ref. 16. This shows that LDA + U is a suitable scheme for the cases under study. Generally, DFT underestimates or overestimates the physical properties due to the approximations used for the exchange-correlation term. As these intermetallic systems are correlated compounds, therefore the LDA+U is more effective on these materials as compared to other exchange-correlation potentials, i.e., LDA and LDA+U+SOC, which underestimate the lattice constants

Table 1. Calculated and experimental structural properties like lattice constant (a_0) in unit Å, volume (V_0) in (a.u.)^3, bulk modulus (B) in GPa and ground state energy (E_0) in Ry of ScTM (TM = Co, Rh, Ir, Ni, Pd, Pt, Cu, Ag and Au) by LDA, LDA + U and LDA + U + SOC.

Materials		LDA	LDA + U	LDA + U + SOC	Exp.	Others
ScCo	a_0	3.014	3.150	3.0349	3.160[a]	3.13[c]
	V_0	184.722	210.9	188.6350		
	B	106.182	94.33	147.6379		122.5[c]
	E_0	−4307.370	−4306.976	−4307.383		
ScRh	a_0	3.163	3.201	3.152	3.205[a]	3.22[c], 3.254[d]
	V_0	213.527	221.3	211.41		
	B	106.755	144.52	77.76		161[c], 169[d]
	E_0	−11086.563	−11092.390	−11086.597		
ScIr	a_0	3.168	3.209	3.162	3.206[a]	3.23[c]
	V_0	214.559	223.00	213.45		
	B	230.906	192.88	195.98		168.5[c]
	E_0	−37221.335	−37232.601	−37221.775		
ScNi	a_0	3.080	3.149	3.091	3.165[a]	3.169[b]
	V_0	197.194	210.701	199.38		
	B	107.854	128.857	140.502		109[b]
	E_0	−4561.887	−4565.724	−4561.893		
ScPd	a_0	3.239	3.282	3.237	3.283[a]	3.206[b], 3.329[d]
	V_0	229.251	238.595	228.869		
	B	136.139	155.899	135.480	128[c]	112.6[b], 137[d]
	E_0	−11609.813	−11615.771	−11609.852		
ScPt	a_0	3.235	3.269	3.228	3.270[a]	3.307[b]
	V_0	228.523	235.4870	227.035		
	B	172.463	159.518	153.667	162.8[c]	139.62[b]
	E_0	−38398.064	−38409.315	−38398.563		
ScCu	a_0	3.173	3.239	3.169	3.256[a]	
	V_0	215.492	229.329	214.782		
	B	107.359	95.747	109.9818		
	E_0	−4830.018	−4833.878	−4830.030		
ScAg	a_0	3.346	3.422	3.3137	3.416[a]	3.439[d]
	V_0	252.717	270.4591	245.5576		
	B	66.282	85.3627	56.502		99[d]
	E_0	−12149.930	−12155.949	−12149.983		
ScAu	a_0	3.324	3.378	3.3136	3.373[a]	
	V_0	247.935	260.1168	245.5269		
	B	102.297	131.6965	121.8447		
	E_0	−39599.945	−39611.977	−39600.479		

Note: [a]Ref. 16, [b]Ref. 32, [c]Ref. 33 and [d]Ref. 21.

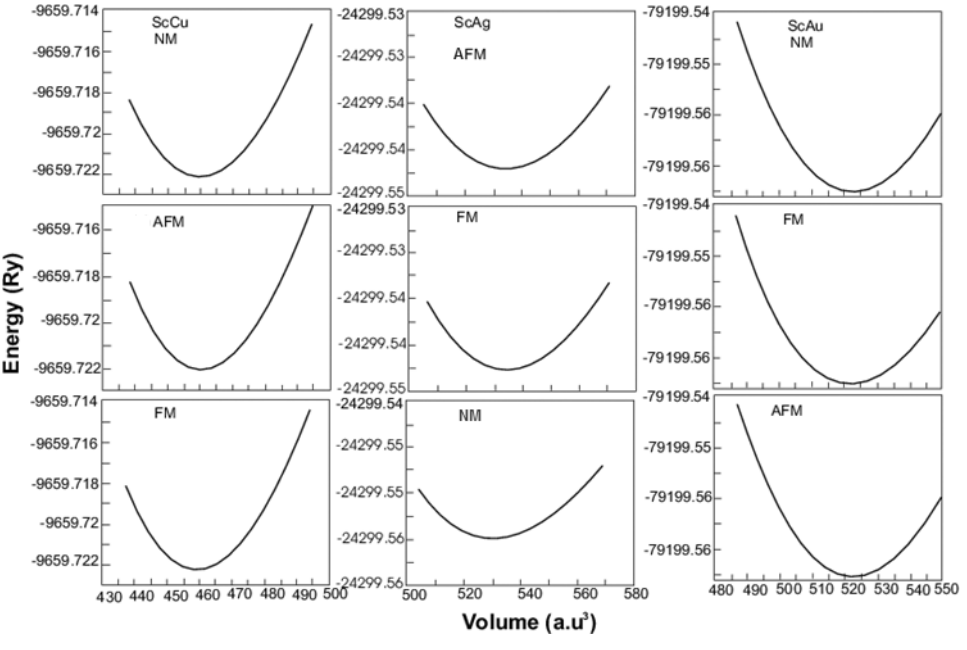
of the present compounds with maximum differences of 4.6% and 3.9%, respectively. Bulk modulus can be used to show the degree of hardness of a material. The results presented in Table 1 show an increasing trend in bulk moduli of the materials, i.e., 94.33, 144.52, 192.88, 128.857, 155.899 and 159.518 GPa for ScCo, ScRh, ScIr, ScNi, ScPd and ScPt, respectively, while this trend is broken down for ScCu, ScAg and ScAu. The value decreases for ScCu (95.747 GPa) and then increases in the sequence of ScAg (85.362 GPa) and ScAu (131.696 GPa), respectively. This shows

that ScAg is a soft material as compared to ScCu and ScAu due to the greater melting points of Cu (1085°C) and Au (1064°C) as compared to Ag (962°C).[28–32]

To study the stable magnetic phase of ScTM intermetallics, double cell optimizations are performed for each compound in different magnetic phases like nonmagnetic (NM), ferromagnetic (FM) and anti-ferromagnetic (AFM) ones. The calculated optimization curves of these compounds are shown in Figs. 1(a)–1(c) and the corresponding ground state energies for all the three magnetic phases, nonmagnetic, ferromagnetic and anti-ferromagnetic phases are presented in Table 2. It is clear from Table 2 and Figs. 1(a)–1(c) that ScCo, ScPd, ScPt and ScCu have lowest energies in their ferromagnetic phase; ScIr, ScNi and ScAu have lowest energies in the anti-ferromagnetic state, whereas ScAg has the lowest energy in its nonmagnetic phase. Hence, ScCo, ScPd, ScPt and ScCu compounds are more stable in the ferromagnetic state, ScIr, ScNi and ScAu are more stable in anti-ferromagnetic phase, whereas ScAg is more stable in the nonmagnetic phase.

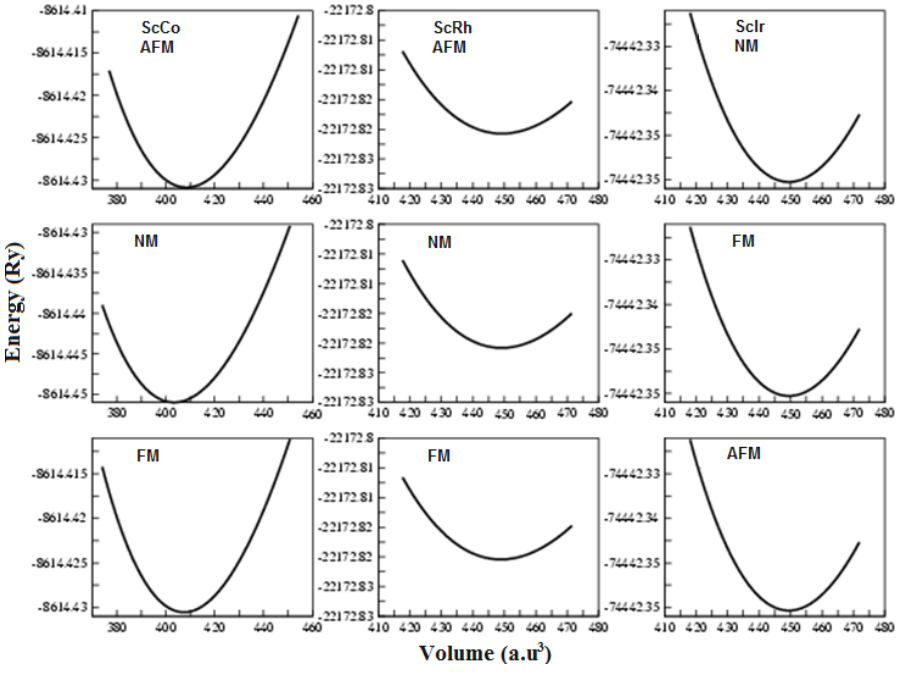
3.2. *Electronic properties*

Electronic structure plays a key role in determining many physical properties of a material. The total and partial densities of states (TDOSs and PDOSs, respectively)

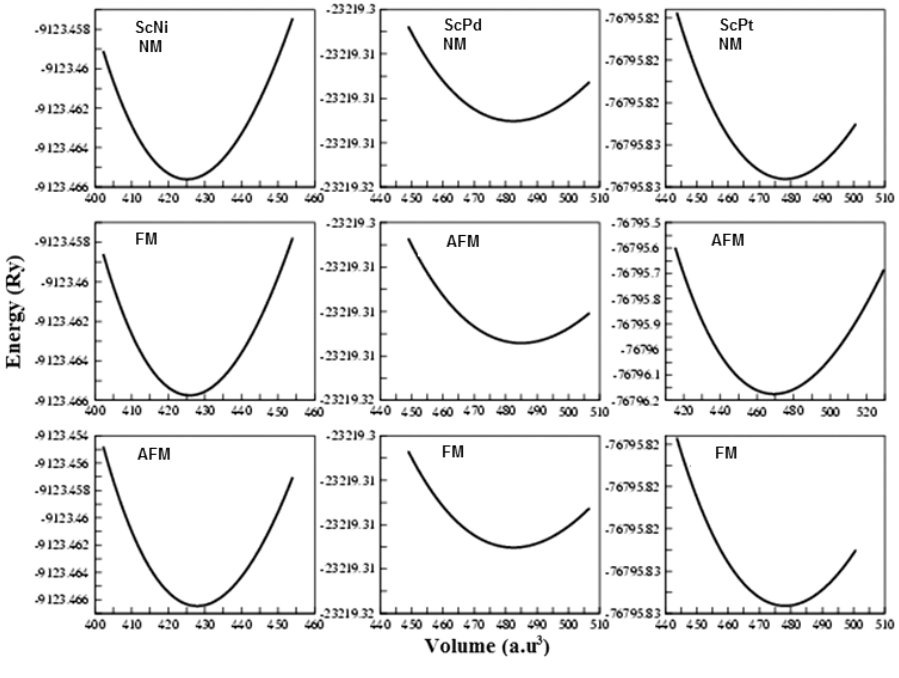


(a)

Fig. 1. (a) Optimization plots of ScTM (TM = Cu, Ag and Au) for the stability of the magnetic states. (b) Optimization plots of ScTM (TM = Co, Rh and Ir) for the stability of the magnetic states. (c) Optimization plots of ScTM (TM = Ni, Pd and Pt) for the stability of the magnetic states.



(b)



(c)

Fig. 1. (*Continued*)

Table 2. Calculated magnetic energies of NM, FM and AFM phases of the double cell and U/W ratios of the unit cell of ScTM (TM = Co, Rh, Ir, Ni, Pd, Pt, Cu, Ag and Au) compounds.

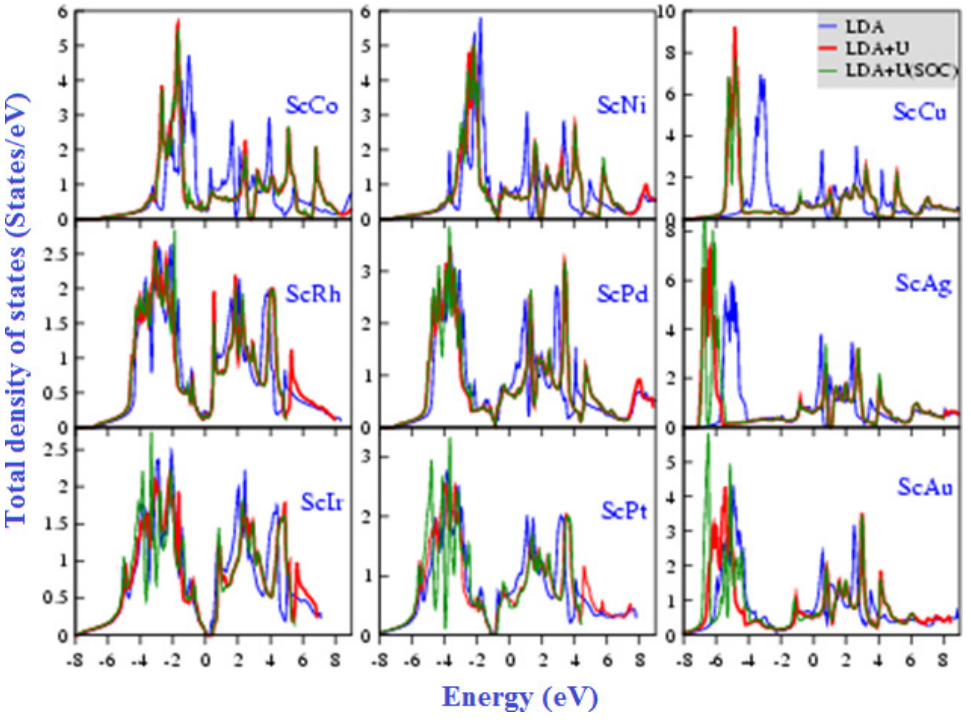
Compounds	E_{NM} (Ry)	E_{FM} (Ry)	E_{AFM} (Ry)	U/W (eV)
ScCo	−8614.430856	−8614.450993	−8614.430552	1.8571
ScRh	−22172.820724	−22172.820812	−22172.82043	0.8253
ScIr	−74442.350246	−74442.350267	−74442.350358	1.4950
ScNi	−9123.4656000	−9123.465750	−9123.466460	0.7177
ScPd	−23219.312562	−23219.313555	−23219.312577	1.5975
ScPt	−76795.834028	−76795.834552	−76795.834110	4.0153
ScCu	−9659.722139	−9659.722394	−9659.722163	6.2558
ScAg	−24299.554958	−24299.547728	−24299.547414	6.6033
ScAu	−79199.562584	−79199.562629	−79199.562711	0.5212

calculated by LDA, LDA + U and LDA + U + SOC for all these compounds are plotted in Figs. 2(a)–2(c). Figure 2(a) explains the TDOSs of these intermetallic systems by LDA, LDA + U and LDA + U + SOC. In all these plots, the Fermi levels are crossed by the densities of states. Hence, all these compounds are predicted to be metals. Figure 2(b) shows the PDOSs of Sc and TM d-states. The above figure reveals the origin of the metallic nature of these compounds. From the figure it can be seen that in ScCo, ScRh, ScIr, ScNi, ScPd and ScPt compounds, the Fermi levels are crossed by the d-states of both Sc and TM elements with dominant contributions of Co, Rh, Ir, Ni, Pd and Pt d-states, whereas in ScCu, ScAg and ScAu compounds, the Fermi level is also crossed by the densities of both Sc and TM d-states. In the above instance, the dominant participant is Sc d-state which is due to the fact that in the Cu, Ag and Au cases the d-states are completely filled. The same phenomenon is also reported by Fatima *et al.*[33] for such types of compounds. Figures 2(c)–2(e) explain the effects of SOC in these intermetallics. Without SOC the Sc and TM (Co, Rh, Ir, Ni, Pd, Pt, Cu, Ag and Au) d-states split into two substates e_g and t_{2g}, where e_g-state is high in energy as compared to the t_{2g}-state. After applying SOC the d-states (e_g and t_{2g}) further split into subenergy states such that e_g-state splits into d_{z^2} and $d_{x^2y^2}$ and t_{2g}-state splits into $d_{zx} + d_{yz}$ and d_{xy} energy bands. Figure 2(c) also provides microlevel information about these participated states across the Fermi level. In ScCo compound without SOC the Fermi level is crossed by the t_{2g}-d-state of Sc and e_g-d-state of Co. After applying SOC the dominant participated states at the Fermi level are Sc-$d_{zx} + d_{yz}$ and Co-$d_{x^2y^2}$ energy bands. In ScRh, without SOC the Fermi level is crossed by both the energy states e_g and t_{2g} of Sc, having the maximum contribution in the conduction region, whereas the e_g-state of Rh is localized in the valence region, while e_g crosses the Fermi level. After applying SOC, Sc-d-state splits into five further subenergy bands such as d_{z^2}, d_{xy}, $d_{x^2y^2}$ and $d_{xz} + d_{yz}$, whereas Rh-d-state is also split into the same number of energy states. In the case of Rh, the most dominant energy state is $d_{x^2y^2}$ which crosses the Fermi level, as shown in Fig. 2(c). A similar trend is observed for ScIr. Figures 2(d) and 2(e) explain similar phenomena for

ScNi, ScPd, ScPt, ScCu, ScAg and ScAu compounds without SOC and with SOC effect.

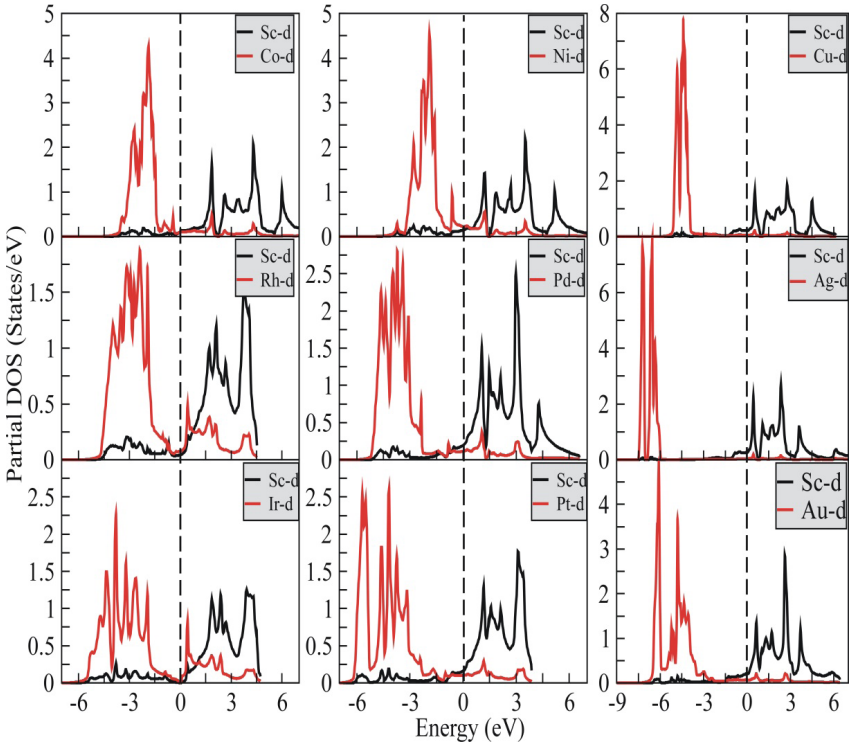
U optimization plays an important role in the determination of strength of the electronic correlations effects in these compounds.[15] Figure 3 shows the width of TM versus valence electron number. It can be seen from the figure that the width of the d-state of the TM increases from $3d$ to $5d$, which shows that the correlation effect decreases in these compounds in the sequence of $3d \rightarrow 4d \rightarrow 5d$, which is in agreement with the same trend reported for TM by Sasioglu *et al.*.[15] This shows that our results are logical and consistent to the reported work of the elemental behavior of TM.

In ScTM compounds, the ratio of Hubbard U parameter to the width of TM d-state (U/W) shows different correlation behavior as compared to the elemental response, see Fig. 4. This is due to the fact that in these compounds different types of bonding and quantum interactions are involved. The calculated values of U/W are 1.8571, 0.8253, 1.4950, 0.7177, 1.5975, 4.0153, 6.2558, 6.6033 and 0.5212

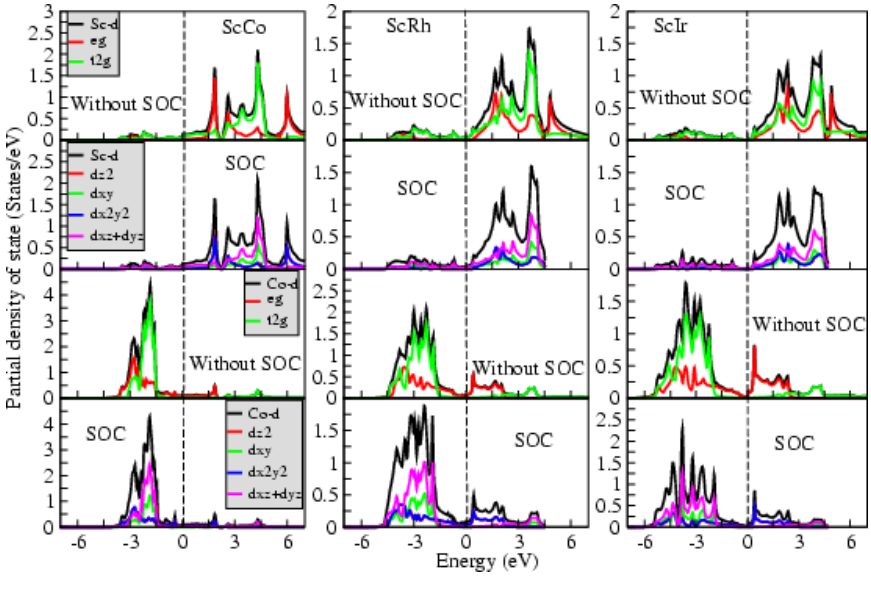


(a)

Fig. 2. (Color online) (a) Total DOSs for ScTM (TM = Co, Rh, Ir, Ni, Pd, Pt, Cu, Ag and Au) compounds. (b) TM d-states' DOSs of ScTM (TM = Co, Rh, Ir, Ni, Pd, Pt, Cu, Ag and Au) compounds. (c) Partial DOSs of ScCo, ScRh and ScIr compounds with SOC and without SOC. (d) Partial DOSs of ScNi, ScPd and ScPt compounds with SOC and without SOC. (e) Partial DOSs of ScCu, ScAg and ScAu compounds with SOC and without SOC.

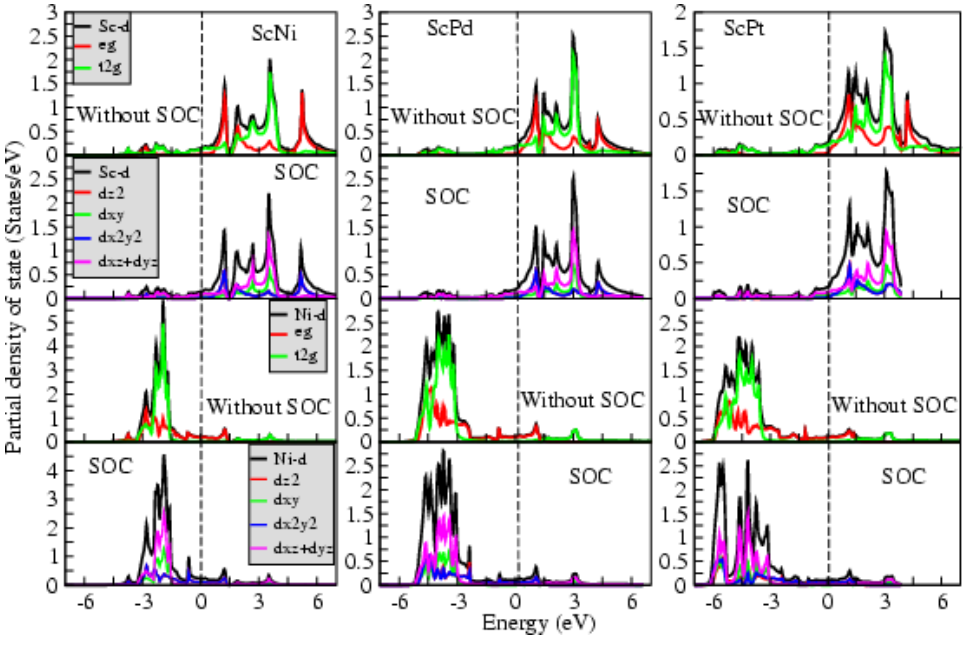


(b)

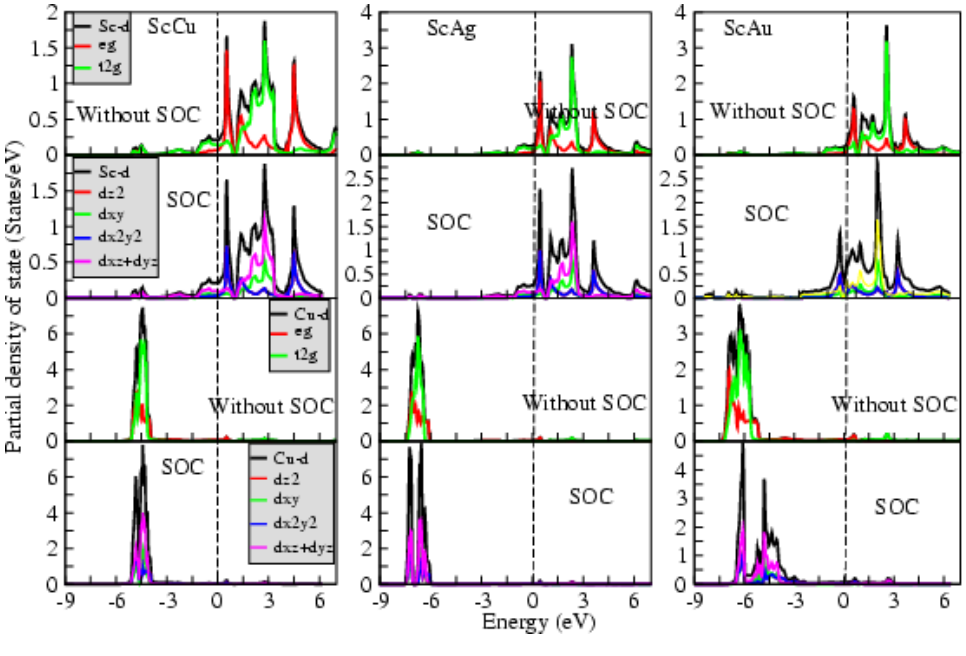


(c)

Fig. 2. (*Continued*)



(d)



(e)

Fig. 2. (*Continued*)

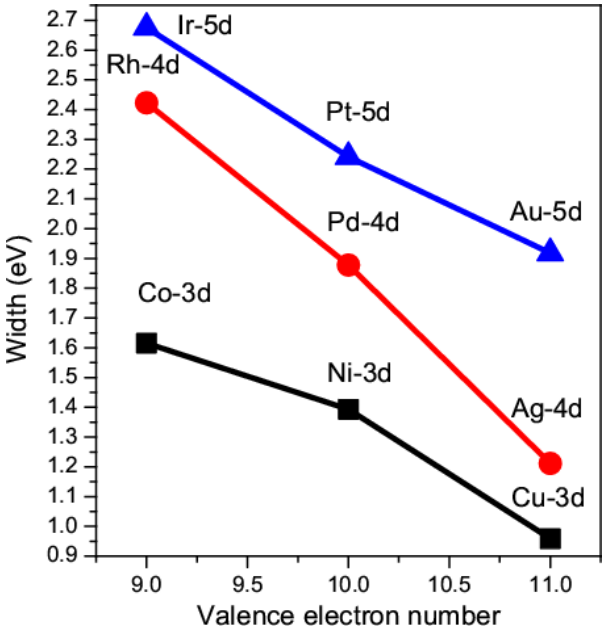


Fig. 3. (Color online) Plot between bandwidth (W) and valance electrons of TM = Co, Rh, Ir, Ni, Pd, Pt, Cu, Ag and Au.

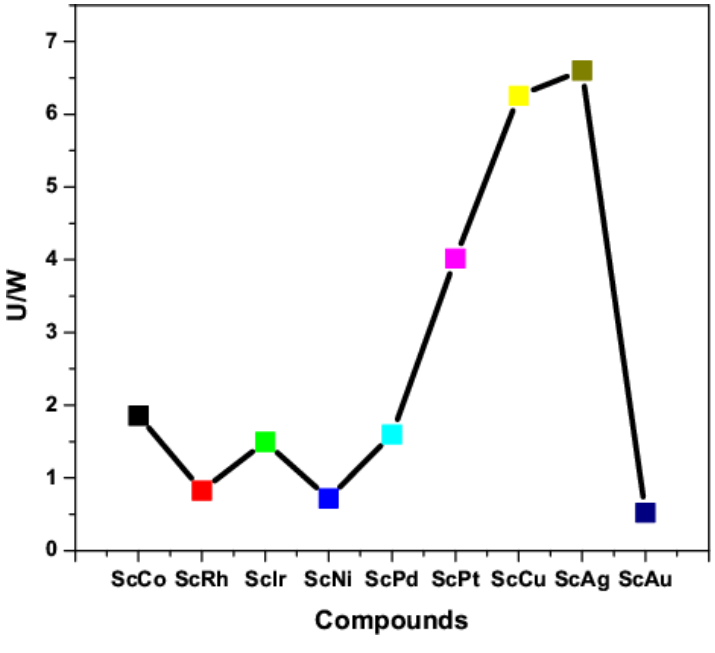


Fig. 4. (Color online) The ratios U/W of the effective Coulomb interaction (U) and the d-state bandwidth (W) for the TM (Co, Rh, Ir, Ni, Pd, Pt, Cu, Ag and Au).

for ScCo, ScRh, ScIr, ScNi, ScPd, ScPt, ScCu, ScAg and ScAu, respectively, see Table 2. It is clear from the table that ScCo, ScIr, ScPd, ScPt, ScCu and ScAg are highly correlated compounds, because their U/W ratio is greater than 1. This property in these compounds leads to a very interesting physical property like unconventional forms of superconductivity.[1–3] While ScRh, ScNi and ScAu are intermediately correlated compounds, because their U/W values are nearly equal to 1.[15] It can be also noted that there is no weakly correlated system in the present set of compounds. The same phenomenon is also observed by Sasioglu *et al.*[15] in particular TM elements like Cu and Ag such that their U/W ratios are greater than 1.

3.3. *Magnetic properties*

From Sec. 3.1 it is confirmed that ScCo, ScRh, ScPd, ScPt and ScCu are ferromagnetic, and ScIr, ScNi and ScAu are anti-ferromagnetic, whereas ScAg is a nonmagnetic material. To study the origin of magnetism in these compounds, LDA, LDA + U and LDA + U + SOC spin-polarized calculations are performed. At the Fermi energy (E_F), electron spin-polarization for a material can be calculated by the equation[34,35]

$$P = \frac{D\uparrow(E_F) - D\downarrow(E_F)}{D\uparrow(E_F) + D\downarrow(E_F)}, \tag{1}$$

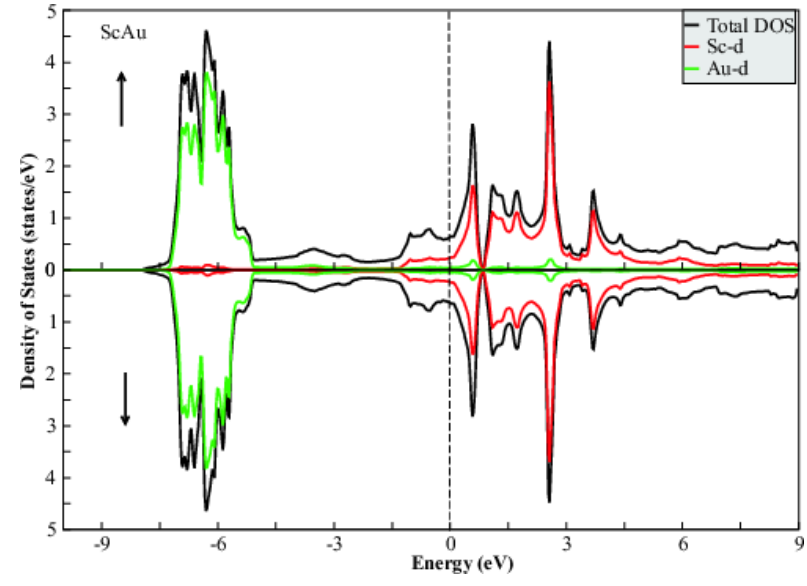
where $D\uparrow(E_F)$ [$D\downarrow(E_F)$] represents the DOS in spin-up (spin-down) channel at the Fermi level. The type of materials can be identified using the value of P such that zero value of P shows nonmagnetic behavior of materials. Spin-polarization of electrons at Fermi level is 100% when the value of $D\uparrow(E_F)$ is zero (nonzero) and the value of $D\downarrow(E_F)$ is nonzero (zero). These types of calculations are very important to understand the magnetic nature of materials. The calculated spin and orbital contributions of the magnetic moments are listed in Table 3 for ScTM compounds.

It can be seen from the table that for ScCo the interstitial magnetic moment inside the muffin-tin sphere as calculated by LDA is 0.0049 μ_B, by LDA + U it is -0.3425 μ_B and by LDA + U + SOC it is -0.3374 μ_B. The spin magnetic moments in the series of ScTM compounds are 0.0011, -0.3317 and -0.3241 μ_B for Sc and -0.0316, 0.8611 and 0.08265 μ_B for Co, whereas the orbital magnetic moment calculated by LDA + U + SOC for Sc is 0.0076 μ_B and for Co is 0.0637 μ_B. The total magnetic moment per ScCo cell, i.e., $M^{\text{Total}}(\text{spin}) + M^{\text{Total}}(\text{orbital}) = \text{Total}$, is 0.2363 μ_B. It can be observed that in ScCo compound, Sc atom and the interstitial region are found with negligible negative magnetic moments. Thus, the net spin magnetic moment is dominated by the 3d-state electrons of the transition atom (Co), as shown in Fig. 5(d). In the case of ScNi, the interstitial magnetic moment inside muffin-tin sphere calculated by LDA is -0.0025 μ_B, by LDA + U it is 0.0019 μ_B and by LDA + U + SOC it is -0.0018 μ_B. The spin magnetic moments of Sc are -0.0017, -0.0001 and -0.0017 μ_B and for Ni they are 0.0168, -0.0172 and -0.0013 μ_B, whereas the orbital magnetic moment by LDA + U + SOC for Sc

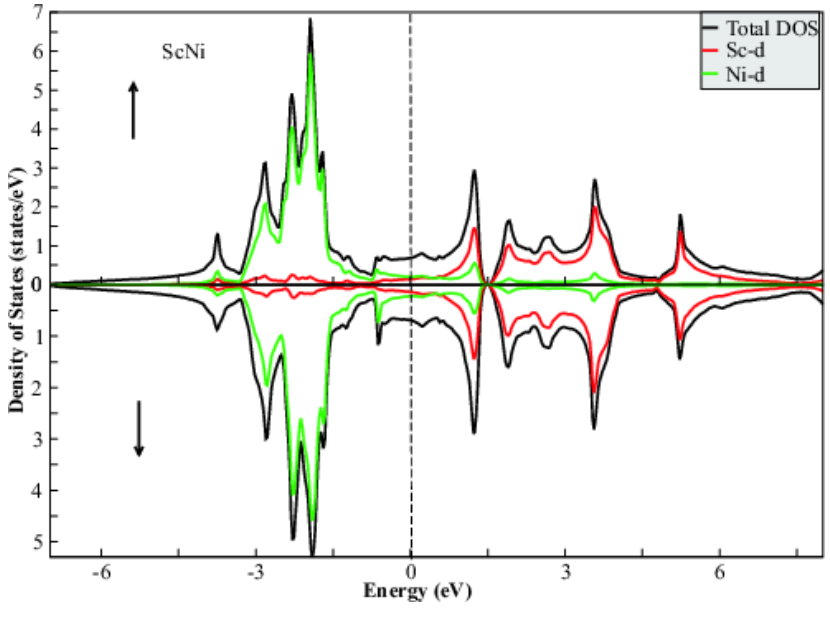
Table 3. Calculated spin magnetic moments in the interstitial region (M^{int}), spin magnetic moments per atom inside the muffin-tin sphere ($M^{\mathrm{Sc}}/M^{\mathrm{TM}}$), total spin magnetic moments inside muffin-tin spheres per cell (M^{Total}), orbital magnetic moments per atom inside the muffin-tin sphere ($M^{\mathrm{Sc}}/M^{\mathrm{TM}}$), orbital total magnetic moments per cell (M^{Total}) and total magnetic moments per cell ($M^{\mathrm{Total}}(\mathrm{spin}) + M^{\mathrm{Total}}(\mathrm{orbital}) = \mathrm{Total}$) of ScTM (TM = Co, Rh, Ir, Ni, Pt, Pd, Cu, Ag and Au) compounds by LDA, LDA + U and LDA + U + SOC.

Compounds	Sites	LDA	LDA + U	LDA + U + SOC		
		MTMT		Spin	Orbital	Total
ScCo	M^{int}	0.0049	−0.3425	−0.3374	—	
	M^{Sc}	0.0011	−0.3317	−0.3241	0.0076	
	M^{Co}	−0.0316	0.8611	0.08265	0.0637	
	M^{Total}	−0.0256	0.1868	0.1649	0.0714	0.2363
ScNi	M^{int}	−0.0025	0.0019	−0.0018	—	
	M^{Sc}	−0.0017	−0.0001	−0.0017	0.0001	
	M^{Ni}	0.0168	−0.0172	−0.0013	0.0008	
	M^{Total}	0.0125	−0.0154	−0.0049	0.0009	−0.0039
ScCu	M^{int}	0.0001	0.0039	0.0044	—	
	M^{Sc}	0.0003	0.0059	0.0057	0.0000	
	M^{Cu}	−0.0004	0.0016	0.0011	0.0000	
	M^{Total}	−0.0000	0.0114	0.0113	0.0000	0.0114
ScRh	M^{int}	−0.0031	−0.0054	−0.0081	—	
	M^{Sc}	−0.0024	−0.0027	−0.0071	0.0003	
	M^{Rh}	0.0012	−0.0012	0.0091	0.0009	
	M^{Total}	−0.0042	−0.0095	−0.0060	0.0013	−0.0047
ScPd	M^{int}	−0.0001	0.0002	0.0006	—	
	M^{Sc}	0.0007	0.0035	0.0011	0.00009	
	M^{Pd}	−0.0015	−0.0053	0.0000	0.00002	
	M^{Total}	−0.0008	−0.0016	0.0017	0.00011	0.0018
ScAg	M^{int}	0.0003	0.0002	0.0009	—	
	M^{Sc}	0.0007	0.0025	0.0016	0.0000	
	M^{Ag}	−0.0007	−0.0004	0.0001	−0.0000	
	M^{Total}	0.0003	0.0022	0.0026	0.0000	0.0026
ScIr	M^{int}	−0.0018	−0.0025	−0.0012	—	
	M^{Sc}	−0.0012	−0.0021	−0.0012	0.0001	
	M^{Ir}	0.0029	0.0048	0.0023	0.0002	
	M^{Total}	−0.0000	0.0000	−0.0001	0.0003	0.0003
ScPt	M^{int}	0.0004	−0.0008	0.0002	—	
	M^{Sc}	0.0027	0.00013	0.0004	0.0000	
	M^{Pt}	0.0018	−0.0002	0.0001	0.0000	
	M^{Total}	0.0051	0.0002	0.0007	0.0000	0.0007
ScAu	M^{int}	0.0007	0.0007	0.0005	—	
	M^{Sc}	0.0027	0.0040	0.0009	−0.0001	
	M^{Au}	−0.0015	−0.0013	−0.0002	−0.0000	
	M^{Total}	0.0020	0.0034	0.0012	−0.0001	0.0011

is 0.0001 μ_B and for Ni is 0.0008 μ_B. The total magnetic moment per ScNi cell is −0.0039 μ_B. In ScCu compound the interstitial magnetic moment inside the muffin-tin sphere by LDA is 0.0001 μ_B, by LDA+U it is 0.0039 μ_B and by LDA+U+SOC it is 0.0044 μ_B. The spin magnetic moments are 0.0003, 0.0059 and 0.0057 μ_B for

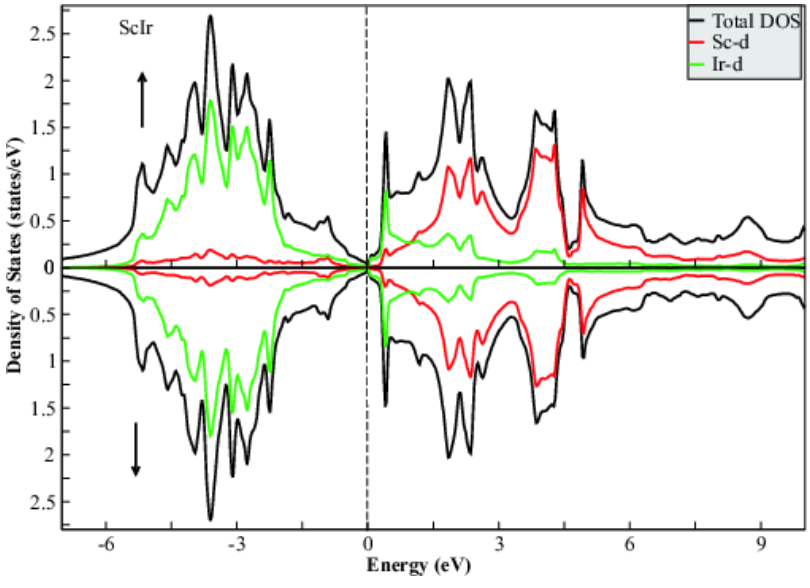


(a)

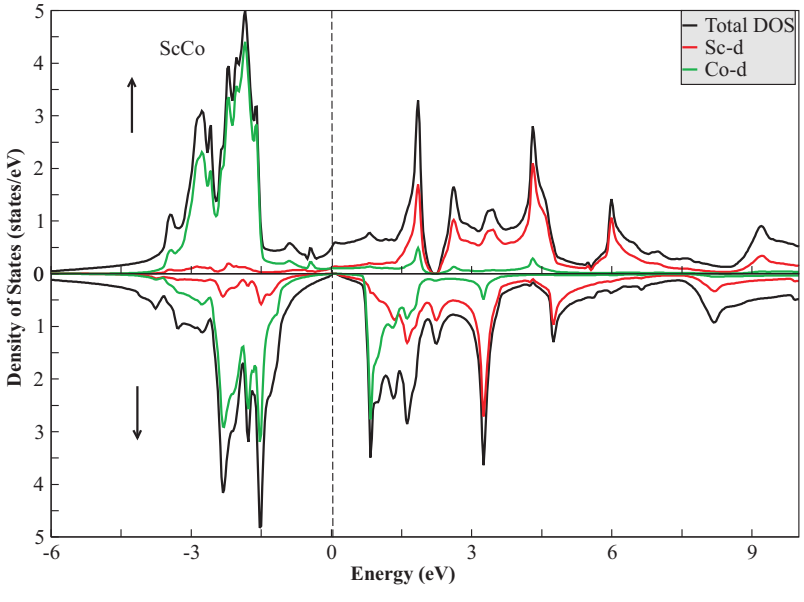


(b)

Fig. 5. (Color online) (a) Double cell AFM-TDOSs for spin-up and spin-down of ScAu compound. (b) Double cell AFM-TDOSs for spin-up and spin-down of ScNi compound. (c) Double cell AFM-TDOSs for spin-up and spin-down of ScIr compound.



(c)



(d)

Fig. 5. (*Continued*)

Co and are -0.0004, 0.0016 and 0.0011 μ_B for Cu. The orbital magnetic moment by LDA$+U+$SOC for Sc is 0.0000 μ_B and for Cu is 0.0000 μ_B. The total magnetic moment per ScNi cell $[M^{\text{Total}}(\text{spin}) + M^{\text{Total}}(\text{orbital}) = \text{Total}]$ is 0.0114 μ_B. The

interstitial magnetic moment and Sc magnetic moment are negligible which means that in the total magnetic moment the dominant contribution is due to the TM d-state. In ScCu, the dominant contribution is observed due to d-state of Sc element, because Cu d-state is completely filled while the Sc d-state is partially filled. A similar trend is also seen in ScRh, ScPd, ScAg, ScIr and ScPt compounds.

To confirm the anti-ferromagnetic behavior of these compounds, we performed the double cell self-consistent field calculations. The spin-dependent total densities of states of these compounds are presented in Figs. 5(a)–5(c). As it is clear from Fig. 5(a)–5(c) that DOSs of ScNi, ScIr and ScAu compounds in both spin channels are mirror reflections, it confirms the metallic anti-ferromagnetic nature of these compounds.

4. Conclusions

In summary, first-principles calculations are performed to study the correlations and SOC effects in ScTM compounds. The lattice constants are calculated by LDA, LDA + U and LDA + U + SOC and we found that the LDA + U results are well consistent with the available experimental results. U optimization for each compound is performed. Furthermore, U/W ratio is used to determine correlation strength of each compound. It was found that ScTM (TM = Co, Ir, Pd, Pt, Cu and Ag) compounds are highly correlated whereas ScTM (TM = Rh, Ni and Au) are intermediately correlated compounds. SOC effects are also discussed for all materials and particularly shown for ScPt compound. The calculated density of states shows the metallic behavior of these compounds. Metallic behavior is attributed to the d-state of either scandium or TM elements. The stable magnetic phase of these compounds is also determined. It is found that ScCo, ScRh, ScPd, ScPt and ScCu are ferromagnetic, ScIr, ScNi and ScAu are anti-ferromagnetic, whereas ScAg is a nonmagnetic material.

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