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Electronic structure and magnetic properties of selected UTX compounds: LDA + U approach

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Abstract

We present calculations of a set of UTX compounds (where T is a transition metal and X is a p element) in the framework of density functional theory applying the LSDA + U exchange–correlation energy functional. As the parameters U and J for these compounds are not known, we varied them in effort to reproduce experimental uranium magnetic moments. Using the obtained electronic structures we discuss the magnetism and the effects of hybridization. Our results are in improved agreement with experimental findings.

1. Introduction

Many of the UTX compounds (where T is a transition metal and X is a p element) crystallize in the layered structure of ZrNiAl type (hexagonal, space group 189, $P\bar{6}2m$) with two alternating layers. One layer ($z = 0$) contains a transition metal (denoted T_1) and a p element, and the other ($z = 1/2$) contains the transition metal T_2 and U atoms [1]. T_1 and T_2 occupy different crystallographic positions.

Interlayer exchange coupling of U atoms is relatively weak and depends on the T element. This is the main reason for a large variability of magnetic structures observed in different UTX compounds. For example, UNiGa orders antiferromagnetically while UCoGa orders ferromagnetically. Small substitutions of Co into UNiGa lead to ferromagnetic order. URhAl and UIrAl are also ferromagnets, unlike UCoAl, which is an enhanced Pauli paramagnet, which undergoes a metamagnetic transition to the ferromagnetic state even in small magnetic fields ≈ 0.6 T. This variability is one of the reasons why these ternary uranium intermetallics are currently the focus of interest of many experimental [1–4] and theoretical groups [2, 6–8]. Recently, Antonov *et al* performed an LSDA + U analysis of UTAI (T = Co, Rh and Pt). They succeeded in explaining satisfactorily the results of x-ray magnetic circular dichroism experiments, but their calculations failed to reproduce the experimental uranium magnetic moments [5].

An important characteristic of individual compounds is the degree of localization of U 5f states. All are essentially itinerant, but still the degree of localization is reflected in the magnitude of the U magnetic moments [1, 2, 9]. While UNiAl and UPtAl exhibit higher magnetic moments (the U moments are approximately $1.3 \mu_B$), the moments of UCoAl and UCoGa are lower. This is usually attributed to a different level of hybridization of U 5f states with transitional element d electrons.

The competition between localization and itinerancy of uranium 5f electrons imposes a difficulty on all types of calculations. Standard *ab initio* calculations in the framework of density functional theory (DFT) are based on the local spin density approximation (LSDA) for the exchange–correlation energy [10]. This scheme however fails in describing systems with strongly correlated electrons, not only in the case of lanthanides and actinides [2]. In the case of systems with 4f electrons, which are mostly very well localized, one usually can improve calculation by employing the so-called open-core scheme, in which hybridization of 4f electrons with others is artificially switched off and these electrons are treated as core-like. This scheme can also be used in some uranium-based systems, where it is known that U 5f electrons are well localized, as in UPd₃ [11]. On the other hand, standard band calculation, where the 5f electrons are treated as valence Bloch electrons, performs quite well in cases of strongly itinerant 5f electrons.

However, the degree of localization of the 5f electrons in UTX compounds varies, and thus it would be preferable to have one consistent scheme, which allows all cases to be treated using the same approach. So we turned our attention to the LSDA + *U* method, which includes orbitally dependent terms in the LSDA exchange–correlation potential. To mention a few cases, LSDA + *U* was successful in describing the magnetic properties of UGe₂ [12] and also in the analysis of x-ray magnetic circular dichroism experiments performed on UTX compounds [5]. However, one should also bear in mind that LSDA + *U* is a semi-empirical theory. As such, there is no guarantee that LSDA + *U* will improve results over LSDA, when applied to a new class of materials. In this paper, we present a systematic study of the magnetic properties of a class of UTX compounds using LSDA + *U*, and *a posteriori* we conclude that LSDA + *U* allowed us to improve the description of the magnetic properties of the compounds studied in comparison to results presented in the existing literature.

We concentrated our attention on ferromagnetic phases of selected UTX compounds. We present, for the first time to the best of our knowledge, full-potential fully relativistic LSDA + *U* calculations exploring a realistic range of *U* and *J* parameters in an effort to obtain uranium magnetic moments that are consistent with experiment. These calculations lead to band structures, which allow us to explain some magnetic properties of the compounds studied. Moreover, using the *U* and *J* values obtained we calculated the equilibrium volume, which is considerably improved with respect to experiments in comparison to standard LSDA calculations.

The main new aspect of our treatment is the exploration of a realistic range of *U* and *J* parameters, analogously to the work by Shick and Pickett [12]. For example, Gasche *et al* [8] performed magnetic calculations using an orbital polarization method. Their treatment is based on the linear muffin-tin orbital method in the atomic spheres approximation (LMTO-ASA), which neglects the nonspherical parts of the potential in the atomic spheres. Their calculations failed to reproduce the magnetic properties. Kučera *et al* [13] and Kuneš *et al* [6] did calculations using a full-potential method with spin–orbital interaction included; however, in UTX compounds LSDA strongly underestimates the orbital moments, and that is a reason why their calculations did not reproduce the uranium magnetism well enough. More recently, Antonov *et al* [5] employed LMTO-ASA including LSDA + *U* with two different values of *U*—an atomic one $U = 2$ and 0.5 eV—but none of them leads to experimental uranium

magnetic moments. That is why a more careful exploration of LDA + U parameter space is desired.

2. Details of calculations

We performed calculations in the framework of density functional theory. Kohn–Sham equations were solved by the full-potential augmented plane waves plus local orbitals (APW + lo) method, which is implemented in the WIEN2k code [14]. This method is a recent improvement over the full-potential linearized augmented plane waves method (LAPW). It maintains all the advantages and high numerical accuracy but offers higher efficiency, because well converged results can be obtained with much smaller numerical basis sets in comparison to the older LAPW method [15].

Because of the high atomic number of uranium, relativistic calculations are necessary. Core states are calculated using the four-component fully relativistic solver of Kohn–Sham–Dirac equations, while valence states are treated in a scalar-relativistic approach, with spin–orbit interaction (SO) included using a second-variation step method. Relativistic local orbitals for the description of U $6p_{1/2}$ states are included [16]. Such calculations are typically in good agreement with more demanding fully relativistic four-component approaches, as for example the relativistic full-potential local orbitals method [17].

Most of the calculations were performed using the following parameters. The radii of atomic spheres were 2.8 au (atomic units, 1 au = 0.529 17 Å), 2.5 and 2.4 au for U, T and X respectively. The wavefunction expansion parameter $RK_{\max} = 7.5$ was used. This corresponds to approximately 85 plane wavefunctions per atom. Brillouin zone integration was performed using the modified tetrahedron method with 60 k -points in the irreducible wedge of the Brillouin zone. We carefully tested the convergence of the results presented with respect to the parameters mentioned and found them to be fully sufficient for all presented characteristics of the compounds studied.

We also tested two different implementations of the LDA + U method, namely the around mean field (AMF) and a method with a partial correction to self-interaction [14]. Since their results are similar we decided to use the AMF method, because by construction it is better suited for systems with a lower degree of localization, which should be the case for the UTX compounds. The LDA + U potential is implemented in a rotationally invariant way in both cases. In these calculations we varied the parameters U and J , which were used to describe the onsite Coulomb (direct and exchange) interactions. Considering the atomic values $U = 2.0$ eV and $J = 0.55$ eV [12] we varied the effective U in the range from 0.2 to 1.0 eV with three different J values, namely 0.33, 0.44 eV, and an atomic value 0.55 eV.

Assuming that LDA + U is appropriate for the description of the magnetism of UTX compounds (note the discussion of applicability of LDA + U in the introductory section), we *heuristically* expect that the value of J does not change dramatically from its atomic value, and that the value of U should not be lower than value of J . We admit that on this level such a calculation loses its *ab initio* character, but on the other hand, we will show that these heuristically derived values allow us to obtain valuable results. As a figure of merit for the calculations we take the saturated magnetic moments. Optimization of U and J thus leads to a dependence between them. The total energies of the corresponding calculations differ by less than 1 mRyd, and therefore we cannot select proper values based on the minimum of the total energy.

For completeness, we also tried to obtain U and J parameters in an *ab initio* way for the case of UPtAl, for which we tested various approaches. These are summarized in the last part of the paper. In principle, they confirm the correct order of magnitude of our U and J values, though *ab initio* values are usually higher than the values we used in the previous part.

Table 1. Collected experimental data (structure and saturated uranium magnetic moment; see references in the text), optimized U and J values and corresponding calculated total, orbital and spin magnetic moments of U, respectively.

	UIrAl	UPtAl	URhAl	UCoAl	UFe _{1/2} Ni _{1/2} Al	UCoGa	UNiGa
a (pm)	695.8	701.4	696.5	667.5	674.1	666.46	669.53
c (pm)	401.4	412.5	401.9	396.6	394.7	392.65	400.2
x_U	0.594	0.5785	0.5804	0.5788	0.5788	0.580018	0.575
$x_{Al,Ga}$	0.256	0.2395	0.2361	0.2358	0.2358	0.239151	0.234
$\mu_{U,exp}$ (μ_B)	0.965	1.384	0.94	~ 0.6	0.62	0.63	1.3
U (eV)	0.5	0.8	0.5	0.6	0.57	0.5	1.0
J (eV)	0.44	0.44	0.33	0.33	0.33	0.44	0.44
$\mu_{U,th}$ (μ_B)	0.94	1.35	0.96	0.59	0.62	0.62	1.31
μ_L (μ_B)	2.16	2.98	2.31	1.62	1.71	1.70	2.85
μ_S (μ_B)	-1.22	-1.63	-1.36	-1.04	-1.09	-1.08	-1.54

We also tested how much the results of LDA + U calculations depend on the starting density matrix, which can be important in calculations of compounds containing rare-earth atoms. Experience has shown that the converged self-consistent electronic structure does not depend on the starting density matrices in those cases, where U and J parameters are smaller than the bandwidth of 5f states. In all treated UTX compounds this bandwidth exceeds 2 eV, which is well above the upper limit of the interval of U parameters used (1 eV).

3. Results and discussion

In the following subsections we describe the results for UTX compounds, namely UPtAl, UIrAl, URhAl, UCoAl, UCoGa, UFe_{1/2}Ni_{1/2}Al and UNiGa. Structure parameters [1] were taken from available low temperature experimental data. It will be shown that we are able to reproduce lattice parameters with improved accuracy in comparison to standard LSDA calculations. Structure parameters together with measured saturated moments are listed in table 1.

3.1. URhAl

We found that approximately for $U = 0.9$ eV – $1.2J$ we obtain a magnetic moment in agreement with experiment. Based on the arguments mentioned above and in agreement with the results of Shick *et al* [12], we propose that effective values for U and J are *approximately* 0.5 and 0.33 eV, respectively. With these parameters we obtained a uranium magnetic moment of 0.956 μ_B . The calculated orbital moment is 2.31 μ_B , which is in fair agreement with the experimental value of 2.1 μ_B . Moreover, the theoretical $-\mu_L/\mu_S = 1.71$ is near the experimental ratio of 1.81 [18]. This is a considerable improvement, since LSDA with spin-orbital interaction included gives values 1.4 μ_B for orbital moment and 1.30 for the ratio to the spin moment [6].

The experimental magnetic moments of the two types of Rh atoms are 0.28 and 0.03 μ_B [18], which should be compared with the theoretical spin moments of 0.07 and 0.05 μ_B . They agree to order of magnitude and in sign. The small deviation indicates that there may be a weak (though non-negligible) orbital polarization. To take this into account more accurately would require us to include an orbital dependent potential LDA + U also for the rhodium sites. As we are mainly interested in the uranium magnetism, this has not been done in this work.

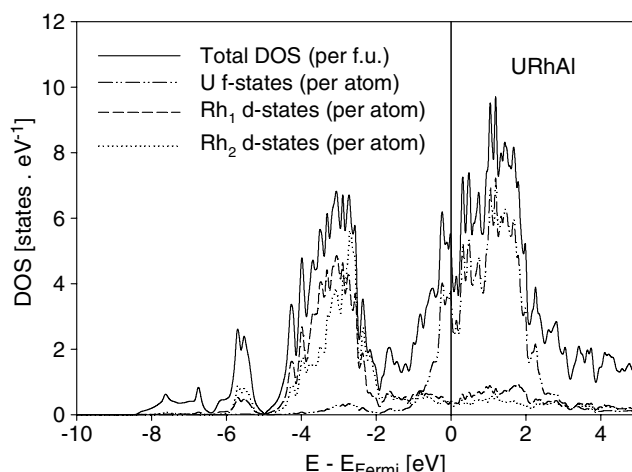


Figure 1. Total density of states (per formula unit) and projections on individual transitional metal d states and uranium f states (per atom) of URhAl.

We should also mention that our values of magnetic moments are related to moments inside the atomic spheres and there is a non-negligible contribution from the interstitial region of size $-0.14 \mu_B/\text{f.u.}$, which partially belongs to all sites but mainly to conduction electrons. The experimental value of polarization of conduction electrons is $-0.11 \mu_B$ [18].

Rhodium is the only 4d transitional element that is studied in the present set of compounds. In comparison to other UTX compounds, the Rh 4d bands (figure 1) are centred around -3 eV . That is a lower binding energy than for the 5d bands of Pt and Ir, which are centred more or less at -4 eV , and higher than the 3d bands of Co and Ni centred slightly below -2 eV . These are described in detail in the following sections. The effects of hybridization of 5f states with d states are comparable with those of UIrAl, leading to uranium magnetic moments of similar magnitude (see table 1).

3.2. UIrAl and UPtAl

Comparison of these two compounds is interesting, since their transition elements are neighbours in the periodic table, but their magnetism is rather different. The uranium magnetic moment in UIrAl is much smaller and more itinerant than in UPtAl.

The calculated electronic densities of states support this experimental finding. Inspecting the 5d and 5f projections of the respective densities of states (see figure 2), we can see the effects of hybridization, which are rather different from each other. The 5d bands of Pt are relatively well separated from the uranium 5f bands, and their hybridization is low. They are also narrower (the lattice parameters of UPtAl are larger than those of UIrAl) and lead to higher moments on U sites. To compare real space localization of magnetic moments, we calculated magnetization density maps. Despite the narrower U 5f bands in UPtAl we did not observe any remarkable difference in localization of the magnetic moments around uranium sites between UPtAl and UIrAl in real space. The volume of the UIrAl unit cell is smaller, which leads to wider Ir 5d bands that hybridize more (in comparison to UPtAl) with the U 5f bands. This hybridization reduces the uranium magnetic moment, whereas it increases the transition metal magnetic moment (Ir: $0.06 \mu_B$, Pt: $0.03 \mu_B$), which is antiparallel to the uranium spin magnetic moment. The transition metal magnetic moment is lower by a factor

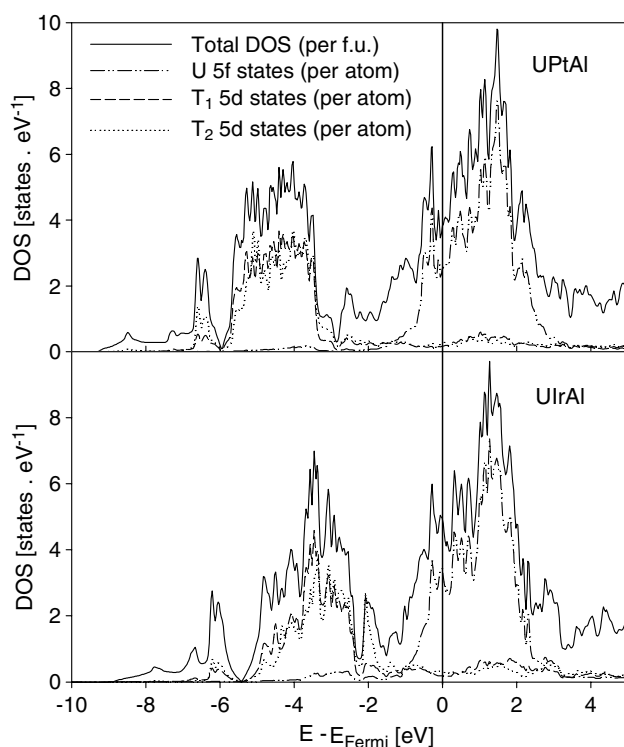


Figure 2. Total density of states (per formula unit) and projections on individual transitional metal d states and uranium f states (per atom) of (a) UPtAl and (b) UIrAl.

of 15 or 40, respectively. The hybridization between spin-up uranium 5f bands and transition metal 5d bands draws electrons from the transition metal spin-up bands, thus creating a spin moment antiparallel to the total U spin moment. The stronger the effect of hybridization, the higher the transition metal spin moment.

Orbital moments of transition metal elements are small due to weak spin-orbit interaction (at least for 3d and 4d) and band broadening. On the other hand, the orbital magnetic moment of uranium atoms is large. Its size is roughly twice the size of the spin moment, but of opposite sign, in qualitative agreement with Hund's rules, however both of reduced size. This reduction can be attributed to the itinerancy of the uranium 5f electrons. Also relativistic effects play a role here. The combination of orbital and spin magnetic moment leads to a total magnetic moment that is parallel to the transition metal magnetic moments.

We succeeded in reproducing the magnetic moment of UPtAl with $U = 0.8$ eV and $J = 0.44$ eV. In this case, the spin magnetic moment was $-1.63 \mu_B$ and orbital magnetic moment $2.98 \mu_B$. These values are consistent with the set c in table II of [2], taking into account that our calculated values should be compared to saturated magnetization. Comparing to previous works by Gasche [8] and Kučera *et al* [13], our values represent a considerable improvement of overall agreement with experiment.

Using the obtained U and J values for UPtAl, we calculated the energy versus volume curves at a fixed c/a ratio equal to the experimental value. We found that the equilibrium volume in the LSDA + U method is in better agreement with experiment than that of the standard LSDA method (with or without spin-orbit interaction). An interesting detail is that

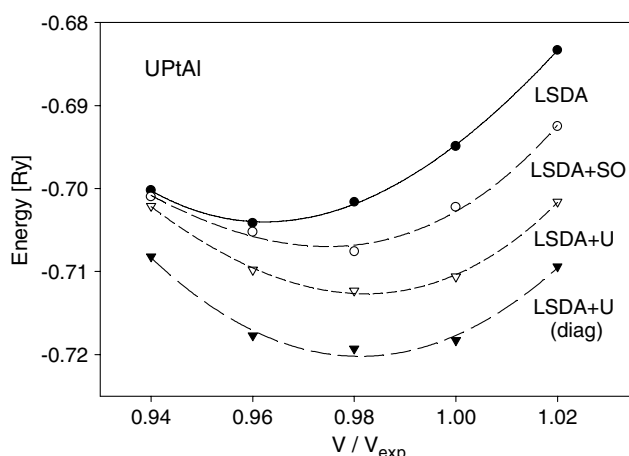


Figure 3. Energy versus volume curves for standard LSDA (full circles), LSDA with spin-orbit interaction (empty circles), LSDA + U with spin-diagonal orbital potential (full triangles) and LSDA + U with complete orbital potential, i.e. spin non-diagonal parts included (empty triangles). In both LSDA + U calculations spin-orbit interaction was included.

including a spin-nondiagonal part of the orbital potential (crossterm) to the self-consistent cycle improves that agreement further (see figure 3). The following results were obtained (V_{eq} is the calculated equilibrium volume and V_{exp} is the experimental low-temperature unit cell volume): $V_{\text{eq}}/V_{\text{exp}} = 0.963$ in the standard LSDA calculation, but including spin-orbit interaction improves this ratio to $V_{\text{eq}}/V_{\text{exp}} = 0.975$. LSDA + U calculation without the crossterm leads to $V_{\text{eq}}/V_{\text{exp}} = 0.981$. Calculation with the crossterm leads to the slightly better ratio $V_{\text{eq}}/V_{\text{exp}} = 0.982$. This good agreement with experiment justifies our use of low temperature experimental values for the lattice parameters in our calculations.

In the case of UIrAl, the best agreement with experiment was obtained for $U = 0.5$ eV and $J = 0.44$ eV. The calculated total magnetic moment with these parameters is $0.944 \mu_{\text{B}}$ (the experimental value is $0.965 \mu_{\text{B}}$ [19]). Its orbital and spin contributions are 2.16 and $-1.22 \mu_{\text{B}}$, respectively. Experimental values for spin and orbital magnetic moments are—to our best knowledge—not known.

We also performed an energy versus volume calculation for UIrAl. Results for this compound confirm the improved agreement with experiment, as in the case of UPtAl. The result in standard LSDA treatment $V_{\text{eq}}/V_{\text{exp}} = 0.963$ improves to 0.970 , 0.972 and 0.988 for calculations including spin-orbit interaction, spin-diagonal parts of LSDA+ U orbital potential, and full LSDA + U potential, respectively.

3.3. UCoAl and UFe_{1/2}Ni_{1/2}Al in virtual crystal approximation

UCoAl is a paramagnet in its ground state, but a small magnetic field is sufficient to cause a metamagnetic transition, making the system ferromagnetic [20]. Also small amounts of Fe substituting Co lead to a ferromagnetic alloy [21]. In this sense UCoAl is very near to the onset of ferromagnetism. One must note that a standard LSDA calculation (with or without spin-orbital interaction) predicts a ferromagnetic ground state. Using U and J parameters predicted by us we checked the ground state with an LSDA + U calculation and that also predicts a ferromagnetic ground state. In fact, the stabilization energy is even larger, namely approximately 70 meV/f.u. Calculated stabilization energies of LSDA and LSDA with SO calculations are in agreement with published results [22].

In contrast to UCoAl, the alloy $\text{UFe}_{1/2}\text{Ni}_{1/2}\text{Al}$ is ferromagnetic in its ground state [22]. We treated this alloy in the virtual crystal approximation (VCA). Experimental structure parameters (which are fairly different from UCoAl) were applied, and Fe and Ni elements were replaced by an ‘average’ element, i.e. Co. The ferromagnetic ground state was correctly reproduced by our VCA calculations as well as the value of the experimental magnetic moment (see table 1). Moreover, there is a clear tendency to the stabilization of the ferromagnetic state in $\text{UFe}_{1/2}\text{Ni}_{1/2}\text{Al}$ with respect to UCoAl. The difference of total energies of ferromagnetic state and paramagnetic state rose to approximately 200 meV/f.u. Thus we can conclude that the change of magnetic properties of the ground state between $\text{UFe}_{1/2}\text{Ni}_{1/2}\text{Al}$ and UCoAl is to a large extent a consequence of different lattice parameters.

3.4. UCoGa and UNiGa

Comparison of UCoGa and UNiGa will be relatively analogous to the case of UPtAl and UIrAl. UCoGa is a ferromagnet and UNiGa is an antiferromagnet, but a rather low magnetic field of $B_c \approx 1$ T is able to switch the magnetic moments into the ferromagnetic arrangement. UCoGa and UNiGa differ by size of the magnetic moment and the degree of localization on the uranium site. The saturated uranium magnetic moment in UNiGa ($1.3 \mu_B$, [1]) is larger by factor of 2 than in UCoGa ($0.63 \mu_B$, [23]); see table 1.

The band structure calculation leading to the correct magnetic moments on uranium sites reveals other details. The 3d bands are narrower (≈ 2 eV) in comparison to systems with 5d electrons (≈ 3 eV). Their centres are higher in energy and their hybridization with 5f bands is stronger.

Transition metal magnetic moments are larger, at least in the case of Co. It is interesting that the magnetic moments on the Co atoms are very similar for both Co sites, and both are antiparallel to the spin moments at the U site. This is not true for the Ni sites. The Ni atom, which is in same plane as the U atoms, has a much lower magnetic moment than the other Ni in the $z = 0$ plane, and is aligned parallel to the U spin moment.

Plots of densities of states reveal a different 5f–3d hybridization in these systems. As can be seen from figure 4, the Ni d bands in UNiGa are deeper in energy by nearly 1 eV in comparison to the Co d bands in UCoGa. Although the 5f bands are somewhat broader in UNiGa, their hybridization with 3d is weaker. Due to this weakening the 5f bands lead to much higher magnetic moments than in UCoGa.

4. Calculation of U and J parameters for UPtAl

In the existing literature (see for example [24–26]), there are different approaches on how to calculate the parameters U and J . Usually they are based on a supercell calculation, where one fixes the occupancy of the f electrons of one selected atom and switches off the corresponding hybridization with other electrons. This can be done most easily by means of the open-core calculation. Here the U 5f electrons are treated as core-like states, which do not hybridize with valence states and whose occupancy is fixed. It can be shown that derivatives of the 5f orbital energy with respect to occupancies can be related to the parameters U and J . This of course is based on the assumption that the orbital energy is calculated correctly, which is not strictly the case in systems with strongly correlated f electrons (note that LDA + U is not applicable here, since the f electrons are not treated as ‘valence’ states). Nevertheless, we do not have a better approach at hand, and argue that, even when we do not have correct absolute values of orbital energies, their trends while varying orbital occupancies might mimic the correct ones.

It is clear that such a calculation would be a very difficult task in our systems, because a $2 \times 2 \times 2$ supercell would contain 24 f.u. of UPtAl, i.e. 72 atoms. The symmetry will be

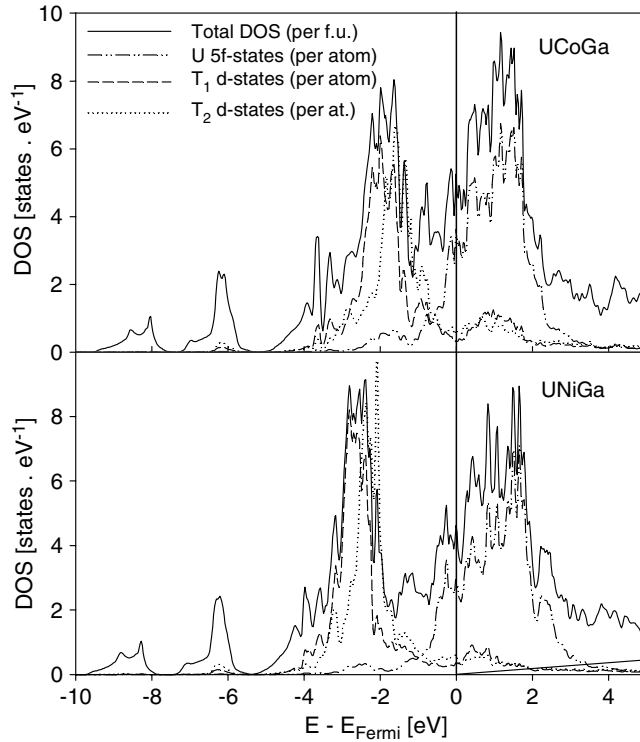


Figure 4. Total density of states (per formula unit) and projections on individual transitional metal d states and uranium f states (per atom) of (a) UCoGa and (b) UNiGa.

lowered in comparison to normal calculations, because we will have to treat one uranium site differently. These are the reasons why we did not try to perform such calculations.

To have an idea of the magnitudes of the U and J parameters, we decided to do a simpler, however less accurate, calculation. We treated all U 5f electrons as core states, and no supercell is constructed. The parameter U , i.e. the screened Slater integral F^0 , is calculated as the difference between orbital energies $e_f(n_\uparrow; n_\downarrow)$ using the formula $e_{f\uparrow}(\frac{n}{2} + \frac{1}{2}; \frac{n}{2}) - e_{f\uparrow}(\frac{n}{2} + \frac{1}{2}; \frac{n}{2} - 1) - e_{f\downarrow}(\frac{n}{2} + \frac{1}{2}; \frac{n}{2}) + e_{f\downarrow}(\frac{n}{2} + \frac{1}{2}; \frac{n}{2} - 1)$, where n is the occupancy of the f states, and $e_F(n_\uparrow; n_\downarrow)$ is the corresponding Fermi level [25]. Results of these calculations lead to U values between 2.2 and 2.8 eV, depending on n . For $n = 2.5$ (occupancy in the self-consistent LSDA + U calculation) we obtained $U = 2.51$ eV. In such a calculation, however, we have three open-core uranium atoms per unit cell. Increasing n in all of them causes a decrease of electronic density of the other valence states that is three times stronger than in the case where we alter only one uranium atom in a supercell. So the change of converged electronic density due to charge renormalization is larger and the effect of screening is weaker. Therefore one can expect that this is an upper bound, which we consider as an upper limit of U in UPTAl.

To obtain the J parameter, we varied $n_{f\uparrow}$ and $n_{f\downarrow}$ in such a way that their sum remained constant (and equals the converged LSDA + U value of 2.5). Then one can estimate J using the following formula: $J = \partial(e_{f\uparrow} - e_{f\downarrow}) / \partial(n_{f\uparrow} - n_{f\downarrow})$. We obtained a value of J of 0.43 eV, which agrees very well with our value 0.44 eV. Of course, this excellent agreement is to some extent fortuitous. On the other hand, the calculated J value should not contain such a large error as in the case of U , and its agreement indicates that we are near the ‘correct’ J for UPTAl.

5. Conclusions

We have succeeded in describing the magnetism of selected UTX compounds and obtained saturated magnetic moments which allowed us to propose corresponding U and J parameters. By using these parameters we obtained, in contrast to [8], spin and orbital magnetic moments that are in good agreement with available experimental data coming from neutron diffraction. Moreover, we improved the agreement with experiment in our calculation of equilibrium lattice constants. The proposed values of U and J are of the same magnitude as those deduced from first principles calculations, that have been performed for the UPtAl compound.

Acknowledgments

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