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Magnetic properties of $DyCo_5$ and $TbCo_5$ intermetallics from the electronic structure calculations

G.I. Miletić*, Ž. Blažina

Laboratory for Solid State Chemistry, Division of Materials Chemistry, Institute Rudjer Bošković, P.O. Box 180, 10002 Zagreb, Croatia

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Abstract

LSDA and LSDA + U calculations, with spin–orbit coupling (SOC) included, were performed for $DyCo_5$ and $TbCo_5$ intermetallic compounds. In the case of magnetic moments, LSDA − SOC calculations give results in good agreement with the experimental data. However, LSDA has shown to be unable to predict relative stabilities of ferromagnetic and ferrimagnetic configurations of the 4*f* and 3*d* spin sublattices giving the wrong result that the ferromagnetic configuration is more stable. LSDA + U method cures this problem and gives correct result. Additionally, within the accuracy of available experimental data, the corresponding effective exchange fields are in reasonable agreement with experiment.

Keywords: Magnetically ordered materials; Rare earth intermetallics; DFT calculations

1. Introduction

Rare earth-transition metal (RE-TM) intermetallics are attracting considerable scientific interest since they offer a wide basis for development of permanent magnets. These investigations are guided by both, technological and fundamental reasons. Among the RE-TM intermetallics, hexagonal Haucke compounds (structure type $CaCu_5$, space group $P6/mmm$) of the $RECo_5$ composition are one of the most interesting subclasses which exhibit high Curie temperatures and high magnetocrystalline anisotropies with the wide known example of $SmCo_5$ [1,2].

Reviews on earlier experimental research can be found in [1,2] while the theoretical work (up to 1998) based on the density functional theory-DFT [3,4] is reviewed in [5].

It is well known that the fundamental magnetic properties of the RE-TM intermetallics arise from two groups of electrons: very localized 4*f* and more itinerant 3*d*. Today it is commonly accepted that 5*d* electrons ferrimagnetically couple spin magnetic moments of the 4*f* and 3*d* subsystems through the 4*f*–5*d* intraatomic exchange interaction and the 3*d*–5*d* hybridization [6,7].

Theoretical description of magnetism of the RE-based compounds within basic DFT approximation (local spin density approximation-LSDA) was often restricted to the so-called open core treatment of the 4*f* electrons since LSDA places partially filled 4*f* spin subband at the Fermi level which influences the ground state properties and can lead, for example, to a wrong prediction of the relative stability of different magnetic orderings [8].

Although the open core treatment has proven to be useful in the treatment of 4*f* electrons, the necessary condition for its usefulness is a strong localization of 4*f* electrons and one can expect that this will be fulfilled for heavier rare earths.

It is therefore interesting to mention a possible case where both, ferrimagnetic orientation of the 4*f* and 3*d* spin magnetic moments and applicability of open core approximation, could be questionable. In $SmCo_5$ better agreement between calculated and experimental total magnetic moments was obtained assuming that Sm and Co spin magnetic moments align ferromagnetically and not ferrimagnetically [9]. Possible ferromagnetic coupling of Sm and Co spin magnetic moments was explained as a

*Corresponding author. Fax: +385 1 468 0084.
E-mail address: gmiletic@irb.hr (G.I. Miletić).

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consequence of the 4*f*–3*d* hybridization implying that open core approximation is inapplicable in that case [10]. Since it is usually accepted that 4*f* and 3*d* spin magnetic moments couple ferrimagnetically, the assumption that the 4*f* and 3*d* spin magnetic moments in $SmCo_5$ couple ferromagnetically [9] rises an interesting question, which is important both for theoretical work and the interpretation of experimental data. According to [9] no direct measurement was performed to reveal type of ordering (ferro or ferri) in $SmCo_5$.

The subject of the present paper is the electronic structure and some magnetic properties (magnetic moments and the relative stabilities of the ferromagnetic and ferrimagnetic orderings of 4*f* and 3*d* spin sublattices) of the rare earth intermetallics $DyCo_5$ and $TbCo_5$. Calculations were performed within LSDA and, to improve description of the 4*f* states, LSDA + *U* method [8] was additionally employed. For a more complete comparison of the various treatments of 4*f* states, calculations with 4*f* states treated as an open core states were also performed in the case of $DyCo_5$.

2. Computational details

Full-potential calculations were performed with APW + lo basis set [11] as implemented in program WIEN2k [12]. Exchange-correlation potential was calculated within LSDA as prescribed by Perdew and Wang [13] and, to obtain better description of 4*f* states, by LSDA + *U* method [8]. For double counting correction in LSDA + *U* prescription of Anisimov et al. [14] was used since it was regarded as more appropriate for the very localized 4*f* electrons (see [15,16]).

Spin-orbit coupling (SOC) along with scalar-relativistic approximation was included using second variational procedure [17,18]. According to experimental data, magnetization direction is in the plane normal to *c*-axis for both $DyCo_5$ and $TbCo_5$ [19], therefore, direction [1 0 0] was used in the present calculations.

LSDA − SOC calculations were performed at first and, after reaching selfconsistency, LSDA + *U* − SOC calculations were started with density matrices (and other quantities) obtained from LSDA − SOC calculation and with the U_{4f} parameter equal to 0.1 Ry and the J_{4f} parameter equal to 0.06 Ry. After reaching selfconsistency, the U_{4f} parameter was gradually increased up to 1.0 Ry in steps of 0.1 Ry while the J_{4f} parameter was kept constant. Each LSDA + *U* − SOC calculation (except the first one) was started with density matrices and other quantities obtained from the previous LSDA + *U* − SOC calculation.

For G_{max} (cut-off for Fourier expansion of charge density) a value of 14.0 was taken, for RK_{max} (*R*-the smallest of muffin-tin radii, K_{max}-plane wave cut-off; RK_{max} determines number of augmented plane waves used in calculation) a value of 7.0. Brillouin zone was sampled with $15 \times 15 \times 16$ *k*-mesh, the radii of muffin-tin spheres were 2.5 a.u. for RE atoms and 2.3 a.u. for Co atoms. Structural data for $DyCo_5$ and $TbCo_5$ are given in Table 1.

Table 1
Structural data for $DyCo_5$ and $TbCo_5$ [1,20]

Compound	*a* (Å)	*c* (Å)
$DyCo_5$	4.926	3.988
$TbCo_5$	4.950	3.979

$CaCu_5$ type

Atom	Position	*x*	*y*	*z*
RE	1(a)	0	0	0
Co	2(c)	1/3	2/3	0
Co	3(g)	1/2	0	1/2

3. Results and discussion

3.1. $DyCo_5$

According to the data given in Table 2 LSDA − SOC calculations for ferrimagnetic configuration of 4*f* and 3*d* spin magnetic moments resulted in total (spin + orbital) atomic magnetic moments which are in good agreement with experimental data [21]. In addition, Co magnetic moments are also in good agreement with previous calculations [22–25]. Due to magnetization direction used in present calculations, the symmetry is lower than that of the original space group and the 3(*g*) site splits in two groups of atoms. Superscripts on the position labels in Table 2 indicate the number of Co atoms in each of these groups. The corresponding experimental data were given according to the original space group (*P*6/*mmm*) [21].

The total magnetic moment obtained in LSDA − SOC calculation is $1.05\mu_B$/f.u. while experimental values obtained from magnetization measurements on single crystals are $1.40\,\mu_B$/f.u. [26] and $1.71\,\mu_B$/f.u. [27].

It is interesting to note that 4*f* and 5*d* spin magnetic moments have an opposite orientation in the case of ferromagnetic configurations of 4*f* and 3*d* spin magnetic moments. As follows from [6,7] selfpolarized 3*d* states will, through the 3*d*–5*d* hybridization, polarize 5*d* states always antiparallel to itself. Consequently, in ferromagnetic configuration of 4*f* and 3*d* spins 3*d*–5*d* hybridization induces 5*d* spin moment which is opposite to both 4*f* and 3*d* spin moments.

However, in spite of agreement between calculated and experimental values of magnetic moments, LSDA − SOC treatment of 4*f* electrons as valence electrons gives a wrong prediction of the relative stability of ferrimagnetic and ferromagnetic ordering of Dy and Co spin magnetic moments in $DyCo_5$. The present LSDA − SOC calculations incorrectly predict that ferromagnetic ordering is more stable than ferrimagnetic, the energy difference being 18.5 mRy. Additionally, LSDA calculations without SOC result in even worse agreement with experiment;

Table 2
Magnetic moments in $DyCo_5$ from LSDA − SOC calculation for ferrimagnetic and ferromagnetic configurations of 4*f* and 3*d* spin magnetic moments and from neutron diffraction experiment performed at 4.2 K [21]

Atom	μ^{spin}	μ_{4f}^{spin}	μ_{4f}^{orb}	μ_{5d}^{spin}	μ_{3d}^{spin}	μ_{3d}^{orb}	μ_{tot}	μ_{tot}^{exp} [21]
Ferrimagnetic								
Dy	4.82	4.62	3.84	0.15			8.65	8.8 ± 0.3
Co(2*c*)	−1.48				−1.50	−0.10	−1.58	-1.66 ± 0.10
Co$(3g)^1$	−1.52				−1.54	−0.08	−1.59	-1.63 ± 0.10
Co$(3g)^2$	−1.52				−1.54	−0.11	−1.63	-1.63 ± 0.10
Interstitial					0.41			
Ferromagnetic								
Dy	4.56	4.62	3.19	−0.06			7.75	
Co(2*c*)	1.52				1.54	0.12	1.64	
Co$(3g)^1$	1.52				1.54	0.10	1.61	
Co$(3g)^2$	1.52				1.54	0.16	1.68	
Interstitial					−0.35			

ferromagnetic configuration is now for 24.2 mRy more stable than ferrimagnetic configuration. As mentioned above, this is a known failure of LSDA when applied to systems containing 4*f* electrons [8]. It should also be mentioned that the same problem with LSDA was recently noted in the study of lanthanide impurities in the Fe host [28]. In [28], among other results, it was indicated that LSDA + *U* method is able to reproduce correctly the relative stability of the ferromagnetic and ferrimagnetic configurations of the 4*f* and 3*d* spin magnetic moments.

On the other hand, it was earlier shown that open core treatment of 4*f* states provides good description of relative stabilities of ferrimagnetic and ferromagnetic ordering of 4*f* and 3*d* spin magnetic moments in RE-TM intermetallics [22,29–31]. In particular, the use of open core approximation together with the so-called two-sublattice model enabled calculation of the effective exchange fields B^{ex} for many RE-TM intermetallics which are in very good agreement with experimental data [22,29–31]. Within the two-sublattice model the exchange field is connected to the difference of total energies of ferromagnetic and ferrimagnetic configurations of 4*f* and 3*d* spin magnetic moments [22,29–31]: $E_{ferro} - E_{ferri} = 4\,\mu_B B^{ex} S_{RE} Z_{RE}$ where $2\mu_B S_{RE}$ is 4*f* spin magnetic moment and Z_{RE} the number of RE atoms in the unit cell which equals to one in the present case.

To obtain a more complete picture we also performed calculations with 4*f* states treated as open core states with the number of 4*f* electrons fixed to 9 and 4*f* spin magnetic moment fixed to $5\mu_B$. Open core calculation correctly predicts that the ferrimagnetic configuration of 4*f* and 3*d* spin sublattices is more stable than the ferromagnetic one, the energy difference being 10.9 mRy. This energy difference corresponds to the exchange field of 256 T. This is in reasonable agreement with previously calculated value (also within open core approximation) of 216 T [22]. Experimentally determined values vary very much: 172 T [32], 160 T [33] and 315 T [34]. In [32], as a possible explanation of seemingly too low values of the exchange field extracted from measurements in $TbCo_5$, $DyCo_5$ and $HoCo_5$, authors offered anisotropy of 3*d* sublattice which was not included in their analysis and mutual orthogonality of easy magnetization directions of RE and Co sublattices. All this indicates that values of B^{ex} found in experiment should be accepted keeping in mind uncertainties present in the course of their determination. Consequently, a comparison of such experimental values with theoretically calculated values will be also of limited validity.

The open core calculation as an input parameters requires the number and magnetic moment of 4*f* electrons and, on the other hand, LSDA treatment of 4*f* electrons as valence electrons results in an incorrect prediction of the ground state configuration of the 4*f* and 3*d* spin sublattices. It is, therefore, desirable to apply a method which will give reasonable results both about 4*f* magnetic moments and the relative stability of ferrimagnetic and ferromagnetic configurations of the 4*f* and 3*d* spin sublattices. Recently, the LSDA + *U* approach was used to determine B^{ex} in $GdCo_5$ and the authors found very good agreement with the experimental data [35].

Fig. 1 illustrates the difference between total energies of ferromagnetic and ferrimagnetic configurations of 4*f* and 3*d* sublattices obtained in the LSDA + *U* − SOC calculation vs. the value of the U_{4f} parameter. For $U_{4f} \geqslant 0.3$ Ry, LSDA + *U* − SOC approach correctly predicts that the ferrimagnetic configuration is more stable than the ferromagnetic one.

Since both the Coulomb repulsion parameter U_{4f} and the exchange parameter J_{4f} were used here as "free" parameters, it is necessary to comment the choice of their reasonable numerical values. In [28], based on the requirement that the exchange field is constant for all lanthanides and their analysis of literature data, a value of 0.7 Ry was chosen for U_{4f} for all lanthanides. For J_{4f} the value of 0.07 Ry was taken, also for all lanthanides [28].

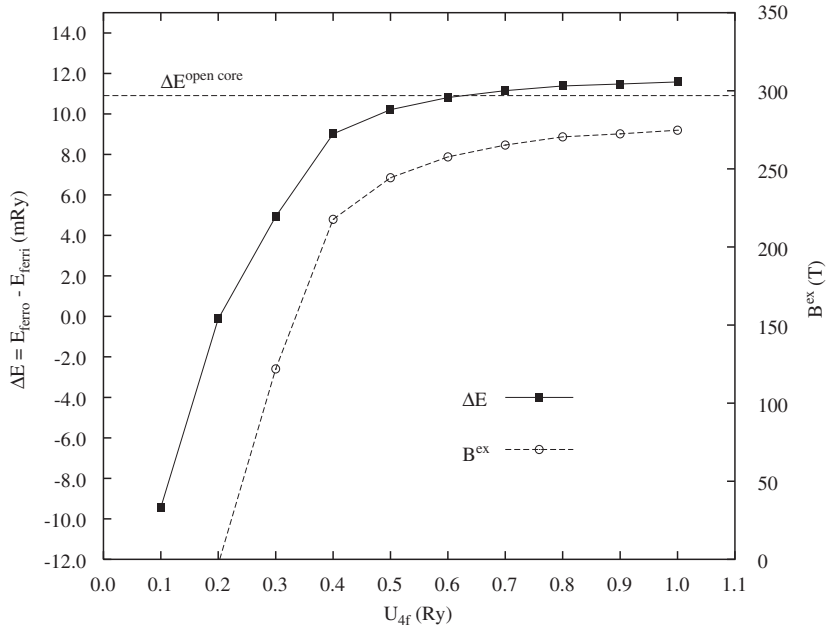

Fig. 1. Differences between total energies of ferromagnetic and ferrimagnetic configurations in $DyCo_5$ obtained in the LSDA + U − SOC calculation and corresponding exchange fields for different values of the U_{4f} parameter. Corresponding open core result is marked with the dashed line.

According to [36] experimental and theoretical value of U_{4f} for Tb span the range of about 0.37–0.44 Ry while J_{4f} parameter remains almost constant (0.05–0.06 Ry) when going from Ce to Tm. Additionally, according to [36], experimental and theoretical values of U_{4f} for Dy are almost equal and are within 0.37–0.44 Ry. One could, therefore, expect that a value of 0.4–0.7 Ry presents a reasonable choice for U_{4f} and a value of 0.05–0.07 Ry for J_{4f} for both Dy and Tb.

It is interesting to note that ΔE almost saturates at the higher values of U_{4f} (Fig. 1). Additionally, LSDA + U − SOC result is very close to the present open core result in the range $U_{4f} \geqslant 0.5$ Ry. In Fig. 1 exchange field vs. U_{4f} is also given. The two-sublattice relation which connects ΔE and B^{ex} (see above) assumes that 4f spin magnetic moments for both configurations of the two spin sublattices are equal to the corresponding free ion value. This is not necessarily true when the 4f electrons are treated as valence electrons. For calculations of the exchange field we therefore used (as in [28]) the following expression: $B^{ex} = (E_{ferro} - E_{ferri})/(|\mu^{ferro}_{4f-spin}| + |\mu^{ferri}_{4f-spin}|)$. Calculated exchange field $B^{ex} = 218$ T corresponding to $U_{4f} = 0.4$ Ry is very close to the theoretical value of B^{ex} obtained earlier [22]. All values of B^{ex} for $U_{4f} \geqslant 0.4$ Ry fall within the range spanned by the experimentally determined values of B^{ex}.

Calculated spin and orbital magnetic moments of 4f electrons vs. U_{4f} parameter are shown in Fig. 2. For ferrimagnetic configuration magnetic moments do not change appreciably for $U_{4f} \geqslant 0.4$ Ry. 4f magnetic moments at $U_{4f} = 0.4$ Ry are: $\mu^{spin}_{4f} = 4.89\mu_B$ and $\mu^{orb}_{4f} = 3.94\mu_B$, both values being greater than the corresponding LSDA − SOC values. In the case of ferromagnetic configuration LSDA + U approach influences more the 4f magnetic moment since the corresponding LSDA − SOC values are: $\mu^{spin}_{4f} = 4.62\mu_B$ and $\mu^{orb}_{4f} = 3.19\mu_B$.

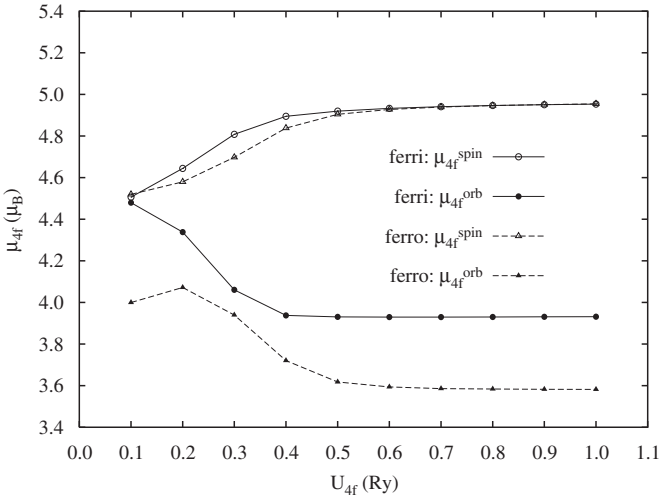

Fig. 2. Spin and orbital magnetic moments of 4f electrons in $DyCo_5$ for ferromagnetic and ferrimagnetic configurations obtained in the LSDA + U − SOC calculation for different values of the U_{4f} parameter.

In Fig. 3 Dy–4f density of states calculated with LSDA − SOC and LSDA + U − SOC are shown. As can be seen from Fig. 3, LSDA places partially filled spin-down 4f states at the Fermi energy. A known effect of introduction of LSDA + U method is also visible in Fig. 3: occupied (unoccupied) states are shifted down (up) in energy, and, consequently, spin-down 4f states are removed from the Fermi energy.

3.2. $TbCo_5$

In Table 3 magnetic moments for the ferrimagnetic and ferromagnetic configurations obtained from LSDA − SOC calculation are presented. It can be seen that calculated Tb magnetic moments for the observed (ferrimagnetic) configuration agree less with experimental values [37] than calculated Dy magnetic moments. The total magnetic moment obtained in the present LSDA − SOC calculation is $0.45\,\mu_B$/f.u. while the value obtained on single crystal is $0.69\,\mu_B$/f.u. [27]. Co magnetic moments calculated in previous calculation [22] agree well with the values obtained in the present study.

LSDA − SOC calculation gives again a wrong prediction about the ground state configuration of two spin sublattices: the ferromagnetic configuration is more stable, the energy difference being 11.5 mRy.

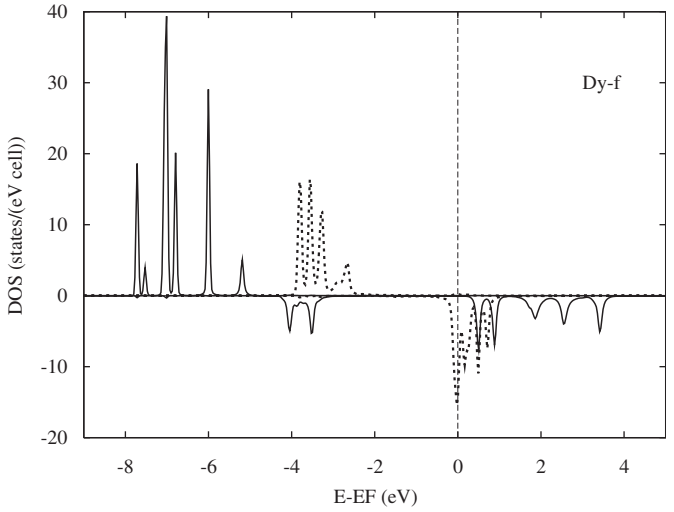

Fig. 3. 4*f* density of states of Dy for two spin directions as calculated in LSDA − SOC and LSDA + *U* − SOC calculations. LSDA − SOC 4*f* density of states is labeled with dotted line, while LSDA + *U* − SOC 4*f* density of states ($U = 0.4$ Ry, $J = 0.06$ Ry) is labeled with full line.

LSDA + *U* − SOC results for difference of total energies of the ferromagnetic and ferrimagnetic configurations and the corresponding exchange fields are shown in Fig. 4.

Again, the application of the LSDA + *U* method exhibits significant improvement over the LSDA results. For $U_{4f} \geqslant 0.2$ Ry ferrimagnetic configuration of the two spin sublattices is more stable. Exchange fields obtained in the present calculation show faster saturation with respect to U_{4f} than in the case of $DyCo_5$. Compared to the previously calculated exchange field of 231 T [22] (within open core approximation), exchange fields obtained in this paper agree well for a wide range of U_{4f} values. For the interval $U_{4f} = 0.4 - 0.7$ Ry, $B^{ex} = 206$–232 T while even for the rather high value of $U_{4f} = 1.0$ Ry, $B^{ex} = 237$ T. Experimentally obtained values of B^{ex} for $TbCo_5$ are 189 T [32] and 190 T [33], the value of B^{ex} corresponding to $U_{4f} = 0.4$ Ry being in best agreement with these experimental data. As mentioned earlier, this experimental values could be too low [32].

Fig. 5 illustrates calculated spin and orbital magnetic moments of 4*f* electrons.

LSDA + *U* results presented in this paper deserve additional comment. It is well known that LSDA + *U* calculation, depending on the initial density matrices of correlated (in the present case 4*f*) states, can easily converge to many different solutions and that it is often not easy to say which one is the "best" (see [28] for more details). In general, such multiple solutions will have different total energies as well as different magnetic moments (e.g. [28]). Therefore, it should be noted that the present results (total energies and, consequently, exchange fields and 4*f* magnetic moments) could be modified if calculations with initial density matrices different from those used here would be performed.

Table 3
Magnetic moments in $TbCo_5$ from LSDA − SOC calculation for ferrimagnetic and ferromagnetic configurations of 4*f* and 3*d* spin magnetic moments and from neutron diffraction experiment performed at 4.2 K [37]

Atom	μ^{spin}	μ^{spin}_{4f}	μ^{orb}_{4f}	μ^{spin}_{5d}	μ^{spin}_{3d}	μ^{orb}_{3d}	μ_{tot}	μ^{exp}_{tot} [37]
Ferrimagnetic								
Tb	6.01	5.77	1.84	0.19			7.85	8.35 ± 0.55
Co(2*c*)	−1.43				−1.45	−0.10	−1.52	-1.55 ± 0.20
Co(3*g*)[1]	−1.50				−1.52	−0.08	−1.57	-1.70 ± 0.10
Co(3*g*)[2]	−1.50				−1.52	−0.11	−1.61	-1.70 ± 0.10
Interstitial					0.44			
Ferromagnetic								
Tb	5.71	5.73	1.44	−0.04			7.15	
Co(2*c*)	1.50				1.52	0.13	1.62	
Co(3*g*)[1]	1.51				1.53	0.09	1.60	
Co(3*g*)[2]	1.51				1.53	0.15	1.65	
Interstitial					−0.32			

The meaning of superscripts on the Co(3*g*) atoms is the same as in Table 2 (see text).

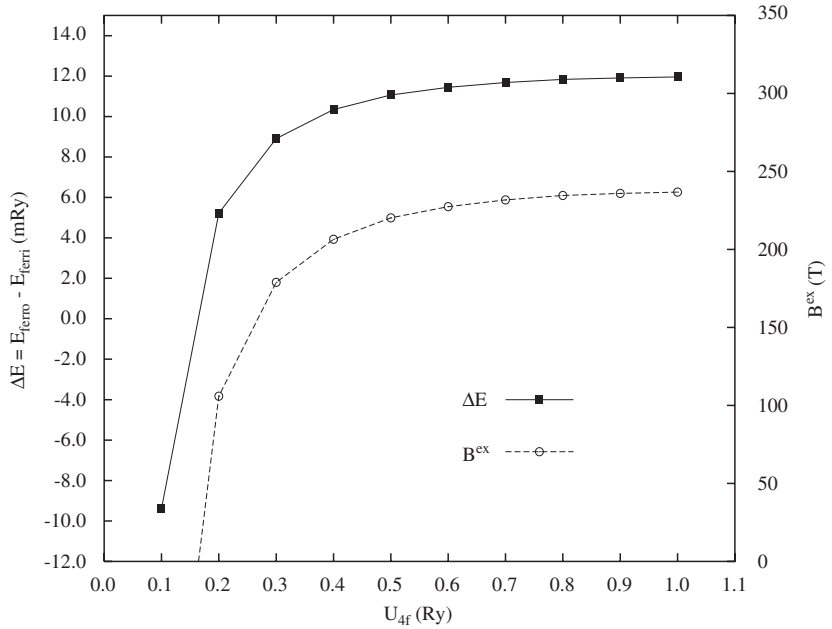

Fig. 4. Differences between total energies of ferromagnetic and ferrimagnetic configurations in $TbCo_5$ obtained in the LSDA + U − SOC calculation and corresponding exchange fields for different values of the U_{4f} parameter.

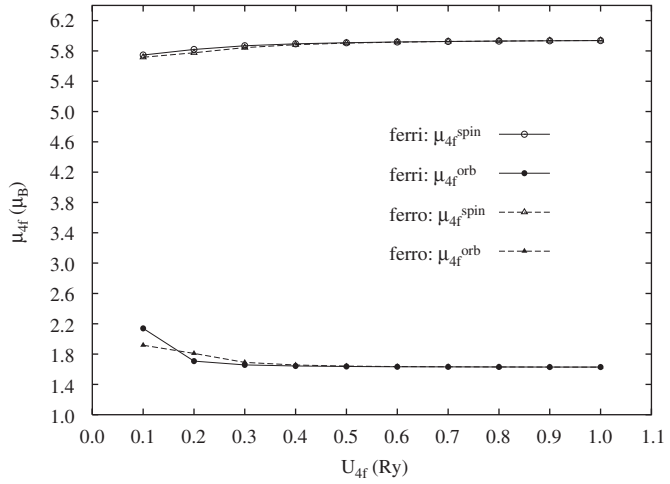

Fig. 5. Spin and orbital magnetic moments of 4f electrons in $TbCo_5$ for ferromagnetic and ferrimagnetic configurations obtained in the LSDA + U − SOC calculation for different values of the U_{4f} parameter.

4. Conclusion

LSDA and LSDA + U calculations for $DyCo_5$ and $TbCo_5$ were performed. In the case of magnetic moments LSDA − SOC calculations give results which are in good agreement with experimental values in the case of $DyCo_5$ and in somewhat worse agreement with the experimental values obtained for $TbCo_5$. On the other hand, they completely fail to reproduce relative stabilities of ferromagnetic and ferrimagnetic configurations of 4f and 3d spin sublattices giving the wrong result that ferromagnetic configuration is more stable in both $DyCo_5$ and $TbCo_5$.

Consequently, LSDA + U method was applied. While keeping agreement between calculated and experimental values of magnetic moments obtained in LSDA − SOC calculations, LSDA + U − SOC results in the case of relative stabilities of ferromagnetic and ferrimagnetic configurations are considerably improved over LSDA − SOC ones. Bearing in mind that the experimentally determined values of the effective exchange fields should be taken with care, one could say that the present results obtained in LSDA + U − SOC calculations are in reasonable agreement with the experimentally obtained values for both $DyCo_5$ and $TbCo_5$.

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