Calculation of magnetic anisotropy energy in $SmCo_5$

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$SmCo_5$ is an important hard magnetic material, due to its large magnetic anisotropy energy (MAE). We have studied the magnetic properties of $SmCo_5$ using density functional theory (DFT) calculations where the Sm *f* bands, which are difficult to include in DFT calculations, have been treated beyond the local density approximation (LDA), within the LDA + *U* formalism. The large MAE comes mostly from the Sm *f*-shell anisotropy, stemming from an interplay between the crystal field and the spin-orbit coupling. We found that both are of similar strengths, unlike some other Sm compounds, leading to a partial quenching of the orbital moment (*f* states cannot be described as either pure lattice harmonics or pure complex harmonics), an optimal situation for enhanced MAE. A smaller portion of the MAE can be associated with the Co-*d* band anisotropy, related to the peak in the density of states at the Fermi energy. Our result for the MAE of $SmCo_5$, 21.6 meV/f.u., agrees reasonably with the experimental value of 13-16 meV/f.u., and the calculated magnetic moment (including the orbital component) of $9.9\mu_B$ agrees with the experimental value of $8.9\mu_B$.

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The permanent magnet intermetallic compound $SmCo_5$ has been studied extensively experimentally[1,2] and theoretically.[3–11] The interest in these materials is fueled by their large magnetic anisotropy energy (MAE), which is defined as the difference between the ground-state energies due to rotation of the magnetic field (magnetization direction). It is generally understood that the main source of the large MAE in $SmCo_5$ and other Sm-Co magnets is large magnetic single-site anisotropy of the Sm *f* shell.[9,12–14] In simple terms, this means the strong spin-orbit coupling tries to align the Sm *f* shell with the magnetic field, causing the *f* shell to rotate with the field. Sm atoms in a lattice interact with the crystal field, and the energy of this interaction depends on the orientation of the Sm *f* shell in the lattice. This is the leading contribution to the MAE. Note that if the crystal field is too small, the *f* shell rotates freely with the magnetic field, producing no MAE, while if the spin-orbit is too small, the orbital moment is quenched and again no MAE appears. We will see below that in $SmCo_5$ both interactions are comparable, producing a large MAE.

This basic understanding has existed for a long time, and has been the basis of several model calculations, where atomic calculations for Sm have been combined with the crystal field parameters derived from first principles calculations.[15] However, first principles calculations which could provide a quantitative analysis of different components of the MAE in $SmCo_5$ are still missing, to the best of our knowledge. In this paper we report such calculations, using an all-electron, full-potential, relativistic linearized augmented plane wave (FLAPW) method with an extension beyond the local density approximation (LDA), LDA+*U*, which accounts for Coulomb correlations in the *f* shell.

Our analysis is organized as follows. We start by looking at the ''Co part'' of the MAE, the part *not* related to the Sm single-site anisotropy. We do this by investigating YCo_5 which forms in the same crystal structure as $SmCo_5$ but contains no *f* electrons. We calculate the MAE for YCo_5 and for the hypothetical Co_5 compound (corresponding to YCo_5 with Y removed) to elucidate the role of Y, and analyze the electronic origin of the MAE using the force theorem. We then move to $SmCo_5$, where we compute the MAE as a function of the Coulomb repulsion parameter *U*. These results demonstrate the nature of the Sm *f* states which shows strong competition between the crystal field and the spin-orbit interactions.

For our electronic structure calculations we have used the self-consistent FLAPW method.[16] The local density approximation of Perdew and Wang[17] and the generalized gradient approximation (GGA) of Perdew, Burke, and Ernzerhof[18] were used for the correlation and exchange potentials. Calculations were performed using the WIEN package.[19] Local orbital extensions[20] were included in order to accurately treat the upper core states and to relax any residual linearization errors. A well converged basis consisting of approximately 300 LAPW basis functions in addition to the local orbitals was used with the Y and Sm sphere radii set to 2.115 a.u. and the Co sphere radii to 2.015 a.u. The results varied only within a few percent for reasonable choices of atomic radii (2.0–3.0 a.u.). In our previous study[11] on YCo_5 we established that the plane-wave cutoff parameters $RK_{\max}$ and $G_{\max}$ of 9 and 14, respectively, are suffucient for MAE calculations, so the same parameters were used in this work. Spin-orbit (SO) interaction was incorporated using a second variational procedure,[21] where all states below the cutoff energy 1.5 Ry were included. The most recent version of the WIEN code, WIEN2K, includes the so-called $p_{1/2}$ extension,[16,22] which accounts for the finite character of the wave function at the nucleus for the $p_{1/2}$ state that cannot be adequately represented as a linear combination of a finite number of solutions of the radial Schrödinger equation with $l=1$. Self-consistent calculations were performed with 80 **k** points in the irreducible Brillouin zone, and increasing to 180 **k** points changed the MAE by only ~0.1 meV/f.u.

The crystal structure of $SmCo_5$ and YCo_5 is that of $CaCu_5$ ($P6/mmm$, No. 191). The experimental values of *a* and *c*/*a* used in the calculation are 9.452 a.u. and 0.792 for $SmCo_5$

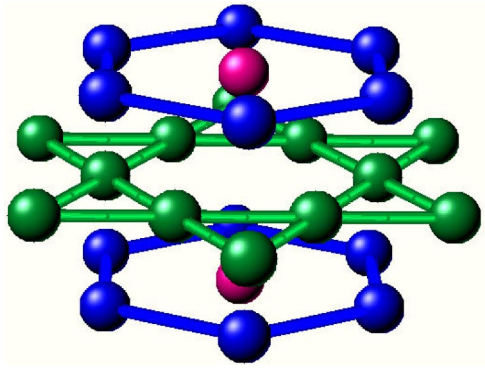

FIG. 1. Crystal structure of $SmCo_5$. Shown are two layers of hexagonal Co(2c) with a *kagomé* lattice of Co($3g$) atoms lying between. The Sm atoms lie in the middle of the hexagons in the Co($2c$) layers.

and 9.313 a.u. and 0.806 for YCo_5. Optimized values of the c/a ratio and volume were the same as the experimental values to within ~2%. The Co sites are separated into two sets of inequivalent atoms, Co(2c) having two-fold multiplicity and Co($3g$) having three-fold multiplicity (Fig. 1). Including spin-orbit coupling into the calculation lowers the symmetry when the field lies along the plane (to $Pmmm$, No. 47), separating the 3 atoms corresponding to Co($3g$) into two inequivalent sites which have multiplicities of 2 and 1, respectively. To eliminate a systematic error[11] we performed the calculation for both magnetization directions using the same, highest *common* symmetry group ($Pmmm$, in this case).[23]

In our previous work,[11] we found the MAE of YCo_5 to be 0.32 meV/Co, which is 0.44 meV/Co lower than the experimental number of 0.76 meV/Co.[24] What is important for our discussion is that both experimental and calculated numbers are substantially larger than the MAE of the hcp Co (0.065 meV/Co).[25] The question arises whether this enhancement is due to a different mutual arrangement of the Co ions, a charge transfer between Y and Co, or the MAE associated with the Y ions. To answer this question, we performed calculations for a hypothetical Co_5 compound defined as YCo_5 with Y removed with the positions of all cobalt atoms unchanged. We found MAE of 0.28 meV/Co (compared to 0.32 meV/Co in YCo_5), proving that the reason for the relatively large MAE in YCo_5 is a favorable arrangement of the Co atoms.

We can actually pinpoint the microscopic origin of this large MAE. The MAE depends on subtle differences in the electronic structure under rotations of the external magnetic field. While our actual calculations used two self-consistent energies for the two field directions, it is convenient to analyze the results using the force theorem.[26] According to this theorem, one can start from the same charge density (which is converged without spin orbit), and then apply the spin orbit within one iteration for the two different magnetization directions $\mathbf{e}_1$ and $\mathbf{e}_2$. One then sums the eigenvalues for the occupied states in both cases, the difference of these sums corresponding to the MAE, good to second order in the change in the electron charge density:

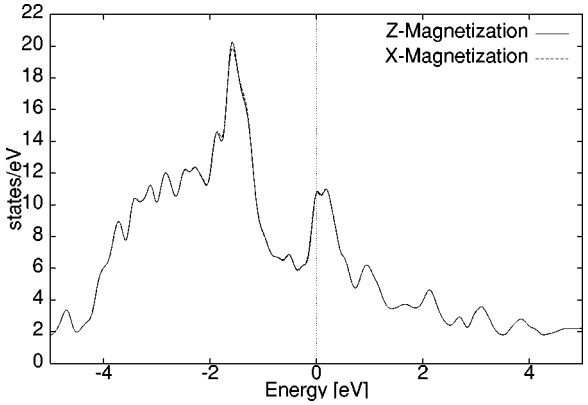

FIG. 2. Calculated density of states (DOS) using the force theorem for magnetization along the Z axis and along the X axis in YCo_5. The difference is only noticeable around the peak near -1.5 eV.

$$\mathrm{MAE} \approx \Sigma_i^{\mathrm{occ}} \epsilon_i(\mathbf{e}_1) - \Sigma_i^{\mathrm{occ}} \epsilon_i(\mathbf{e}_2). \quad (1)$$

We used the force theorem to produce the DOS plots for YCo_5 shown in Fig. 2. The two plots are practically indistinguishable on this scale, except near -1.5 eV, which shows a slight variation near the top of the peak. Also notice the smaller Co d-band minority peak which crosses the Fermi level on its left side. We now plot the corresponding difference in the one-electron energy [Eq. (1)] against the number of valence electrons (Fig. 3). Below full occupation (48 electrons), there are positive and negative variations to the running value of the MAE which generally average to zero. At full occupation, 48 valence electrons, the MAE shows a small positive contribution (~1.5 meV/f.u.), in agreement with the results found by taking the energy difference of two self-consistent calculations. This corresponds to the differences under rotation of the magnetization direction in the Co d-band minority peak which is cut by the Fermi level (Fig. 2). Dopant atoms change the DOS and, hence, the calculated

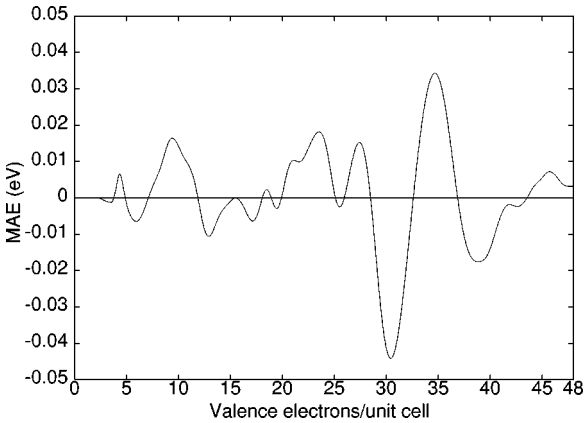

FIG. 3. Using the calculated density of states (DOS) of YCo_5 (Fig. 2) for the two magnetization directions, the product of the energy and the difference in the DOS are plotted as a function of valence electrons/unit cell. At full occupation, 48 valence electrons, a small (~1.5 meV/f.u.) positive contribution to the MAE is related to the Co d peak near the Fermi energy.

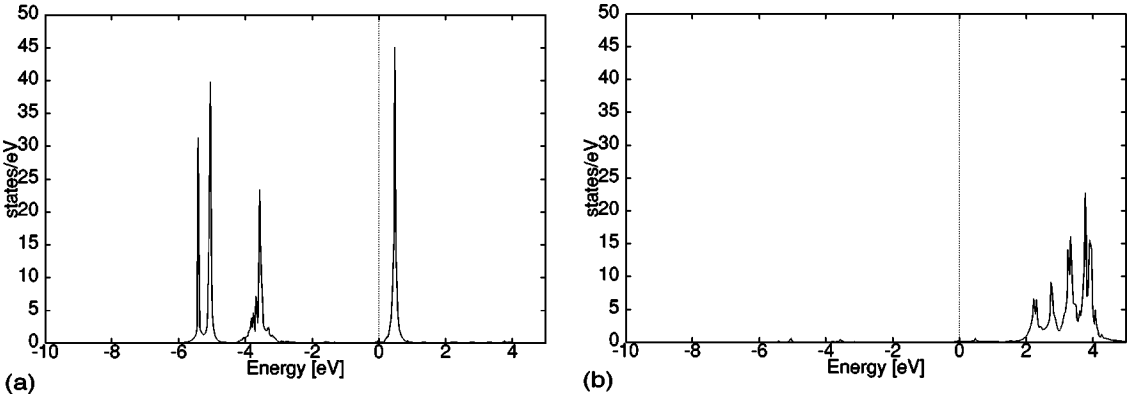

FIG. 4. Calculated (a) spin up and (b) spin down density of states (DOS) for the Sm *f* orbitals with GGA and LDA+*U* (SIC-LDA, GGA) in $SmCo_5$ including spin orbit. The lowest spin-up peak corresponds to $m=+3$, the second to a combination of $m=+2$, $+1$. The highest valence band peak is composed of $m=0$, $+2$, -2 and $m=+1$, -1, $+3$, -3. The conduction band peak is composed of $m=-2$ and $m=-3$, -1.

MAE enough so that one cannot blindly trust the results of a rigid shift of the Fermi energy, but this plot indicates that small amounts of Fe doping may initially increase the MAE before it decreases and changes sign, as has been seen experimentally[27] and theoretically.[28]

Several difficulties are encountered going from YCo_5 to $SmCo_5$. Computationally, the main difference between the two compounds is that Sm includes an open *f* shell that cannot be described in the framework of the conventional LDA theory. Indeed, uncorrected DFT (whether LDA or GGA) calculations incorrectly pin all of the *f* orbitals at the Fermi energy (E_F) in $SmCo_5$ and other systems containing unfilled *f* orbitals. In order to circumvent this problem, the previous electronic structure calculations[9,12–14] for $SmCo_5$ did not treat the *f* orbitals as valence electrons but as unhybridized core electrons. However, the width of the *f* bands is ~ 1 eV, much too large for this approximation. Since the single-site MAE of Sm is due to the asphericity of the *f* shells,[29] in other words, to the interaction of this shell with the crystal field, understanding the exact shape and occupation of the *f* orbitals is crucial. Therefore we applied a Hubbard *U* correction to the *f* orbitals which naturally splits the *f* bands into lower and upper Hubbard bands with nearly integer occupancies.

While the LDA+*U* method seems the proper procedure for handling the localized Sm *f* orbitals, the question remains which form of the LDA+*U* should be used. There are several prescriptions, differing mainly in the way the double counted energy components are subtracted off.[30] The two most common are referred to in the WIEN code[19] as SIC and AMF [the former name is misleading from the physical point of view, so Mazin *et al.*[30] suggested an acronym FLL (fully localized limit)]. As discussed by Mazin *et al.*,[30] the FLL prescription is more appropriate for well localized orbitals, such as *f* electrons in $SmCo_5$, so it was used in our calculations.[31]

The LDA+*U* method includes two parameters *U* and *J* that have no rigorous definition in a solid. In an atom, one way to define *U* and *J* is *via* the derivatives of the energy of the atomic level with respect to their occupancies[32]

$$U_f=\frac{\partial \varepsilon_{f\uparrow}}{\partial n_{f\downarrow}}, \tag{2}$$

$$J_f=\frac{\partial(\varepsilon_{f\uparrow}-\varepsilon_{f\downarrow})}{\partial(n_{f\uparrow}-n_{f\downarrow})}. \tag{3}$$

We have applied these formulas to a quasiatom residing in a potential well defined by the DFT crystal potential, which is especially easy within the LMTO technique (the details of this procedure will be reported elsewhere). This gives for $SmCo_5$ $U_f \approx 5.2$ eV and $J_f \approx 0.75$ eV, which, as the subscripts explain, will act on the Sm *f* orbitals in the DFT calculation. Note that this approach overscreens the Coulomb interaction by forcing all screening charge into one atomic sphere, therefore such calculated U_f may be slightly underestimated.

The effect of including LDA+*U* in the calculation can be seen by looking at the spin-up [Fig. 4(a)] and spin-down [Fig. 4(b)] contribution of the Sm *f* orbitals to the density of states (DOS). With just DFT-GGA, the Sm *f* orbitals form a narrow band pinned at E_F (not shown). The addition of *U* and *J* shifts the unoccupied spin-minority *f* band up by approximately $(U-J)/2$ and splits the spin minority *f* band into the lower and the upper Hubbard bands, separated roughly by $U-J$. Furthermore, LDA+*U* enhances the Hund's second rule coupling[33] and tries to unquench the orbital moment by making the orbital moment projection *m* a good quantum number. Without spin orbit there is no Hund's second rule coupling, and orbital moment is quenched, that is, each *f* band includes the same amount of $m=3$ character, as of the $m=-3$ character, etc. Spin orbit in combination with Hubbard *U* favors pure *m* states. This scenario holds, for instance for such Sm compounds as $SmAl_2$ and SmZn, where the individual spin and orbital moments are known experimentally,[34] and the orbital moment is between -4.5 and $-5\mu_B$, roughly as expected from Hund's second rule, in agreement with LDA+*U* calculation with a sufficiently large *U*.[35] In $SmCo_5$, however, the crystal field is sufficiently strong to prevent total unquenching, and as a result the

TABLE I. f-occupation matrix for $SmCo_5$ ($U=5$ eV, magnetization direction is 001). The first column lists the eigenvalues, the other the corresponding eigenvectors in terms of spherical harmonics with given m.

e value	3	2	1	0	−1	−2	−3
0.96	0.81	0	0.05	0	0	0	0.14
0.95	0	1.	0	0	0	0	0
0.95	0.12	0	0.79	0	0	0	0.09
0.95	0.01	0	0.04	0	0.77	0	0.17
0.94	0	0	0	0.66	0	0.35	0
0.04	0.06	0	0.12	0	0.22	0	0.61
0.02	0	0	0	0.35	0	0.66	0

f-occupation matrix is not diagonal in the m representation (Table I), and the orbital moment is reduced to $-2.8\mu_B$ (within the calculation).

This can be also illustrated by the DOS for $SmCo_5$, and comparing with the f-occupation matrix (Table I). The lowest peak in the DOS [Fig. 4(a)] is clearly dominated by $m=3$, corresponding to the first state in the table. The next peak includes two states: a pure $m=2$ state and a nearly pure $m=1$ state. The third peak is also composed of two closely lying peaks, one of character $m=0, +2, -2$, and a second of character $m=+1, -1, +3, -3$. The conduction band peak also contains two closely lying peaks, one with mostly $m=0$ and an admixture of $m=-2$, and the second of $m=-1$ with an admixture of $m=-3$. The two empty states are very close in energy and correspond, one to $m=-2$ with an admixture of $m=0$, and the other to $m=-3$ with an admixture of $m=-1$. Note that if we apply LDA+U to scalar relativistic calculations, the charge state of the f shell remains the same, but now the bands are formed by the real lattice harmonics, with the two E_{2u} states forming the unoccupied upper Hubbard bands and, correspondingly, the E_{1u}, B_{1u}, B_{2u}, and A_{2u} states forming the occupied bands. The distance between the lowest (E_{1u}) and the highest (A_{2u}) occupied states gives us a gauge of the crystal field strength: ~ 0.1 Ry (Fig. 5).

A technical problem with LDA+U calculations is that, unlike conventional DFT calculations, localized orbitals such as f states can converge to a number of metastable configurations.[35] There is no guarantee that the configuration shown in Fig. 5(a) is the true ground state. However, we used different starting configurations but were never able reach a self-consistent configuration with pure m states. The calculated magnetic moment, which depends crucially on the orbital configuration, agrees with experiment. The calculated spin moment is $12.2\mu_B$, and the Sm orbital moment is $-2.8\mu_B$, while the Co orbital moments are about $0.1\mu_B$ each, leading to the total moment of $9.9\mu_B$, to be compared with the experimental value of $8.9\mu_B$.[36,37] As mentioned, fully unquenched orbital moment would be between -4.5 and $-5\mu_B$,[35] thus reducing the total moment to 7.2–$7.7\mu_B$ and increasing the disagreement with the experiment by a factor of 2–3.

The calculated MAE of $SmCo_5$ comes from two sources. One is the MAE of the Co sublattice, analogous to that in YCo_5. The other is the single-site anisotropy of the Sm f shell. The strong spin-orbit effect on the Sm f shell is necessary due to the small MAE resulting when the spin-orbit effects are weak compared to crystal field effects, as in YCo_5. If there were no crystal field effects in $SmCo_5$, the f states would be pure m states, so the direction of the orbital quantization axis would always coincide with the magnetic field, by virtue of the spin-orbit interaction. Assuming a crystal field interaction much weaker than the spin orbit, we observe that the energy of the f shell with its orbital moment aligned along 001 or along 100 comes from the dependence of the crystal field energy on the orientation of the f shell. The stronger the crystal field, the larger the MAE. The fact that the calculated f bands in $SmCo_5$ are not pure m states indicates that the crystal field in this compound is strong, comparable with the spin-orbit interaction. In fact, our preliminary calculations for a sister compound Sm_2Co_{17} (Ref. 38) indicate that the f states there are much closer to pure m-states than those in $SmCo_5$, that is, that the crystal field there is weaker, in agreement with the reduced MAE per Sm in Sm_2Co_{17}.[39]

As discussed above, the single site MAE is defined by a delicate balance between the crystal field, the spin-orbit interaction, and the Hubbard repulsion. Since the LDA+U method implements the principal aspects of the latter, we do

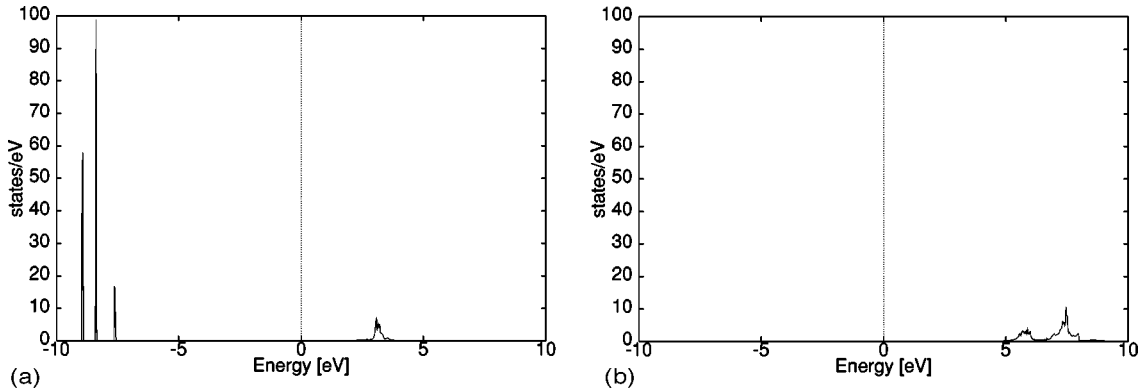

FIG. 5. Calculated (a) spin up and (b) spin down density of states (DOS) for the Sm f orbitals with GGA and LDA+U (SIC-LDA, GGA) in $SmCo_5$ without spin orbit. The occupied bands consist of, correspondingly, the E_{1u}, the B_{1u} and B_{2u}, and the A_{2u} states while the conduction bands consist of the two E_{2u} states.

expect to have a reasonable description of MAE within this method. However, the accuracy of such calculations is necessarily limited. A good understanding of this can be gained by comparing the MAE calculated within two different versions of the WIEN code. Using the WIEN2K package,[19] in WIEN2K.01 the Hubbard correction is applied *before* solving the second-variational spin-orbit equations, while in the WIEN2K.02 version it is done *simultaneously*. We obtain an MAE of 12.6 meV/f.u. using the former version, and 21.6 using the latter. Both compare favorably with the experimental number of 13–16 meV/f.u.[40–44] emphasizing, however, the sensitivity of the result to the treatment of the correlation effects.

It is worth noting that *without* the LDA+U correction, in DFT-GGA, the calculated MAE was -11.1 meV/f.u. (note the wrong sign: the easy axis in the plane rather than axial), with the spin moment of $12.9\mu_B$ and an orbital moment of $-1.5\mu_B$. Also, calculations from the Dresden group,[9] otherwise similar to ours [we agree on the MAE in YCo_5 (Ref. 11)], but with f electrons treated as an ''open core,'' produced MAE of only ~ 7 meV/f.u.; presumably, such ''atomic'' description of the f electrons underestimate the crystal field effects.

Since the parameter U is not very well defined, it is always instructive to check the dependence of the results on U, particularly since the above mentioned quasiatomic procedure tends to underestimate U. Indeed, we found that if U is reduced to ≈ 4 eV the upper Hubbard bands are too close to the Fermi level and the MAE is substantially overestimated (~ 40 meV/f.u.). On the other hand, when U was increased to 6.0 eV the MAE, as expected, changed little. It is also worth noting that using LDA (Ref. 17) instead of GGA (Ref. 18) improves the total magnetic moment ($8.6\mu_B$, with the experimental value being $8.9\mu_B$), but worsens the MAE (26.0 meV/f.u., to be compared with 21.6 meV/f.u. in GGA for the same value of U, or with the experiment, 13–16 meV/f.u.). Interestingly, both in YCo_5 and $SmCo_5$ the GGA results are in better agreement with the experiment for the MAE than LDA, although in the former compound calculations underestimate the MAE, and in the latter overestimate.

To conclude, we have performed first principle calculations of the magnetic properties of $SmCo_5$ using a highly accurate LAPW code including the LDA+U formalism. We obtained much better agreement with experiment than previous methods which treated the f orbitals as open core rather than valence states. Comparing the calculation for $SmCo_5$ with YCo_5 and with the hypothetical $\square Co_5$ we conclude that the MAE of the Co sublattice comes from a favorable arrangement of the Co atoms, which leads to a peak in the spin-minority DOS at the Fermi level. The MAE of the Sm f shell comes from the interplay between the spin-orbit coupling, which tends to align the f shell according to the magnetization direction and the crystal field, that aligns it according to the crystal lattice. In $SmCo_5$ both interactions appear to be of approximately the same strength, which makes $SmCo_5$ such an exceptionally hard magnet even compared with other Sm-Co compounds.

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[1] H.R. Kirchmayr and C.A. Poldy, J. Magn. Magn. Mater. **8**, 1 (1978).
[2] R.J. Radwanski and J.J.M. Franse, Int. J. Mod. Phys. B **7**, 782 (1993).
[3] S.K. Malik, F.J. Arlinghaus, and W.E. Wallace, Phys. Rev. B **16**, 1242 (1977).
[4] L. Nordstrom, M.S.S. Brooks, and B. Johansson, J. Phys.: Condens. Matter **4**, 3261 (1992).
[5] J. Trygg, L. Nordstrom, and B. Johansson, *Physics of Transition Metals*, edited by P.M. Oppeneer and J. Kubler (World Scientific, Singapore, 1993), p. 745.
[6] M. Yamaguchi and S. Asano, J. Appl. Phys. **79**, 5952 (1996).
[7] G.H.O. Daalderop, P.J. Kelly, and M.F.H. Schuurmans, Phys. Rev. B **53**, 14 415 (1996).
[8] M. Yamaguchi and S. Asano, J. Magn. Magn. Mater. **168**, 161 (1997).
[9] L. Steinbeck, M. Richter, and H. Eschrig, J. Magn. Magn. Mater. **226-230**, 1011 (2001).
[10] L. Steinbeck, M. Richter, and H. Eschrig, Phys. Rev. B **63**, 184431 (2001).
[11] P. Larson and I.I. Mazin, J. Appl. Phys. **93**, 6888 (2003).
[12] M. Richter, P.M. Oppeneer, H. Eschrig, and B. Johansson, Phys. Rev. B **45**, 13 919 (1992).
[13] P. Novak and J. Kuriplach, IEEE Trans. Magn. **MAG-30**, 1036 (1994).
[14] K. Hummler and M. Fähnle, Phys. Rev. B **53**, 3272 (1996).
[15] M. Fähnle, K. Hummler, M. Liebs, and T. Beuerle, Appl. Phys. A: Mater. Sci. Process. **57**, 67 (1993).
[16] D.J. Singh, *Planewaves, Pseudopotentials, and the LAPW Method* (Kluwer Academic, Boston, 1994).
[17] J.P. Perdew and Y. Wang, Phys. Rev. B **45**, 13 244 (1996).
[18] J.P. Perdew, K. Burke, and M. Ernzerhof, Phys. Rev. Lett. **77**, 3865 (1996).
[19] P. Blaha, K. Schwarz, G.K.H. Madsen, K. Kvasnicka, and J. Luitz, WIEN2K, An Augmented Plane Wave + Local Orbitals Program for Calculating Crystal Properties, Karlheinz Schwarz, Technische Universitat Wien, Austria, 2001.
[20] D.J. Singh, Phys. Rev. B **43**, 6388 (1991).
[21] D.D. Koelling and B. Harmon, J. Phys. C **10**, 3107 (1977); P. Novak (unpublished).
[22] J. Kunes, P. Novak, R. Schmid, P. Blaha, and K. Schwarz, Phys. Rev. B **64**, 153102 (2001).
[23] R.W.G. Wyckoff, *Crystal Structures* (Krieger, Melbourne, FL, 1986), Vol. 2.
[24] K.H.J. Buschow, A.M. van Diepen, and H.W. De Wijn, Solid State Commun. **15**, 903 (1974); S.G. Sankar, V.U.S. Rao, E. Segal, W.E. Wallace, W.G.D. Frederick, and H.J. Garrett, Phys. Rev. B **11**, 435 (1975): R.J. Radwanski, J. Magn. Magn. Mater. **62**, 239 (1984).
[25] D.M. Paige, B. Szpunar, and B.K. Tanner, J. Magn. Magn. Mater. **44**, 239 (1984).

[26] M. Weinert, R.E. Watson, and J.W. Davenport, Phys. Rev. B **32**, 2115 (1985), and references therein.
[27] F. Rothwarf, H.A. Leupold, J. Greedan, W.E. Wallace, and Dilip K. Das, Int. J. Magn. **4**, 267 (1973).
[28] P. Larson, I.I. Mazin, and D. A. Papacontantopoulos (unpublished).
[29] S. Buck and M. Fähnle, J. Magn. Magn. Mater. **166**, 297 (1997).
[30] A. G. Petukhov, I. I. Mazin, L. Chioncel, and A. I. Lichtenstein, Phys. Rev. B **67**, 153106 (2003).
[31] As a test, we also performed calculations using LDA+U-AMF; the results for the orbital moment were considerably worse ($-1.5\mu_B$ compared to $-2.8\mu_B$) and the calculated MAE was heavily overestimated.
[32] V. I. Anisimov, O. Gunnarsson, Phys. Rev. B **43**, 7570 (1991).
[33] I. V. Solovyev, A. I. Liechtenstein, and K. Terakura, Phys. Rev. Lett. **80**, 5758 (1998).
[34] H. Adachi, H. Ino, and H. Miwa, Phys. Rev. B **59**, 11 445 (1999).
[35] H. Gotsis and I.I. Mazin (unpublished).
[36] T.-S. Zhao, H.-M. Jin, G.-H. Gua, X.-F. Han, and H. Chen, Phys. Rev. B **43**, 8593 (1991).
[37] J. Deportes, D. Givord, J. Schweitzer, and F. Tasset, IEEE Trans. Magn. **MAG-12**, 1000 (1976).
[38] P. Larson, I.I. Mazin, and D.A. Papaconstantopoulos (unpublished).
[39] Zhi-gang Sun, Shao-ying Zhang, Hong-wei Zhang, and Bao-gen Shen, J. Phys.: Condens. Matter **13**, 2001 (2001).
[40] B. Szpunar, Acta Phys. Pol. A **60**, 791 (1981).
[41] T.-S. Zhao, H.-M. Jin, R. Grossinger, X.-C. Kou, and H.R. Kirchmayr, J. Appl. Phys. **70**, 6134 (1991).
[42] D.-L. Leslie-Pelecky and R.L. Schalek, Phys. Rev. B **59**, 457 (1999).
[43] C.H. Chen, M.S. Walmer, M.H. Walmer, W. Gong, and B.-M. Ma, J. Appl. Phys. **85**, 5669 (1999).
[44] I.A. Al-Omari, R. Skomski, R.A. Thomas, D. Leslie-Pelecky, and D.J. Sellmyer, IEEE Trans. Magn. **MAG-37**, 2534 (2001).