

# Electron correlation beyond the local density approximation: self-interaction correction in gadolinium

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## Abstract

We report on detailed first-principles calculations which focus on the magnetic and structural properties of the (0001) surface of gadolinium. The electronic correlation within the localized 4f states is treated within the self-interaction correction (SIC), thus going beyond the local spin-density approximation. The ferromagnetic ground state is predicted correctly if the SIC is applied; the effect of surface relaxations on Heisenberg exchange parameters and on the Curie temperature are addressed by Monte Carlo calculations. The SIC also has a profound effect on the dispersion of the d surface states, due to hybridization of the 4f states with the 5d valence states. The best agreement with photoemission experiments is obtained within the transition state approximation, which takes into account the orbital relaxation. The Rashba spin-orbit coupling in the d surface states is fully captured by our relativistic multiple scattering approach.

(Some figures in this article are in colour only in the electronic version)

## 1. Introduction

Density functional theory (DFT) is the most widely used method for electronic structure calculations. Despite the success of the local spin-density approximation (LSD) to DFT, there are serious shortcomings: the properties of 3d metal oxides are described badly, the band gaps of semiconductors are underestimated, in *f*-systems the density of states is in strong disagreement with experiment, in some cases the LSD gives qualitatively wrong results for Mott–Hubbard insulators, to name a few. Some of the discrepancies are due to the restriction of DFT to describe the ground state properties, but some failures can be attributed to the partial cancellation of the spurious self-interaction of an electron with itself, which is present in the Kohn–Sham (KS) effective potential. This kind of systematic error can be corrected by removing the self-interaction from the total energy functional [1]. Application of the self-interaction correction (SIC) to transition metal oxides (TMOs) [2] and wide-gap semiconductors [3], for example, shows promising results. Another method to study TMOs and semiconductors is LDA + *U* [4], which adds an on-site Coulomb interaction to the LSDA functional [5]. LDA + *U* was used to study other systems with localized electrons such as

gadolinium [6]. However, in this method the on-site Coulomb interaction *U* is an adjustable parameter and is chosen to optimize agreement with experiment.

Gd is a prototype for investigation of the electron correlation. Correct treatment of the strongly localized 4f states changes the ground state magnetic ordering from antiferromagnetic to ferromagnetic. Other properties of Gd also improve when the electron correlation is taken into account. The surface states of Gd(0001), which are mostly  $d_{z^2}$  majority states, hybridize with the localized 4f majority states. As we will see later the SIC of the localized states has a significant effect on the surface states and is essential. So far, to our knowledge, all studies on Gd bulk and Gd(0001) have been done by means of LDA + *U* or a 4f-core model [6–8]. In this paper we report the results of an *ab initio* investigation of the SIC in the bulk and on the (0001) surface of Gd.

Applying the SIC to calculate the ground state properties of Gd, e.g. magnetic ordering and local magnetic moments, is very successful. For excited states, it appears that the binding energies of the SI-corrected localized levels are significantly too large when compared to those determined from spectroscopical data, i.e. from photoemission intensities. This ‘overcorrection’ of the SIC is attributed to the orbital

relaxation. SIC calculations are ground state calculations and one cannot expect accurate results for excited states. In our calculations we used the transition state approximation (TSA), that is an average of two ground state potentials (LSD and SIC potentials), to obtain a better agreement with experiments that are associated with the excited states.

The paper is organized as follows: in section 2 local SIC and TSA are explained in detail. Section 3 is devoted to the calculated magnetic properties of Gd bulk and Gd(0001). The surface states and the effect of the Rashba splitting on the surface states are also studied. The paper ends with a summary in section 4.

## 2. Computational aspects

First-principles calculations were performed within the framework of multiple scattering theory, using scalar-relativistic and relativistic Korringa–Kohn–Rostoker (KKR) computer codes. The self-consistent KKR scheme allows us to treat semi-infinite systems. Consequently, the entire system comprises the Gd bulk, the surface region (six Gd layers and four vacuum layers), and the vacuum region. The image potential barrier is mimicked by so-called empty spheres.

Spin–orbit coupling is included by solving the Dirac equation in our relativistic layer KKR code. The layer- and wavevector-resolved spectral density

$$N_{al}(E, \vec{k}_{\parallel}) = -\frac{1}{\pi} \text{Im Tr } G_{al,al}^+(E, \vec{k}_{\parallel}) \quad (1)$$

provides detailed information on the electronic structure. Here,  $G^+(E, \vec{k}_{\parallel})$  is the side limit of the site-diagonal Green function at energy  $E$  and in-plane wavevector  $\vec{k}_{\parallel}$ . The trace is over the muffin-tin sphere of site  $a$  in layer  $l$ . The spectral density can be decomposed with respect to spin and angular momentum, to give access to the relevant properties.

All calculations are performed with the experimental structural parameters of  $a = 6.866$  bohr and  $c/a = 1.59$  [9]. The interlayer distance at the surface is reduced with respect to the bulk, as has been determined experimentally [10]. A surface relaxation of 4% contraction is taken into account.

### 2.1. Self-interaction correction

The self-interaction correction, which is implemented according to [11] in terms of local orbital- and spin-dependent potentials, is applied to the electronic states of Gd. Based on this method, the degree of localization is determined by the energy derivative of the single-site phase shift, that is the Wigner delay time [12]. For a localized state, characterized by the main quantum number  $n$ , angular momentum  $L = (l, m)$ , and spin  $\sigma$ , the charge density is

$$n_{L\sigma}^{(n)\text{SIC}}(\vec{r}) = -\frac{1}{\pi} \int_{E_1}^{E_2} \text{Im } G_{L\sigma, L\sigma}(\vec{r}, \vec{r}; \epsilon) d\epsilon, \quad (2)$$

where  $E_1$  and  $E_2$  lie slightly below and above the energy of the state ( $nL\sigma$ ). This charge density is used to construct the effective self-interaction potential,

$$V_{\text{eff}, L\sigma}^{(n)\text{LSD-SIC}}(\vec{r}) = V_{\text{eff}, \sigma}^{\text{LSD}}(\vec{r}) + V^{\text{SIC}}(\vec{r}), \quad (3)$$

where

$$V^{\text{SIC}}(\vec{r}) = -V_{\text{H}}[n_{L\sigma}^{(n)\text{SIC}}](\vec{r}) - V_{\text{xc}}^{\text{LSD}}[n_{L\sigma}^{(n)\text{SIC}}, 0](\vec{r}). \quad (4)$$

Hence, the Hartree (H) and the exchange–correlation (xc) potential of the localized state are explicitly subtracted from the effective potential. Note that this correction vanishes for delocalized states.

For each SI-corrected channel ( $n\tilde{L}\tilde{\sigma}$ ), indicated by a tilde, the ( $\tilde{L}\tilde{\sigma}$ ) element of the single-site scattering matrix  $t^{(n)}$ , calculated within the local spin-density approximation, is replaced by that obtained from the SI-corrected potential,

$$\tilde{t}_{L\sigma}^{(n)} = t_{L\sigma}^{(n)}(1 - \delta_{L\sigma, \tilde{L}\tilde{\sigma}}) + t_{\tilde{L}\tilde{\sigma}}^{(n)\text{LSD-SIC}} \delta_{L\sigma, \tilde{L}\tilde{\sigma}}. \quad (5)$$

The resulting scattering matrix  $\tilde{t}^{(n)}$  is then used to calculate the SI-corrected scattering-path operator which enters the KKR Green function [13]. The self-interaction is thus corrected self-consistently, without any adjustable parameter. Further, the set of SI-corrected channels is determined by total energy minimization. For Gd it turns out that all 4f majority states have to be corrected.

At present, there is no relativistic version of the SIC. To investigate the effect of the SIC on effects which are mediated by the spin–orbit coupling—in particular the Rashba effect in the majority surface state—we thus proceed as follows. We employ a scaling transformation of the (radial) Dirac equation which allows us to switch between the fully relativistic (including spin–orbit coupling) and the scalar-relativistic description (excluding spin–orbit coupling) [14]. This transformation is applied only to the SI-corrected 4f majority levels, thus keeping the relativistic description for all other electronic states, in particular for the d surface states. By this means we rely on the non-relativistic SIC but in a relativistic framework.

### 2.2. Transition state approximation

In the calculation of the ground state properties, e.g. magnetic ordering and local magnetic moments, the SI correction is applied with full strength. For excited states, it appears that the binding energies of the SI-corrected localized levels are significantly too large when compared to those determined from spectroscopical data, i.e. from photoemission intensities. This ‘overcorrection’ of the SIC is attributed to the orbital relaxation.

The density functional theory of Hohenberg, Kohn, and Sham applies only if the occupation numbers of the orbitals are either zero or one. If the occupancy of one of the single-particle states has been changed, one has to generalize the theory by including the occupation number, as was done by Janak [15]. According to Janak’s theorem, the derivative of the total energy  $E$  with respect to the orbital occupation is equal to the eigenenergy  $\epsilon_{\alpha}$  of the corresponding orbital,

$$\frac{\partial E}{\partial f_{\alpha}} = \langle \psi_{\alpha} | H^{\text{LSD}} | \psi_{\alpha} \rangle = \epsilon_{\alpha}, \quad (6)$$

where  $H^{\text{LSD}}$  is the LSD Hamiltonian and  $f_\alpha$  is the occupation number of the orbital  $\psi_\alpha$ . The relaxation energy  $\Delta E_{\text{relaxed}}$  is calculated by removing an electron from an occupied state,

$$\Delta E_{\text{relaxed}} = - \int_0^1 \epsilon_\alpha(f_\alpha) df_\alpha. \quad (7)$$

The total energy  $E$  includes the relaxation of all orbitals due to the change of the occupation number. Several ways to calculate the removal energy have been proposed [16] but they lead to unphysical effects [17].

We start from the Taylor expansion of the eigenvalue as a function of the occupation number in the neighborhood of  $F_\alpha$ ,

$$\epsilon_\alpha(f_\alpha) \approx \epsilon(F_\alpha) + (f_\alpha - F_\alpha) \left( \frac{\partial \epsilon}{\partial f_\alpha} \right)_{f_\alpha=F_\alpha}. \quad (8)$$

The restriction to the first order is justified if the eigenvalue depends almost linearly on its occupation number [18, 19]. Inserting (8) into (7) and integrating from  $f_\alpha = 1$  to  $1 - p$  gives

$$E(f_\alpha = 1 - p) - E(f_\alpha = 1) = -p\epsilon_\alpha(F_\alpha) + \left[ \frac{p^2}{2} - p(1 - F_\alpha) \right] \left( \frac{\partial \epsilon_\alpha}{\partial f_\alpha} \right)_{f_\alpha=F_\alpha}. \quad (9)$$

To have a method similar to Koopmans' theorem one would need the eigenvalues at full occupancy. For  $F_\alpha = 1$  and  $p = 1$ ,

$$\Delta E_{\text{relaxed}} = -\epsilon_\alpha(1) + \frac{1}{2} \left( \frac{\partial \epsilon_\alpha}{\partial f_\alpha} \right)_{f_\alpha=1}. \quad (10)$$

The first term is the energy of the fully occupied orbital  $\alpha$ . The second term accounts for the orbital's relaxation. This term includes a 'non-Koopmans'-like correction (relaxation of the localized state) and the relaxation energy (relaxation of the other orbitals). In many applications to localized states, the relaxation is significant. To achieve an accurate electron removal energy, this term has to be included in the energy calculation. Using the Hellmann–Feynman theorem [20], the second term on the right-hand side of (10) can be written as

$$\frac{\partial \epsilon_\alpha}{\partial f_\alpha} = \langle \psi_\alpha | \frac{\partial H^{\text{LSD}}}{\partial f_\alpha} | \psi_\alpha \rangle. \quad (11)$$

If the relaxation of other orbitals is neglected (in analogy to Koopmans' theorem), then (11) reduces to

$$\frac{\partial \epsilon_\alpha}{\partial f_\alpha} = \langle \psi_\alpha | u_\alpha + \rho_\alpha \frac{\partial \epsilon_{\text{xc}}}{\partial \rho} | \psi_\alpha \rangle, \quad (12)$$

where  $u_\alpha$  is the Coulomb potential associated with orbital  $\alpha$  and  $\epsilon_{\text{xc}}$  is the exchange–correlation energy per particle. For  $f_\alpha = 1$ , the first term is the self-Coulomb interaction of an electron. The second term is the change of the exchange–correlation energy (to first order in the occupation number) of the system due to removing one electron from the orbital  $\alpha$ . Equation (12) can be interpreted as the self-interaction of an orbital whose occupation number is reduced. Adding this positive term to the energy of the orbital  $\alpha$  increases the removal energy calculated within the LSD. Thus, the

removal energy of a localized orbital with corrected potential  $V_\alpha$  becomes

$$\Delta E_{\text{unrelaxed}} = -\langle \psi_\alpha | H^{\text{LSD}} | \psi_\alpha \rangle - \frac{1}{2} \langle \psi_\alpha | V_\alpha^{\text{SIC}} | \psi_\alpha \rangle. \quad (13)$$

This is the unrelaxed removal energy when an electron is removed from orbital  $\alpha$ . The removal energy is larger than its experimental counterpart because the relaxation of other orbitals is neglected.

As is apparent from (13), the removal energy of the orbital  $\alpha$  is calculated with half strength of the SIC potential associated with this orbital. By this method, i.e. by calculating the LSD and the SIC ground state potentials, one obtains removal energies with good accuracy [3, 17]. Following previous works we call this approach the transition state approximation (TSA).

### 2.3. Exchange parameters and Curie temperature

The self-interaction correction also affects the exchange interaction among the Gd sites. To address this issue, we calculated the Curie temperature of both the bulk and the surface. The Curie temperature is calculated within the Heisenberg model by Monte Carlo simulations (MCSs). The exchange parameters  $J_{ij}$  are calculated by means of the Liechtenstein formula [21]. The critical temperature is determined accurately by the fourth-order Binder cumulant [22].

## 3. Results and discussion

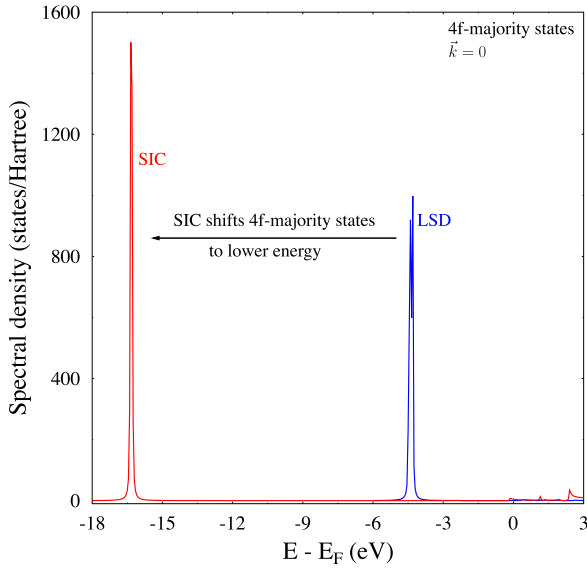
### 3.1. Magnetic structure

The total energy minimization implies that all 4f majority states have to be SI corrected. As a result, their binding energies increase sizably from about 5.0 eV for LSD to about 17.0 eV for SIC (figure 1). Consequently, these states become more localized.

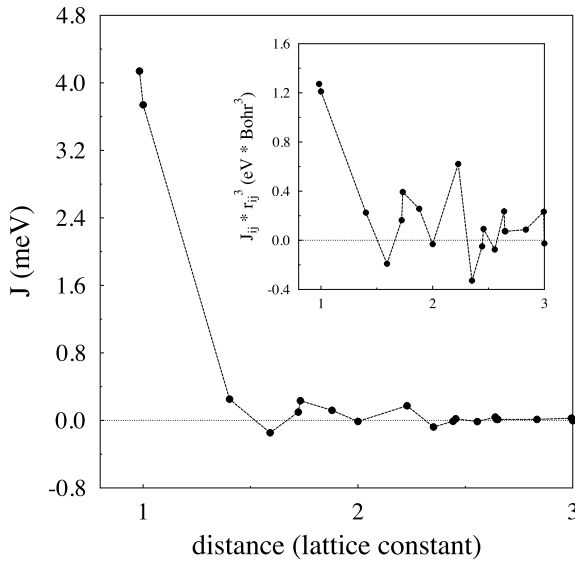
The magnetic ground state is changed from antiferromagnetic ordering, as obtained within the LSD approximation, to ferromagnetic ordering upon application of the SIC. The LDA +  $U$  method also predicts the magnetic ordering ground state and the magnetic moment correctly but relies on adjustable parameters. In LDA +  $U$  calculations the change of magnetic ordering was attributed to the removal of the 4f minority states from the Fermi level to larger energies [6, 7]. A small shift of the minority states is found in our calculations as well; it is a result of the charge redistribution.

For the ferromagnetic ground state, Heisenberg exchange parameters  $J_{ij}$  were computed for Gd bulk (figure 2). For the first three nearest neighbors the coupling is ferromagnetic ( $J_{ij} > 0$ ); the exchange parameters for larger distances change sign and oscillate (inset of figure 2). However, the exchange parameters decrease (in absolute value) rapidly with distance; for example,  $J_{ij}$  of the sixth shell is about 5% of that of the first shell.

To address the effect of the surface relaxation on the exchange parameters, a calculation was performed for two slabs with 12-layer thickness, one unrelaxed, the other with 4%



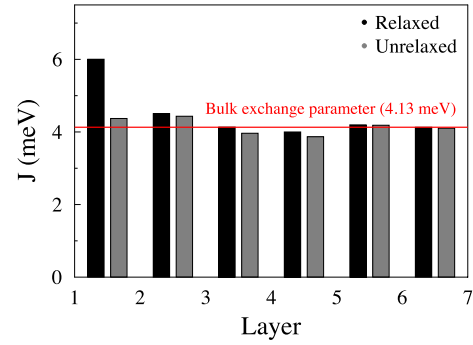
**Figure 1.** Effect of self-interaction correction on the binding energy of 4f majority states in bulk Gd(0001). The spin-resolved spectral density is calculated within the local spin-density (LSD) approximation and within the self-interaction correction (SIC) at  $k_{\parallel} = 0$ .



**Figure 2.** Heisenberg exchange parameters  $J_{ij}$  of Gd bulk (top). To emphasize the oscillations of the  $J_{ij}$ , we show  $J_{ij}r_{ij}^3$  in the inset ( $r_{ij}$  distance of sites  $i$  and  $j$ ).

surface contraction (figure 3). The relaxation has a profound effect on the surface  $J_{ij}$ ; more precisely, this  $J_{ij}$  is increased by about 50%. Thus, we expect a sizable effect on the Curie temperature for the slabs. Please note that in any case the magnetic coupling of the surface layer with the sub-surface layer is ferromagnetic.

We applied MCSs for three 12-layer slabs: (i) with  $J_{ij}$  taken from the bulk calculation (‘bulk’), (ii) with  $J_{ij}$  for the unrelaxed surface (‘unrelaxed’), and (iii) with  $J_{ij}$  for the relaxed surface (‘relaxed’). In accordance with the increasing exchange parameters, in particular those of the first shells,  $T_C$  increases as well: from 320 to 330 K for ‘bulk’ via 330–340 K



**Figure 3.** Effect of the surface relaxation on the Heisenberg exchange parameters. The bars represent  $J_{ij}$  of the first shell with sites located in adjacent layers (black with 4% surface contraction; gray without surface relaxation).

for ‘unrelaxed’ up to 380–400 K for ‘relaxed’. To be more precise, the exchange parameter of the first shell is 4.13 meV for ‘bulk’, 4.37 meV for ‘unrelaxed’, and 6.00 meV for ‘relaxed’. Consequently,  $T_C$  for the ‘bulk’ case matches best the experimental bulk value of 293 K [23]. We also performed MCSs for ‘bulk’ systems with a significantly increased size; in all cases  $T_C$  was within the range reported above. Please note that slabs are free-standing Gd layers with two surfaces. Therefore it is not possible to compare our results directly with experiments [24].

The findings reported in the preceding evidence the importance of the self-interaction correction for the magnetic ordering in systems with correlated electrons. Second, they show the importance of the surface relaxation to the critical temperature. The increased Heisenberg exchange parameters at the surface result in an enhanced  $T_C$  as compared to the unrelaxed system.

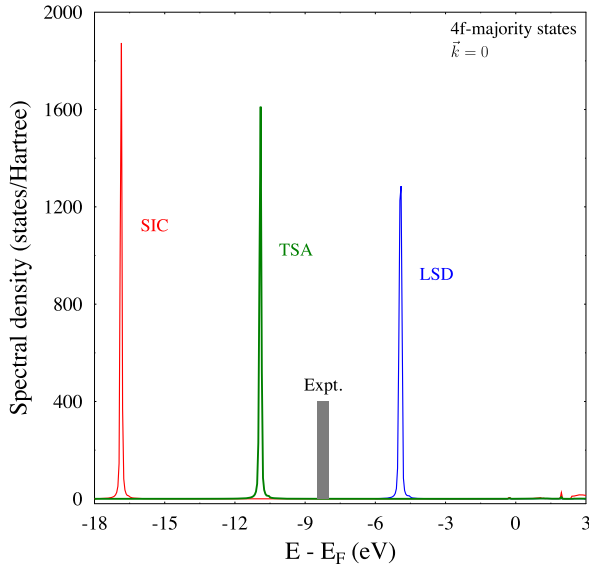
### 3.2. Surface state dispersion and Rashba spin–orbit coupling

So far, all calculated properties, such as magnetic ordering and geometrical constants, were associated with the ground state. To take into account the relaxation of electrons due to an excitation we applied the transition state approximation.

In figure 4 the spectral density of the 4f majority states in Gd(0001) calculated within the LSD, SIC, and TSA is shown. Compared with experimental values (gray bar), the LSD predicts too low a binding energy, while the SIC produces too high a binding energy (cf. the ‘overcorrection’ in figure 1). Applying the TSA, the binding energy increases to 10.5 eV, which is in reasonable agreement with the experimental value (8.0–8.5 eV).

The occupied surface states of Gd(0001) are mostly  $d_{z^2}$  majority states which hybridize with the 4f majority states. Consequently, the treatment of the electronic correlation within the 4f states has an effect on both binding energy and dispersion of the surface states. The d–f hybridization of the surface state can be quantified by the ratio of the d and f contributions to its spectral density  $N$  at  $k_{\parallel} = 0$ . The d–f hybridization of the surface state is larger for SIC ( $d/f = 7$ ) than for LSD ( $d/f = 50$ ), which is at first glance



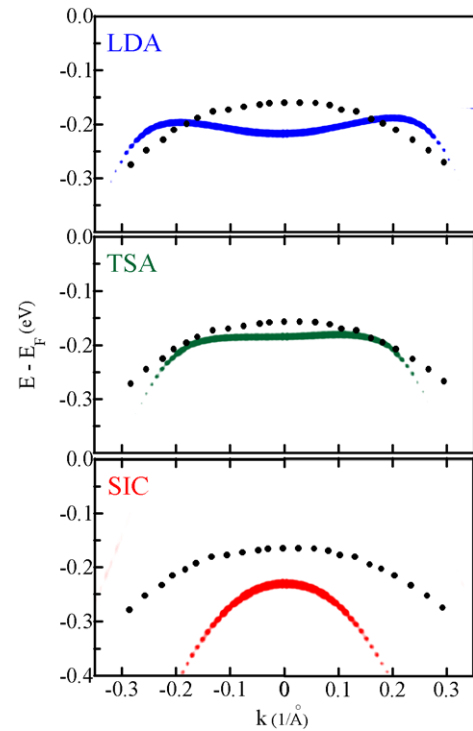


**Figure 4.** Effect of the electronic correlation on the binding energy of 4f majority states in the surface layer of Gd(0001). The spectral density at  $\vec{k}_{\parallel} = 0$  is calculated within the local spin-density approximation (LSD), the self-interaction correction (SIC), and the transition state approximation (TSA). The range of experimental binding energies [6] is marked by the gray bar (of arbitrary height).

counterintuitive. A closer inspection of the spectral density shows that the d contribution to the majority surface state does not change upon application of TSA or SIC. However, spectral weight of f majority character is transferred from the unoccupied to the occupied states and is mixed into the d majority surface state for TSA and SIC. This ‘band-filling’ effect manifests itself in the decreasing d/f ratios and in the increased magnetic moments for TSA and SIC ( $8.0 \mu_B$ ), as compared to LSD ( $8.0 \mu_B$ ).

The majority surface state dispersion of Gd(0001) is shown in figure 5. For the LSD approximation, the binding energy of 0.22 eV at  $\vec{k}_{\parallel} = 0$  ( $\bar{\Gamma}$ ) deviates sizably from the experimental result (0.16 eV, dots). More striking, however, is the positive dispersion at small wavevectors, which does not match the negative dispersion in experiment. Application of the SIC leaves the binding energy almost unchanged (0.23 eV) but results in a strongly negative dispersion, which also does not fit to experiment. The surface state dispersion calculated by the TSA shows a plateau at small  $k_{\parallel}$ , and the binding energy of 0.18 eV almost hits that of the experiment.

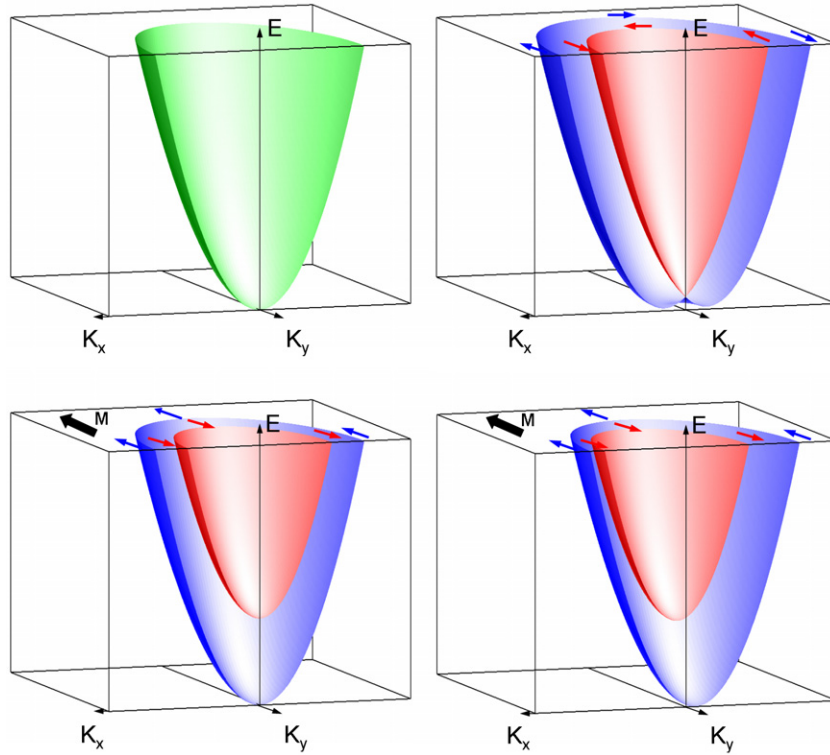
In a non-magnetic crystal with inversion symmetry the electronic states are not spin polarized, due to Kramers’ degeneracy. The spin degeneracy is the result of both time-reversal and inversion symmetry. At surfaces the inversion asymmetry results, via the spin-orbit coupling (SOC), in a splitting in the dispersion relation. At a magnetic surface, spin degeneracy is lifted by the exchange interaction and majority spins are aligned along the quantization axis. The effect of the spin-orbit interaction is mainly modification of the energy dispersion, i.e. moving the dispersion relations with respect to each other. Figure 6 depicts the spin structure of split surface states at a non-magnetic and a magnetic surface.



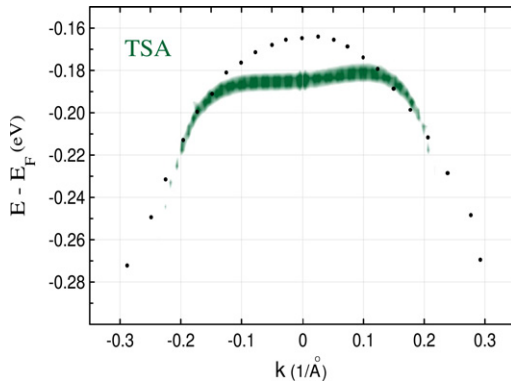
**Figure 5.** Effect of electronic correlations on the  $d_{z^2}$  majority surface state of Gd(0001). The spectral densities calculated within the local spin-density (LSD) approximation, the transition state approximation (TSA), and the self-interaction correction (SIC) are shown along the  $\bar{M}-\bar{\Gamma}-\bar{M}$  line of the surface Brillouin zone. Experimental data (dots) are reproduced from [8].

The spin-orbit interaction and magnetism are taken into account on equal footing in our relativistic layer KKR code. For clarity, we reproduce the TSA data from figure 5 and add eye-guiding horizontal lines in figure 7. As a consequence of the Rashba SOC, the surface state dispersion, as obtained from the spectral density at the surface, becomes asymmetric in the direction normal to the in-plane magnetization. As in experiment, the maximum of the dispersion is shifted off the Brillouin center to positive  $\vec{k}_{\parallel}$ . We note in passing that magnetization reversal ( $\vec{M} \rightarrow -\vec{M}$ ) mirrors the dispersion, that is  $E(\vec{k}_{\parallel}, \vec{M}) = E(-\vec{k}_{\parallel}, -\vec{M})$ . Further, the dispersion maximum of the associated d minority state (not shown here) is shifted oppositely to that of the majority surface state.

From figure 7 one might conclude that the Rashba effect is overestimated in theory. One possible reason could be too large an asymmetry of the surface state confinement, which essentially determines the size of the Rashba effect. Although we cannot rule out this explanation, there may be a few other explanations for this mismatch between theory and experiment. (i) The TSA is a first-order perturbation to SIC and LSD; it does not rely on an adjustable parameter. Thus, the curvature of the surface states could perhaps be better described within LDA +  $U$  but at the cost of the adjustable parameter  $U$  (which is fitted to experimental data). (ii) The effective mass of surface states is sometimes overestimated in KKR, in which the vacuum region is described by so-called empty muffin-tin spheres on the parent lattice (here



**Figure 6.** The schematic spin structure of Rashba-split and exchange-split surface states at a non-magnetic surface (top) and at a magnetic surface (bottom). The left panels show systems with inversion symmetry while the right panels show systems without inversion symmetry. The Rashba spin–orbit coupling in a ferromagnetic two-dimensional electron with in-plane magnetization  $\vec{M}$  removes the inversion symmetry of the spin-split band structure,  $E(+\vec{k}_{\parallel}) \neq E(-\vec{k}_{\parallel})$  for  $\vec{k}_{\parallel} \perp \vec{M}$ .



**Figure 7.** The d majority surface states of Gd(0001) calculated within TSA. The Rashba effect shows up as asymmetry of the dispersion ( $E(\vec{k}) \neq E(-\vec{k})$ ). The in-plane magnetization is perpendicular to  $\vec{k}_{\parallel}$ ,  $\vec{k}_{\parallel}$  along  $\vec{M}-\Gamma-\vec{M}$ . Experimental data (dots) are reproduced from [8].

hcp(0001)). This effect showed up for example in the free-electron-like surface state on Au(111); see [25]. (iii) The experimental dispersion was obtained from the peak positions in angle-resolved photoemission spectra. The maxima are typically rather broad for ferromagnetic systems (about 0.2–0.3 eV FWHM in figure 1(a) of [8]) and, thus, introduce some uncertainty in the detailed dispersion.

Summarizing this section, we conclude that the TSA considerably improves the description of excited states in

systems with electronic correlations, as compared to the LSD approximation and the SIC. Although the agreement with spectroscopical data, e.g. photoemission, is not as good as in LDA + U, we would like to add in favor of the TSA that it does not rely on any adjustable parameters, like the Hubbard parameters U and J in LDA + U approaches [5]. The latter are typically chosen to reproduce experiments.

The hybridization of the 4f majority states (which are treated by SIC) with the d majority surface state has a profound effect on both the binding energy and the dispersion of the latter. On top of the TSA treatment, we have shown that even the Rashba spin–orbit coupling in the surface states is captured correctly. As a result, we conclude that an advanced treatment of the electronic correlation in the localized spin-polarized states is not only important for the magnetic structure but also improves the properties of the valence states.

#### 4. Concluding remarks

The present first-principles study on Gd(0001) shows that the self-interaction correction to the local spin-density approximation improves considerably the description of ground state properties of correlated systems. Its flavor for excited states, i.e. the transition state approximation, is able to describe correctly spectroscopic data. In summary, we have dealt successfully with a complex interplay of electronic correlations, surface relaxation, and spin–orbit coupling on the magnetic ordering, the Curie temperature, and the surface state

dispersion. A key issue in our multiple scattering theoretical calculations is that these do not rely on any adjustable parameter which is related to electronic correlations.

The combination of *ab initio* calculations beyond LSDA and Monte Carlo calculations makes it possible to extend the Curie temperature calculation to more realistic systems, e.g. to Gd(0001)/W(110). This system shows in particular a thickness dependence of the Curie temperature [24].

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