PHYSICAL REVIEW B VOLUME 43, NUMBER 10 1 APRIL 1991

Density-functional calculation of effective Coulomb interactions in metals

V. I. Anisimov* and O. Gunnarsson
Max-Planck-Institut für Festkörperforschung, D-7000 Stuttgart 80,
Federal Republic of Germany

(Received 9 October 1990)

The effective Coulomb interaction between the localized electrons is calculated for Fe and Ce. It is found that a change in the number of 3*d* electrons in Fe is only screened to about 50% inside the Fe atom where the change was made, although perfect (100%) screening was expected for a metallic system like Fe. In Ce, on the other hand, the screening is very efficient. The difference is discussed. For Ce the calculated Coulomb interaction (6 eV) is in good agreement with experiment, while the result (6 eV) for Fe is surprisingly large.

I. INTRODUCTION

For strongly correlated systems, where accurate *ab initio* calculations are difficult to perform, our understanding of the physical properties is often based on a model Hamiltonian approach. An important parameter in such models is the effective Coulomb interaction U between the localized electrons in the system, i.e., the 3*d* electrons in a transition-metal compound and the 4*f* electrons in a rare-earth compound. Traditionally, the parameters in such a model are treated as adjustable parameters and deduced from experiment. Recently, it has become very popular to calculate these parameters using the *ab initio* density-functional (DF) formalism in the local-density (LD) approximation.[1]

The meaning of U has been carefully discussed by Herring.[2] In, e.g., a 3*d* electron system with n 3*d* electrons per atom, U is defined as the energy cost for the reaction

$$2(d^n) \rightarrow d^{n+1} + d^{n-1}, \qquad (1)$$

i.e., the energy cost for moving a 3*d* electron between two atoms which both initially had n 3*d* electrons. Herring[2] emphasized that U is a renormalized quantity. In particular, U contains effects due to screening from other types of electrons, e.g., 4*s* and 4*p* electrons for a 3*d* metal. Thus the number of 4*s* and 4*p* electrons on an atom with $n+1$ 3*d* electrons is reduced and the number on an atom with $n-1$ 3*d* electrons is increased. This screening by 4*s* and 4*p* electrons reduces the energy cost for the reaction Eq. (1). In the Anderson or Hubbard models, for instance, such a screening is not included explicitly and it is then important to introduce it implicitly as a renormalization of U. There are also other renormalization effects for U, in particular due to changes in the radial extent of the orbitals when the number of 3*d* electrons is changed.[2]

Herring[2] argued that for metals the screening by 4*s* and 4*p* electrons is very efficient, and that one therefore ought to consider the reaction

$$2(d^n s^1) \rightarrow d^{n+1}s^0 + d^{n-1}s^2, \qquad (2)$$

i.e., to assume that any change in the number of 3*d* electrons is perfectly screened inside the Wigner-Seitz sphere by a change in the number of 4*s* and 4*p* electrons of the opposite sign. The arguments of Herring for this perfect screening were partly based on screening in a free-electron gas. In Fig. 1 we show the screening charge of a positive point charge in a homogeneous electron gas with the same density as the average density of 4*s* and 4*p* electrons in Fe ($\sim$ 1.1 electrons per atom, $r_s = 2.6\ a_0$). The curve TF was obtained using Thomas-Fermi linear response and the curve LDA was obtained from *linear* response in the LD approximation.[3] The figure illustrates that a large fraction of the screening charge falls inside the Wigner-Seitz sphere with the radius $R_{\rm WS} = 2.66\ a_0$.

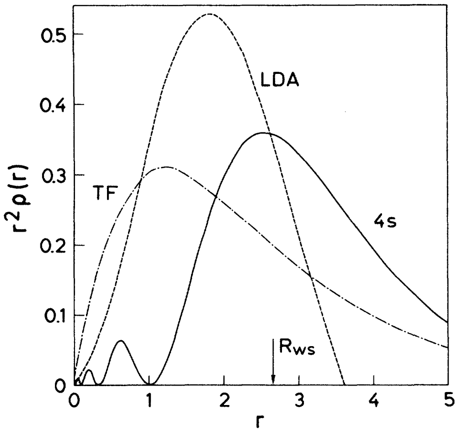

FIG. 1. Screening charges in Fe. The full curve shows $r^2\phi_{4s}^2(r)$, where ϕ_{4s} is the Fe 4*s* wave function calculated for the $3d^7 4s^1$ configuration. The dashed and dash-dotted curves show the results of linear screening in an electron gas using the LD and TF approximations, respectively. r is in units of a_0.

©1991 The American Physical Society

This fraction is 0.66 and 0.92 in the TF and LD approximations, respectively. If nonlinear screening effects are taken into account the screening of a *positive* point charge is substantially more efficient,[4] while the screening of a negative point charge should be somewhat less efficient.

The arguments above are based on screening in an electron gas. For Fe metal the screening is primarily done by the 4*s* and 4*p* electrons. The 4*s* and 4*p* wave functions must be orthogonal to the *s* and *p* core states. This forces the 4*s* and 4*p* wave functions to be located primarily outside the core region. This is illustrated in Fig. 1, where we also show the square of the 4*s* wave function. The 4*s* wave function has its outermost node at about $r = 1\ a_0$ and is rather effectively expelled from the region $r < 1.5\ a_0$. This effectively prevents the screening in Fe from being as efficient as in an electron gas. In this paper we show that because of this, the screening in 3*d* metals is far from perfect while it is quite efficient for 4*f* systems.

In Sec. 2 we discuss the calculation of Coulomb interaction, and in Sec. 3 we present results for Fe and Ce. The results are discussed in Sec. 4.

II. CALCULATION OF F^0_{eff}

In this section we focus on the calculation of the screened Coulomb integral F^0_{eff}, corresponding to the unscreened Slater integral[5] F^0, where

$$F^k = \int_0^\infty r^2 dr \int_0^\infty (r')^2 dr' \frac{r_<^k}{r_>^{k+1}} \phi_{3d}^2(r)\phi_{3d}^2(r'). \tag{3}$$

Here $\phi_{3d}(r)$ is the 3*d* wave function and $r_<$ ($r_>$) is the smaller (larger) of r and r'. To describe multiplet effects the Slater integrals F^2 and F^4 are needed. These are usually deduced from atomic data, since the additional screening effects in a solid appear to be small,[6] and are not discussed further here.

To derive an expression for F^0_{eff} we consider the expression for the interaction energy in Hartree-Fock (HF) for a configuration with the 3*d* states $m_{i_1}\uparrow,\ldots, m_{i_N}\uparrow$, $m_{j_1}\downarrow,\ldots,m_{j_M}\downarrow$ occupied, where m refers to the angular momentum. We write the interaction energy as

$$E_I(m_{i_1}\uparrow,\ldots,m_{i_N}\uparrow;m_{j_1}\downarrow,m_{j_M}\downarrow) = \tfrac{1}{2}F^0_{\text{eff}}n(n-1) + E_x(m_{i_1}\uparrow,\ldots m_{i_N}\uparrow) \tag{4}$$

$$+E_x(m_{j_1}\downarrow,\ldots,m_{j_M}\downarrow) + \Delta E_H(m_{i_1}\uparrow,\ldots,m_{i_N}\uparrow;m_{j_1}\downarrow,\ldots,m_{j_M}\downarrow), \tag{5}$$

where the first term is the spherical part of the Hartree energy related to F^0_{eff}, the second and third term the exchange energies for the spin-up and spin-down exchange energies, respectively, and the fourth term is the nonspherical contributions to the Hartree energy. The total number of 3*d* electrons is n. The term ΔE_H does not enter in the following discussion, since we assume all charge densities to be spherical inside a given atomic sphere [the atomic-sphere approximation[7] (ASA)]. We can then write

$$F^0_{\text{eff}} = E_I\left(\frac{n}{2}+1;\frac{n}{2}\right) - E_I\left(\frac{n}{2};\frac{n}{2}\right) - E_I\left(\frac{n}{2}+1;\frac{n}{2}-1\right) + E_I\left(\frac{n}{2};\frac{n}{2}-1\right), \tag{6}$$

where we have only indicated the number of spin-up and spin-down electrons, since in the ASA it does not matter which m quantum numbers are occupied. We now use the relation[8]

$$\varepsilon_i = \frac{dE}{dn_i}, \tag{7}$$

where ε_i is an eigenvalue to the LDA equation. We then obtain

$$F^0_{\text{eff}} = \varepsilon_{3d\uparrow}\left(\frac{n}{2}+\frac{1}{2},\frac{n}{2}\right) - \varepsilon_{3d\uparrow}\left(\frac{n}{2}+\frac{1}{2},\frac{n}{2}-1\right), \tag{8}$$

where $\varepsilon_{3d\uparrow}$ is the spin-up 3*d* eigenvalue, and the first term gives the difference between the first two terms in Eq. (6).

To calculate F^0_{eff} we now consider a large supercell. The number of 3*d* electrons on one of the atoms in the supercell is varied, and F^0_{eff} is deduced from Eq. (8). In such a calculation the response of the 4*s* and 4*p* electrons to the change in the number of 3*d* electrons is included and the radial extent of the 3*d* orbital is allowed to adjust self-consistently. The calculation therefore includes the important renormalization effects. In doing this calculation we have to avoid double counting of the hopping between the 3*d* orbital and the rest of the system, since this hopping is included explicitly in, for instance, the Anderson model. The hopping integrals connecting all the 3*d* orbitals to other orbitals are therefore put equal to zero.[9,10] This approach has the further advantage that it is easy to force each 3*d* orbital to have the desired occupation number. In the calculation for Fe below, all atoms but one have the 3*d* occupation $n = 7$ ($3d^7 4s^1$), with 3.5 spin-up and 3.5 spin-down electrons. The central atom is given occupation numbers according to Eq. (8) above. The total number of electrons is chosen so that the system is neutral. These calculations are supposed to be performed for an infinite supercell. For a finite supercell we introduce a correction due to the fact that the Fermi energy changes when the number of 3*d* electrons changes. From Eq. (7) we have that the difference between the first two terms in Eq. (6) is then given by $\varepsilon_{3d\uparrow}(\frac{n}{2}+\frac{1}{2},\frac{n}{2}) - \varepsilon_F(\frac{n}{2}+\frac{1}{2},\frac{n}{2})$, where ε_F is the Fermi energy. This follows, since the supercell is always neutral, and the change in the number of 3*d* electrons requires the addition or subtraction of the corresponding number of delocalized electrons at the Fermi energy. We then obtain the expression

$$F^0_{\mathrm{eff}} = \varepsilon_{3d\uparrow}\left(\frac{n}{2}+\frac{1}{2},\frac{n}{2}\right) - \varepsilon_{3d\uparrow}\left(\frac{n}{2}+\frac{1}{2},\frac{n}{2}-1\right) -\varepsilon_F\left(\frac{n}{2}+\frac{1}{2},\frac{n}{2}\right)+\varepsilon_F\left(\frac{n}{2}+\frac{1}{2},\frac{n}{2}-1\right), \qquad (9)$$

which agrees with Eq. (8) if the Fermi energy is unchanged.

III. RESULTS

We have performed calculations, using the linear muffin-tin orbital method in the atomic-sphere approximation.[7] We first consider Fe. In the calculation for Fe we have used a frozen core approximation. Since the $3s$ and $3p$ electrons are rather extended and relatively weakly bound, they can to some extent relax when the $3d$ charge is changed. From atomic calculations, we estimate the effect on F^0_{eff} to be a reduction of 0.5 eV. This number is therefore subtracted from all the frozen core calculations. We have first used a supercell with four atoms. Using the formula (9) we obtained the result $F^0_{\mathrm{eff}} = 5.9$ eV. If the spin polarization is neglected a slightly smaller value (5.6 eV) is obtained. This small difference is not essential, and all the following calculations are therefore nonspin-polarized. We next considered a supercell with 16 atoms, and obtain $F^0_{\mathrm{eff}} = 6.2$ eV using formula (9). This illustrates that the results are rather well converged with the respect to the size of the supercell. We have performed some additional checks of the internal consistency of the results. By using the total energy difference formula (6) we obtain the result 6.3 eV for the 16-atom supercell. The good agreement with the result (6.2 eV) above illustrates that the transition state arguments behind Eq. (9) are accurate. We observe, however, that using Eq. (8), which is not corrected for the change of the Fermi energy in the finite system, leads to the result 5.7 eV, and a somewhat less satisfactory accuracy. For a smaller supercell this discrepancy is larger. As a final test, we have considered a supercell where one atom has the occupancy 8, one the occupancy 6, and all the others the occupancy 7. From this energy $E(d^6+d^8+14d^7)$ we subtract the energy $E(16d^7)$ obtained by letting all 16 atoms in the supercell have the occupancy 7. This gives F^0_{eff} directly according to Herring's definition. The result 6.8 eV does not differ greatly from the other calculations (6.2 and 6.3 eV) for the 16 atom supercell, suggesting that the results are numerically reliable. In these calculations the hopping from the $3d$ levels on *all* the atoms in the super cell was suppressed. This of course influences the $4s$- and $4p$-like electron bands and possibly the ability of these electrons to screen the changes in the $3d$ charge. To check this, we have performed a calculation for a four-atom supercell, where the $3d$ hopping is suppressed only for the central atom. The $3d$ electrons on the other atoms are therefore allowed to participate in the screening as well as in the hybridization with the $4s$ and $4p$ electrons. This calculation leads to the value $F^0_{\mathrm{eff}} = 5.6$ eV, which agrees with the result above (5.6 eV) for a four-atom supercell.

It is now of great interest to check the assumption in previous calculations about perfect screening. We find that the changes in the $3d$ charge is screened to 24% and 29% by the $4s$ and $4p$ electrons, respectively, on the same site. Totally the on-site screening is therefore slightly more than 50%, and it is thus far from perfect. On the neighboring atoms there is in addition about 40% screening. In a renormalized atom calculation, Cox, Coulthard, and Loyd[11] obtained a much smaller value $F^0_{\mathrm{eff}} \sim 2.8$ eV. This is not surprising, since they assumed perfect screening.

We next consider Ce (see Fig. 2). We have performed a calculation for α-Ce using a supercell with four atoms. In this case the outermost core ($5s$ and $5p$) lie ouside the $4f$ orbital, and it is important to include core relaxation explicitly. Thus the core orbitals were recalculated for each $4f$ occupation. This leads to $F^0_{\mathrm{eff}} = 6.1$ eV. The change in the number of $4f$ electrons is screened to about 4% by the $6s$ electrons, 4% by the $6p$ electrons and 97% by the $5d$ electrons inside the Wigner-Seitz sphere. For Ce there is therefore a slight overscreening by about 105%. These results can be compared with calculations by Herbst, Watson, and Wilkins,[12] who used a renormalized atom HF approach. They obtained $U = 5$ eV. This result contains Hund's rules effects from the higher Slater integrals F^2, F^4, and F^6. Thus we subtract the corresponding multiplet effects from our F^0_{eff}, which leads to a value of about 4.6 eV, in good agreement with Herbst, Watson, and Wilkins. We can also compare with calculations by Dederichs *et al.*,[13] who used an impurity calculation and therefore did not make any assumption about the screening. Their calculation is therefore closer to ours, although it contains effects of double counting of the hopping. Dederichs *et al.* obtained the results 6.6 and 8.1 eV for Ce in Ag and Pd, respectively, i.e., slightly

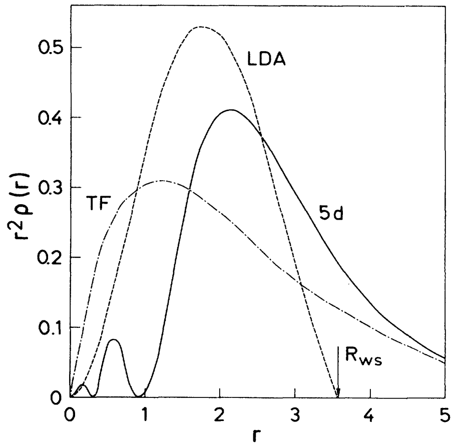

FIG. 2. Screening charges in Ce. The notations are equivalent to Fig. 1. The solid line shows the $5d$ wave function calculated for the configuration $4f^1 5d^1 6s^2$. r is in units of a_0.

larger than our result. Min *et al.* have performed supercell calculations for Ce and obtained $U = 5.4$ eV,[14] which is slightly smaller than our result.

IV. DISCUSSION

As discussed in the Introduction, it has been generally believed that for metals any change in the number of localized electrons is perfectly screened inside the Wigner-Seitz sphere by the delocalized electrons. Our calculations show, however, that for the $3d$ system Fe, the on-site screening is only about 50% while for Ce there is a slight overscreening on the central site. For Fe the screening is done by the $4s$ and $4p$ electrons. As illustrated in Fig. 1, because of the orthogonality to the core electrons, the $4s$ and $4p$ electrons cannot provide such a compact screening charge as would be expected in a free-electron gas with a similar density. The $4s$ wave function is therefore rather effectively excluded from the volume $r < 1.5a_0$. As a result the $3d$ to $4s$ bare Coulomb integral $F^0(3d,4s)$ is only moderately large. Furthermore the $4s$ bandwidth is essentially determined by the square of the wave function at the Wigner-Seitz radius.[7] Since the $4s$ wave function has its maximum close to the Wigner-Seitz radius, the bandwidth is very large and the density of states is small. To illustrate the effect we assume that the screening charge is simply the density of $4s$ and $4p$ states, $N(0)$, close to the Fermi energy times the shift ΔE_s of the $4s$ level due to the change in the number of $3d$ electrons. If the change in the number of $3d$ electrons is unity, the shift is

$$\Delta E_s = F^0(3d,4s) - \delta n_{sp} F^0(4s,4s) - \frac{2(1-\delta n_{sp})}{d}, \tag{10}$$

where δn_{sp} is the change in the number of $4s$ and $4p$ electrons and d is the distance between the nearest neighbors. We have assumed that the $4s$ and $4p$ wave functions have the same radial extent and that the screening charge outside the central sphere, $1-\delta n_{sp}$, is located in the nearest-neighbor spheres. The screening charge is then given by

$$\delta n_{sp} = N(0)\Delta E_s. \tag{11}$$

For Fe wave functions normalized to the Wigner-Seitz sphere we have $F^0(3d,4s) \sim 1.01$ Ry, $F^0(4s,4s) \sim 0.89$ Ry, $d = 4.68a_0$, and $N(0) \sim 2$ states/Ry atom. This gives $\delta n_{sp} = 0.6$, in reasonable agreement with the calculated result $\delta n_{sp} = 0.53$. For Ce the corresponding numbers are $F^0(4f,5d) \sim 0.95$ Ry, $F^0(5d,5d) \sim 0.78$ Ry, $d = 6.48a_0$, and $N(0) \sim 14$ states/Ry atom. This gives $n_{5d} \sim 1.18$ in reasonable agreement with the calculation. We notice that the difference between Fe and Ce is the much larger value of $N(0)$ for Ce. This follows partly because the $5d$ function is somewhat more contracted than the $4s$ function, but in particular because the Wigner-Seitz radius is larger for Ce than for Fe, so that the Ce $5d$ wave function has decayed much more at the Wigner-Seitz radius. The integrals for Fe are slightly larger for Fe than for Ce, because of the effect of renormalizing the wave functions to the Wigner-Seitz radius. Although we find that the $4s$ and $4p$ electrons screen a perturbation in iron rather inefficiently, the situation is completely different if the $3d$ electrons are included. Thus it was found that a core hole in an Mn impurity in CdTe is slightly overscreened if the $3d$ electrons on the *same* site are allowed to participate in the screening.[10] In a similar way we expect, e.g., $3d$ impurities in $3d$ hosts are screened efficiently.

The calculated value of F^0_{eff} appears to be in rather good agreement with experiment for Ce. Thus values in the range 6–7 eV have been deduced from comparison with spectroscopic experiments and model calculations.[15] For Fe the situation seems to be different. Typically F^0_{eff} is expected to be in the range 1–2 eV for the metallic transition metals, with the exception of Ni.[16,6] These estimates often do not include many-body effects in the analysis on the same level as was done for the Ce compounds. Nevertheless it seems that many-body effects cannot fully explain the difference between the calculated and experimentally deduced values of F^0_{eff} for Mn,[17] where a similar result for F^0_{eff} is obtained. This seems to be in contrast to the nonmetallic $3d$ compounds, at least the Ni and Cu compounds, where the present approach appears to give sensible values for F^0_{eff}.[18,9,19,20] We note that in the cases where the screening is far from perfect, the present calculation is expected to overestimate F^0_{eff}. In these cases an appreciable amount of screening charge is located in the spheres which are nearest neighbors to the central sphere, where the number of localized electrons was changed. This charge may be expected to be concentrated in the parts of the spheres which are closest to the central sphere, while the charge is assumed to be spherically symmetric in the ASA applied here. The screening charge then has a smaller effect on the $3d$ level in the central atom, and F^0 is less effectively screened [cf. Eq. (9)]. This effect can be estimated by assuming that all the screening charge outside the central sphere is located exactly outside the central sphere, while in the ASA the charge is effectively located at the center of the neighboring spheres. The correction to F^0_{eff} is then

$$\delta F^0_{\text{eff}} = 27.2 \left[0.5\left(\frac{1}{4.68} - \frac{1}{2.66}\right)\right] = -2.2 \text{ eV}, \tag{12}$$

where 0.5 is the screening charge outside the central sphere, 4.68 is the distance to the nearest neighbor, and 2.66 is the Wigner-Seitz radius. This should be an upper limit to the error due to the ASA. This could reduce the LDA value for F^0_{eff} to about 4 eV, which still appears too large compared with experiment.

V. SUMMARY

The effective Coulomb interaction has been calculated for Fe and Ce as examples of transition metals and rare-earth metals, respectively. It is found that the on-site screening is rather inefficient for Fe ($\sim 50\%$), but very efficient for Ce ($\sim 100\%$). Because of the requirement that the screening orbitals are orthogonal to the core orbital, the screening orbital is more extended than the screening charge in a free-electron gas. As a consequence, the width of the band corresponding to the screening orbital is very large for Fe, making the screening inefficient. For Ce, on the other hand, the Wigner-Seitz radius is rather large compared with the $5d$ orbital, the corresponding band is not so broad, and the screening charge inside the Wigner-Seitz sphere is large. The results for metallic $3d$ systems appear to disagree with experiment, while the results for nonmetallic $3d$ systems and $4f$ systems seem to be in satisfactory agreement with experiment.

ACKNOWLEDGMENTS

We would like to thank J. Zaanen for many helpful discussions.

---

[*] Permanent address: Institute of Metal Physics, Academy of Sciences of the U.S.S.R., Ural Division, Sverdlovsk GSP-170, U.S.S.R.

[1] P. Hohenberg and W. Kohn, Phys. Rev. **136**, B864 (1964); W. Kohn and L.J. Sham, *ibid.* **140**, A1133 (1965); For a recent review see, e.g., R.O. Jones and O. Gunnarsson, Rev. Mod. Phys. **61**, 689 (1989).

[2] C. Herring, in *Magnetism*, edited by G.T. Rado and H. Suhl (Academic, New York, 1966), Vol. IV.

[3] L. Hedin and B.I. Lundqvist, J. Phys. C **4**, 2064 (1971).

[4] Z.D. Popovic and M.J. Stott, Phys. Rev. Lett. **33**, 1164 (1974); C.O. Almbladh, U. von Barth, Z.D. Popovic, and M.J. Stott, Phys. Rev. B **14**, 2250 (1976).

[5] J.C. Slater, *Quantum Theory of Atomic Structure* (McGraw-Hill, New York, 1960), Vol. 1.

[6] E. Antonides, E.C. Janse, and G.A. Sawatzky, Phys. Rev. B **15**, 1669 (1977).

[7] O.K. Andersen, Phys. Rev. B **12**, 3060 (1975); O.K. Andersen and O. Jepsen, Phys. Rev. Lett. **53**, 2571 (1984); O.K. Andersen, Z. Pawlowska, and O. Jepsen, Phys. Rev. B **34**, 5253 (1986).

[8] J.C. Slater, *Quantum Theory of Molecules and Solids* (McGraw-Hill, New York, 1974), Vol. 4; J.F. Janak, Phys. Rev. B **18**, 7165 (1978).

[9] A.K. McMahan, R.M. Martin, and S. Satpathy, Phys. Rev. B **38**, 6650 (1988).

[10] O. Gunnarsson, O.K. Andersen, O. Jepsen, and J. Zaanen, in *Proceedings of the Tenth Taniguchi Symposium on Core-Level Spectroscopy in Condensed Systems*, Kashikojima, 1987, edited by J. Kanamori and A. Kotani (Springer, Heidelberg, 1988), p. 82; Phys. Rev. B **39**, 1708 (1989).

[11] B.N. Cox, M.A. Coulthard, and P. Loyd, J. Phys. F **4**, 807 (1974).

[12] J.F. Herbst, R.E. Watson, and J.W. Wilkins, Phys. Rev. B **17**, 3089 (1978).

[13] P.H. Dederichs, S. Blügel, R. Zeller, and H. Akai, Phys. Rev. Lett. **53**, 2512 (1984).

[14] B.I. Min, H.J.F. Jansen, T. Oguchi, and A.J. Freeman, Phys. Rev. B **33**, 8005 (1986).

[15] J.W. Allen, S.J. Oh, O. Gunnarsson, K. Schönhammer, M.B. Maple, M.S. Torikachvili, and I. Lindau, Adv. Phys. **35**, 275 (1986).

[16] D. van der Marel, G.A. Sawatzky, and F.U. Hillebrecht, Phys. Rev. Lett. **53**, 206 (1984); D. van der Marel, PhD. thesis, Gronningen, 1985 (unpublished).

[17] V. Drchal, O. Gunnarsson, and O. Jepsen (unpublished).

[18] M.R. Norman and A.J. Freeman, Phys. Rev. B **33**, 8896 (1986).

[19] M.S. Hybertsen, M. Schlüter, and N.E. Christensen, Phys. Rev. B **39**, 9028 (1989).

[20] J. Zaanen, O. Jepsen, O. Gunnarsson, A.T. Paxton, O.K. Andersen, and A. Svane, Physica C **153-155**, 1636 (1988); O. Gunnarsson, J.W. Allen, O. Jepsen, T. Fujiwara, O.K. Andersen, C.G. Olsen, M.B. Maple, J.-S. Kang, L.Z. Liu, J.-H. Park, R.O. Anderson, W.P. Ellis, R. Liu, J.T. Markert, Y. Dalichaouch, Z.-X. Shen, P.A.P. Lindberg, B.O. Wells, D.S. Dessau, A. Borg, I. Lindau, and W.E. Spicer, Phys. Rev. B **41**, 4811 (1990).