small-polaron situations [such as for holes in MnO (Ref. 4) and UO_{2+x} (Ref. 6)] would provide a clearer test of the theory.

In summary, we have developed a quantum-mechanical many-electron approach to calculating electron transfer in magnetic insulators. As manifested by the presence of exchange transfer terms, the double-exchange transfer possesses a many-electron character as distinct from the usually assumed one-electron nature. Furthermore, it is demonstrated from first principles that the magnetic nature of the system significantly modifies the temperature dependence of the small-polaron mobility in antiferromagnets but not in paramagnets or ferromagnets.

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Study of the 4f Levels in Rare-Earth Metals by High-Energy Spectroscopies

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The density of the 4f states in all metallic rare earths has been studied with bremsstrahlung isochromat spectroscopy (BIS) and x-ray photoemission spectroscopy (XPS). The final-state multiplet structures of the $4f^{14-n}$ and $4f^n$ configurations observed by BIS and XPS, respectively, are closely related. The elements showing interconfiguration fluctuations are found to have one 4f level in the immediate vicinity of the Fermi level. Correlation energies are extracted directly from the spectra and compared with recent theoretical calculations.

The position of the 4f states above and below the Fermi level (E_F) has been determined for all metallic rare earths in a combined apparatus[1] for bremsstrahlung isochromat spectroscopy (BIS) and x-ray photoelectron spectroscopy (XPS). Both methods have the same surface sensitivity (10–25 Å) which is determined by the inelastic mean free path of 1.5-keV electrons. The measurements were performed in a vacuum in the 10^{-12}-Torr range, allowing good counting statistics without significant surface contamination. The resolution is better than 0.43 eV in BIS[1] and 0.3 eV in XPS.[2] The samples were evaporated *in situ* on a water-cooled holder. In BIS,[3] a beam of monoenergetic electrons impinges on the sample. The process of interest here is the direct deceleration of these electrons in the solid with simultaneous emission of electromagnetic radiation (bremsstrahlung). The electrons then occupy previously empty states above the Fermi level. The photon intensity at the constant energy $\hbar\omega$ = 1486.6 eV (corresponding to the photon energy used in XPS) is recorded as a function of the acceleration potential of the electrons. Disregard-

ing the background contribution and the influence of the matrix elements, the intensities in XPS and BIS spectra are roughly proportional to the density of occupied and unoccupied states, respectively.

Since the open $4f$ shells keep their atomic character in solids, their BIS and XPS spectra show multiplet structures. These correspond to transitions between Hund's-rule ground level of f^n and the accessible final states (S',L',J') belonging to the f^{n+1} configuration for BIS or to the f^{n-1} configuration for XPS. It has been shown theoretically that the relative intensities of the final-state multiplet components formed by photoemission in a $4f$ shell are well approximated by the squares of the fractional parentage coefficients (Q) of the initial ground state.[4] This result is fully confirmed by XPS spectra.[5,6] The following simple physical ideas suggest that BIS spectra can be analyzed in a quite similar way. f^n and f^{14-n} configurations have the same set of (L,S) states.[7] Comparing then a BIS process for an element with $14-n$ $4f$ electrons with an XPS process for an element with n $4f$ electrons, it follows that both initial (L,S) ground states are the same and that both sets of possible (L',S') final states of the configurations $f^{14-(n-1)}$ (BIS) and f^{n-1} (XPS) are also identical. In this situation, it is natural to assume that the intensities of the BIS final-state components are described by the same Q as those involved in the photoemission final states. This has been demonstrated[8] and is well confirmed by the BIS spectra of all rare-earth metals.[9] It must be pointed out that the total angular momentum J of the initial ground states of f^n and f^{14-n} are different and therefore the intensities of the J' multiplets of the BIS final states have been recalculated.

Figure 1 shows the raw spectra of Tb. The in-

tensities of BIS and XPS spectra have been fitted at E_F in order to obtain a continuous function in the whole energy range. The vertical bars indicate the predicted energies and intensities of the final states.[5,6] Peaks of negligible intensity have been omitted and the total intensity of narrowly spaced J' multiplets has been represented at their center-of-gravity position. The energy separations between the different (S',L',J') final states have been taken from uv-absorption measurements in rare-earth ions having the same number of $4f$ electrons as in the XPS and BIS final states.[6] These energy separations have been expanded for XPS and contracted for BIS (8–17% in both cases) to account for the variation of the $4f$ intra-atomic potential resulting from the different nuclear charge: Z in uv absorption, $Z+1$ in XPS, and $Z-1$ in BIS.[6] Theory and experiment are in good agreement. The extended valence states give a nonnegligible intensity contribution above E_F (Fig. 1) and no background correction has been undertaken; nevertheless, the experimental ratio of filled to unfilled $4f$ states is in rough accord with the theoretical value of 8:6. In BIS, the peaks are not as well separated as in XPS. The different instrumental resolutions alone cannot explain this so that final-state lifetimes are shorter above E_F than below it.

The previous discussion has emphasized the atomiclike character of the $4f$-electron excitations in rare-earth metals. We shall now consider only transitions to the lowest final state of the metal, corresponding to the minimum energy required to excite a $4f$ electron to E_F (Δ_-) or to excite an electron from E_F to the first empty $4f$ state (Δ_+). The origin of the energy scale being located at E_F in electron spectroscopies, we have defined here $\Delta_- < 0$ (in opposition to the definition of Herbst and co-workers[10–12] and $\Delta_+ > 0$. De-
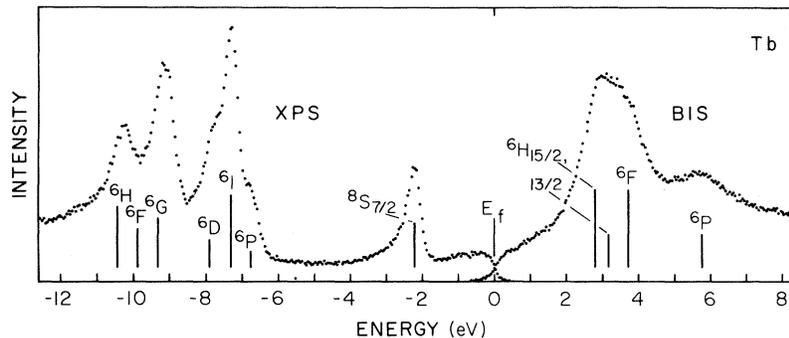
FIG. 1. $4f$ final states observed by XPS and BIS.

tailed calculations of these energies have been performed in the renormalized-atom approach[10-12] and the results have already been found to be in good agreement with XPS results.[5,6] The success of this comparison demonstrates the importance of the screening in the photoemission process of localized states. In the symmetrical BIS process, the additional electron in the $4f$ shell repels one d electron in order to maintain charge neutrality. This $4f^{n+1}$ final state is still highly localized and the renormalized-atom scheme is expected to predict the values of Δ_+ as well. The comparison between experiment and theory[11,12] reported in Fig. 2 confirms this statement, except for a small systematic shift discussed below. A good agreement is also found with previous BIS measurements of La[13] and Ce.[14] A particularly interesting situation is encountered when a $4f$ level approaches E_F. Such atoms can be expected to show spontaneous interconfiguration fluctuations (ICF) if the $4f$ level is pushed to E_F by the chemical environment. Some compounds of Im and Sm provide clear examples of ICF between 2+ and 3+ configurations.[5] It has recently been claimed[15] that surface atoms of metallic Sm are in a divalent configuration, whereas bulk atoms stabilize a trivalent configuration. We find, for Sm, $\Delta_+ = 0.65 \pm 0.2$ eV, which requires a sizable lowering of the $4f$ energy at the surface. The energy position of Δ_- in Ce has not yet been unequivocally
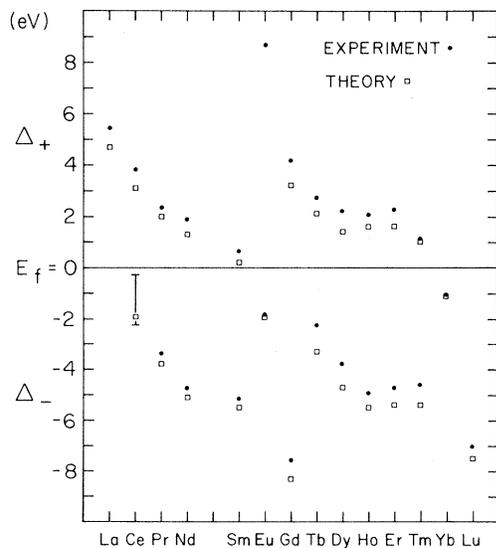
determined[5] but it should not lie far from E_F, since an ICF between 3+ and 4+ has been found in the α phase of the metal and in CeN.[16]

The most important physical consequence resulting from the small $4f$ orbital radius is the high Coulomb correlation energy U which prevents the formation of a $4f$ band when $U > W$ (Hubbard condition,[17] where W is the width of a hypothetical $4f$ band[10]). The order of magnitude of U has already been estimated from photoemission data.[18] Reasonable values lying between 5 and 7 eV are found for insulators and metals. In XPS spectra of mixed-valence compounds, the energy separation between the two photoemission final states originating from the different initial $4f$ populations is precisely the correlation energy. The values obtained in this way for Sm, Tm, and Yb compounds[5] are somewhat larger than the theoretical estimates for metals.[12] Our measurements of Δ_- and Δ_+ by XPS and BIS provide a straightforward and systematic determination of U for all rare-earth metals. Combining the two processes and making an energy balance shows that $\Delta_+ - \Delta_- = U$ ($\Delta_- < 0$), i.e., the minimum energy required to transfer within the metal a $4f$ electron from one atom to the $4f$ shell of another atom. In the example of Fig. 1, it is the energy difference between $^6H_{15/2}$ and $^8S_{7/2}$. The values of U, which can be measured in Fig. 2, are reported in Fig. 3 and compared with recent relativistic estimates.[11,12] The agreement is even better than for the Δ_+ and Δ_- related to E_F. It has been shown that single-particle estimates of U in metals are reduced by a factor of 4 when relaxation and screening are included.[10] In the renormalized-atom approach, the final-state screening

FIG. 2. Comparison of experimental and theoretical (Refs. 11 and 12) values of Δ_- and Δ_+. The experimental Δ_- value for Ce lies within the error bar.
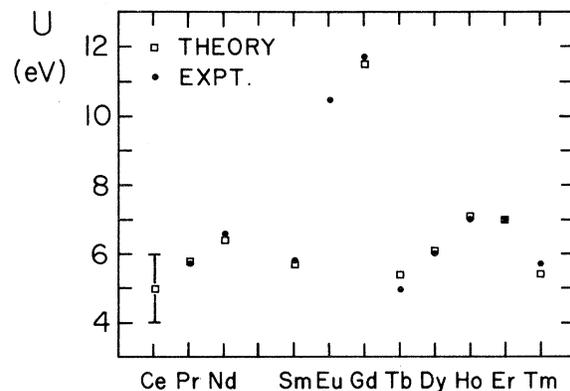
FIG. 3. Comparison of the experimental and theoretical (Refs. 11 and 12) values of the correlation energy U.

charge is constrained within the Wigner-Seitz cell. It appears to be a quite reasonable approximation, even if it does not necessarily minimize perfectly the final-state energy. Any inaccuracy of this type would symmetrically push Δ_- and Δ_+ away from E_F.[10] On the contrary, we observe a small parallel displacement of all the calculated values, which might be explained by the crude location of E_F based on an oversimplified band shape.[12]

We are very grateful to Professor G. Busch for his constant support and interest.

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ERRATA

VACUUM-POLARIZATION EFFECTS ON THOMSON CROSS SECTIONS IN A MAGNETIZED PLASMA. P. Mészáros and J. Ventura [Phys. Rev. Lett. 41, 1544 (1978)].

On page 1545, the caption of Fig. 1(b) should read "values of A including . . . ."

On page 1546 in the fifth line above Eq. (6) the correction term $3\delta(uv)^{-1}$ should have the dependence $(\omega/10^{16})^4$.

The affiliation of the authors both at the time of writing and at present is, for P. Mészáros, Institut für Astrophysik, Max-Planck-Institut für Physik und Astrophysik, 8000 München 40, West Germany, and for J. Ventura, Institut für Extraterrestrische Physik, Max-Planck-Institut für Physik und Astrophysik, 8046 Garching bei München, West Germany.

EFFECTS OF DISORDER ON THE TRANSITION TEMPERATURE AND TRANSPORT PROPERTIES OF A LOW-T_c A15 SUPERCONDUCTOR: Mo$_3$Ge. M. Gurvitch, A. K. Ghosh, B. L. Gyorffy, H. Lutz, O. F. Kammerer, J. S. Rosner, and Myron Strongin [Phys. Rev. Lett. 41, 1616 (1978)].

In the sixth line of the second column on page 1618, the expression "$\rho_{eff} = \bar{\rho}[\frac{2}{3}\langle(\Delta\rho)\rangle^2/\bar{\rho}^2]$" should read "$\rho_{eff} = \bar{\rho}[1 - \frac{2}{3}\langle(\Delta\rho)^2\rangle/\bar{\rho}^2]$." Also in line eleven of the same column, "$\langle(\Delta\rho)^2\rangle \propto l^{-3} \cong \beta\rho^{-3}$" should read "$\langle(\Delta\rho)^2\rangle \propto l^{-3} \cong \beta\bar{\rho}^3$."