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Ab initio studies of magnetism in strongly correlated electron systems

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Abstract

We present an ab initio based method which gives clear insight into the interplay between the band-f hybridization, the band-f coulomb exchange, and the crystal-field interactions, as the degree of 4f localization is varied across a series of strongly correlated cerium systems. The predictions for the ordered magnetic moments, magnetic structure, and ordering temperatures are in excellent agreement with experiment, including the occurrence of a *moment collapse* of non-Kondo origin. In contrast, spin and orbitally polarized ab initio density functional calculations and LDA + U calculations fail to predict, even qualitatively, the trend of the unusual magnetic properties. © 2001 Elsevier Science B.V. All rights reserved.

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Treating the consequences of correlation effects on magnetic behavior in the transitional (neither atomic like nor itinerant) 4f or 5f localization regime, provides one of the central problems of condensed matter physics [1,2]. There is an extremely interesting range of phenomena; treating the theory of these phenomena adequately, and achieving the ability of predicting the behavior of specific materials is particularly difficult [1,2]. An adequate treatment requires treating the interelectronic coulomb interaction, i.e. the correlation effects, as constrained by exchange symmetry [3–6]. In this

paper, we demonstrate an approach for treating these difficulties by predicting the interesting and complex behavior of an important series of cerium compounds.

The isostructural (rock-salt structure) series of the cerium mononictides CeX (X = P, As, Sb, Bi) and monochalcogenides (X = S, Se, Te) have become prototype model systems for study, because of their unusual magnetic properties [7–13]. These strongly correlated electron systems offer the opportunity to vary systematically the chemical environment and cerium–cerium separation on going down the pnictogen or chalcogen column, and hence tailor the degree of 4f localization from the weakly correlated limit in the lighter systems to the strongly correlated limit in the heavier systems

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[7–13]. The calculated single-impurity Kondo temperature, presented below, is much smaller than the magnetic ordering temperature; hence this series lies in the *magnetic* regime of the Kondo phase diagram [14]. Nevertheless, we demonstrate that the sensitivity of the band-f hybridization, band-f coulomb exchange, and crystal-field (CF) interactions to chemical environment gives rise to a variety of interesting unusual magnetic properties, in agreement with experiment across the series, including the occurrence of a non-Kondo moment collapse.

Experimentally, the large magnetic anisotropy changes from favoring $\langle 001 \rangle$ alignment in the pnictides to $\langle 111 \rangle$ in the chalcogenides. The low-temperature ordered magnetic moment increases with increasing lattice constant for the pnictides from $0.80\mu_B$ in CeP to $2.1\mu_B$ in CeSb and CeBi [7,8], while it decreases with increasing lattice constant for the chalcogenides from $0.57\mu_B$ in CeS to $0.3\mu_B$ in CeTe [7–9]. The magnetic moment collapse from CeSb to CeTe, with both systems having about the same lattice constant, is indicative of the sensitivity of the magnetic interactions to chemical environment. The ordering temperature increases from 8 K in CeP to 26 K in CeBi for the pnictides, whereas it decreases from 8.4 K in CeS to 2.2 K in CeTe [7–13,15]. Another unusual feature is the large suppression of the CF splitting, Δ_{CF} , of the $Ce^{3+} 4f_{5/2}$ multiplet between the Γ_7 -doublet CF ground state and the excited Γ_8 -quartet, from values expected from the behavior of the heavier isostructural rare-earth pnictides or chalcogenides [16,17]. This can be understood [18] as arising from band-f hybridization effects.

In this paper, we present material-predictive results from two methods, one *ab initio* based and one *ab initio*, to study the change of magnetic properties across this series. The first, *ab initio* based, method employs the degenerate Anderson lattice model which explicitly incorporates the hybridization and the coulomb exchange interactions on an equal footing [4,5]. This method gives clear insight into the role of the three pertinent interactions: (1) The band-f hybridization-induced inter-cerium magnetic coupling; (2) the corresponding effects of band-f coulomb exchange; and (3) the CF interaction. This approach allows us to understand

the interplay between these interactions as the degree of 4f localization is varied across the series. It predicts magnetic moments, magnetic structures, and ordering temperatures in excellent agreement with experiment. Thus, this approach allows to understand and predict a number of key features of observed behavior. First, is the very low moment and low ordering temperature of the antiferromagnetism observed in CeTe, an incipient heavy Fermion system [19]. We predict the magnetic moment and ordering temperature collapse from CeSb to CeTe, both systems having about the same lattice constant but CeTe having an additional p electron. The earlier work of Sheng and Cooper [4,5] showed that this magnetic ordering reduction is accurately predicted without including any CF effects. An erroneous statement appeared in the recent review article by Santini et al. [20] stating that CF effects played an important role in the calculated results of Sheng and Cooper [4,5]. This is incorrect, since CF effects were *not* included in these calculations. In this paper we show that including the CF effects modifies this behavior only quantitatively. Thus, the origin of the moment collapse is neither of Kondo origin or CF effect. Second, our results demonstrate the great sensitivity of the relative importance of hybridization and coulomb exchange effects on magnetic ordering depending on the degree of 4f localization. The band-f coulomb exchange mediated interatomic 4f–4f interactions are more important for the magnetic behavior of the heavier, more localized, systems; whereas the hybridization-mediated coupling is more important for the lighter, more delocalized systems. Third, we show that for the lighter more delocalized systems the CF interactions are much larger than the inter-cerium interactions and hence dominate the magnetic behavior. Finally, we predict the experimentally observed change of the ground-state magnetic structure from the $\langle 001 \rangle$ AF-IA ($\uparrow\uparrow\downarrow\downarrow$) in CeBi and CeSb to the $\langle 001 \rangle$ AF-I ($\uparrow\downarrow$) in CeAs and CeP. In sharp contrast, the second, *ab initio* method, based on density functional theory within the local density approximation (LDA) [21,22], and on the LDA + U scheme [23] fail to predict, even qualitatively, the trend of magnetism in this series of strongly correlated electron systems.

For the model Hamiltonian of the first method [4]

$$H = \sum_k \varepsilon_k c_k^\dagger c_k + \sum_{Rm} \varepsilon_m f_m^\dagger(R) f_m(R) + \frac{U}{2} \sum_{R, m \neq m'} n_m(R) n_{m'}(R) + H_1, \quad (1)$$

$$H_1 = \sum_{kmR} [V_{km} e^{-i\mathbf{k} \cdot \mathbf{R}} c_k^\dagger f_m(R) + \text{h.c.}] - \sum_{kk'} \sum_{mm'} J_{mm'}(\mathbf{k}, \mathbf{k}') e^{-i(\mathbf{k}-\mathbf{k}') \cdot \mathbf{R}} c_k^\dagger f_m^\dagger(R) c_{k'} f_{m'}(R), \quad (2)$$

the parameters involved, i.e. the band energies ε_k , the f-state energy ε_m , the on-site coulomb repulsion U , the hybridization matrix elements, V_{km} , and the band-f coulomb exchange $J_{mm'}(\mathbf{k}, \mathbf{k}')$, are evaluated on a wholly ab initio basis from non-spin polarized full potential linear muffin tin orbital (FPLMTO) [21] calculations. Note, that the band-f exchange interaction in H_1 is also included in the LDA treatment of the first two terms in Eq. (1). Thus, as in all approaches combining model Hamiltonians with density functional theory (for example LDA + U), this ab initio-based approach includes a certain amount of double counting of the band-f exchange interaction. Our ab initio-based approach is designed to correct for the situation that the treatment of the coulomb interaction involving the rather localized 4f electrons is rather poor within LDA.

Because both the hybridization and coulomb exchange matrix elements are much smaller (~ 0.1 eV) than the intra atomic coulomb interaction U (6 eV), one can apply perturbative techniques and evaluate from first principles the anisotropic two-ion 6×6 interaction matrices, $E_{m_1 m'_1}^{m_2 m'_2}(\mathbf{R})$, which couple the two f-ions [3–5]. The Ce–Ce interactions have three contributions: the wholly band-f coulomb exchange mediated interaction proportional to $J_{mm'}^2$, the wholly hybridization-mediated exchange interaction proportional to V_{km}^4 , and the cross term proportional to $V_{km}^2 J_{mm'}$. The low-temperature magnetic moment and the ordering temperature can then be determined by use of a mean-field calculation [3–5,8]. We have

previously [3–5] applied this method to investigate the magnetic properties of the heavier (i.e., larger lattice constant) cerium systems (CeBi, CeSb, and CeTe). However, these calculations did not take into account the CF interaction and employed a warped muffin-tin LMTO calculation for the parameters entering the model. The excellent agreement found [4,5] with experiment for the magnetic moment and ordering temperature is relatively unaffected by the CF interaction, because the CF interaction in the heavier Ce systems is smaller than the two-ion interactions.

The second method employs ab initio electronic structure calculations, with the 4f states treated as band states, based on the FPLMTO method [21] using (1) only spin polarization, with the orbital polarization included only through the spin–orbit coupling, (2) both spin and orbital polarization [22], and (3) the LDA + U approach [23].

The crystalline field, neglected in the previous calculations [4–6] is expected to affect the magnetic behavior considerably, if it is large. The experimentally observed crystal-field splitting is $\Delta_{\text{CF}}^* = \Delta_{\text{CF}} + \delta\Delta_{\text{CF}}$, where Δ_{CF} is the “bare” CF splitting and $\delta\Delta_{\text{CF}}$ is the hybridization-induced CF splitting. Hybridization between the band states and the f states [Eq. (1) in Ref. [3]] gives rise to a shift of the bare CF energy levels of the 4f state multiplet. The bare CF energy of the $|\Gamma_i\rangle$ state can be evaluated in principle from FPLMTO calculations, namely, $E_{\Gamma_i} = \langle \Gamma_i | V(\mathbf{r}) | \Gamma_i \rangle$, where $V(\mathbf{r})$ is the 4f muffin-tin potential expressed as a sum of lattice harmonics invariant under the f-ion point group operations, and the f electrons are treated as localized rather than itinerant states. In the first method, we treat the 4f states as core states, and allow them to interact only with the spherical component of the effective one-electron potential $V(\mathbf{r})$. Thus, both the hybridization-induced shift of the CF splitting and the interaction of the atomic-like 4f state with the non-spherical components of the potential, giving rise to the CF splitting, are not included in the calculation of the model Hamiltonian parameters. Here, we generalize the first, ab initio based, method to include both the interatomic two-ion 4f–4f coupling and the CF interactions (one-ion term) on an equal footing and to employ a full potential LMTO evaluation of the model

Hamiltonian parameters. While the effect of the full potential on both the hybridization and coulomb exchange interactions is small, including the CF interaction will be shown to play a role as important as the interatomic 4f–4f interactions for understanding and predicting the overall trend in the unusual magnetic properties, as one chemically tunes the degree of 4f localization. The resultant Hamiltonian is

$$H = - \sum_{i,j} \sum_{\substack{\mu,\nu \\ \varepsilon,\sigma}} \zeta_{\mu\nu}^{\varepsilon\sigma}(\theta_{ij}) e^{-i(\mu-\nu+\varepsilon-\sigma)\phi_{ij}} \\ \times c_{\varepsilon}^{\dagger}(j)c_{\sigma}(j)c_{\mu}^{\dagger}(i)c_{\nu}(i) + B_4 \sum_i (O_4^0(i) + 5O_4^4(i)), \quad (3)$$

where the $\zeta_{\mu\nu}^{\varepsilon\sigma}(\theta_{ij})$ are the two-ion interaction exchange matrices rotated to a common crystal-lattice axis [3], and the O_4^0 and O_4^4 are the Stevens operators equivalents acting on the Ce^{3+} free-ion $4f_{5/2}$ multiplet [24]. The effective CF splitting is $\Delta_{\text{CF}}^* = 360B_4$; a positive B_4 value gives the Γ_7 ground state, which is experimentally observed. While work in progress is currently aimed at evaluating the CF splitting on a wholly ab initio basis, in the absence of an ab initio value of the CF interaction in this class of strongly correlated cerium systems, B_4 is evaluated by setting Δ_{CF}^* equal to the experimental values listed in Table 3 [10,17].

In Table 1, we present the calculated values of the zero-temperature cerium magnetic moment from the FPLMTO electronic structure calculations assuming a ferromagnetic structure. Listed in the table are values both with and without the orbital polarization correction, beyond effects of spin–orbit coupling, taken into account. Note, the importance of including the orbital polarization in these 4f correlated electron systems. As expected, in all cases, the orbital polarization is found to be opposite to the spin polarization. Comparison of the total energies predicts that the magnetic anisotropy changes from the $\langle 001 \rangle$ direction in the pnictides to the $\langle 111 \rangle$ in the chalcogenides, in agreement with experiment. LDA calculations for CeSb for an AF–I structure give low spin and orbital moments of $-0.29\mu_B$ and $0.43\mu_B$, respectively, and an energy higher than the ferromagnetic

Table 1

Calculated and experimental [7–11] values of ordered magnetic moments for the cerium systems in μ_B . Listed are the FLMTO values for the spin moment μ_S , orbital moment μ_L , and total moment μ , for spin polarization (SP) only and for both spin and orbital polarization (OP) [22]

	SP			SP + OP			EXP
	μ_S	μ_L	μ	μ_S	μ_L	μ	μ
CeS	– 1.00	0.91	– 0.09	– 1.24	1.99	0.75	0.57
CeSe	– 1.08	1.02	– 0.06	– 1.26	2.07	0.81	0.57
CeTe	– 1.15	1.28	0.07	– 1.31	2.29	0.98	0.30
CeP	– 0.80	0.55	– 0.25	– 0.85	1.27	0.43	0.80
CeAs	– 0.84	0.64	– 0.20	– 0.85	1.42	0.57	0.80
CeSb	– 0.86	0.74	– 0.12	– 0.91	1.61	0.70	2.06
CeBi	– 0.86	0.74	– 0.12	– 0.95	1.69	0.74	2.10

state. Thus, except perhaps for the lighter chalcogenides (CeS and CeSe), comparison of the ab initio and experimental values for the magnetic moment indicates the failure of the LDA calculations to treat properly the correlation effects of the 4f states within the LDA as the degree of 4f correlations increases in the heavier pnictide systems. LDA + U calculations for the heavier systems, CeSb and CeTe, increase the magnetic moment to $2.2\mu_B$ and $1.4\mu_B$, respectively [23]. Similarly, we find that the LDA + U method increases the magnetic moment for the lighter, more delocalized systems, CeP and CeS to $2.0\mu_B$ and $1.9\mu_B$, respectively. Thus, the LDA + U method enhances the magnetic moment across the entire series and fails to predict the trend of magnetic properties. Furthermore, all ab initio calculations fail to predict the moment collapse from CeSb to CeTe, the latter being an incipient heavy Fermion system [19].

In Table 2, we list the values of the $m = m' = \frac{1}{2}$ matrix elements (characteristic matrix elements of the 6×6 exchange interaction matrix) for the first three-nearest-neighbor shells for the light (CeP and CeS) and the heavier compounds (CeSb and CeTe). Listed separately are the three contributions to the interatomic 4f–4f interactions arising from band-f hybridization (V^4), band-f coulomb exchange (J^2), and the cross term. It is important to note that

Table 2

Values of the $m = m' = \frac{1}{2}$ matrix elements of the 6×6 interatomic 4f–4f interaction matrix $E_{m_m m'_m}^{m_m m'_m}(\mathbf{R})$, for the first three nearest-neighbor shells in degrees Kelvin. We list also values of the hybridization induced (E_{V^+}), cross term (E_{V^2J}), and coulomb exchange (E_{J^2}) contributions

	CeP			CeS		
	E_{V^+}	E_{V^2J}	E_{J^2}	E_{V^+}	E_{V^2J}	E_{J^2}
$R = (\frac{1}{2}\frac{1}{2}0)$	2.23	0.64	1.53	0.85	−0.40	1.50
$R = (100)$	6.39	0.27	1.65	−1.60	0.04	−0.80
$R = (1\frac{1}{2}\frac{1}{2})$	−0.08	−0.02	0.16	0.38	−0.16	0.13
	CeSb			CeTe		
	E_{V^+}	E_{V^2J}	E_{J^2}	E_{V^+}	E_{V^2J}	E_{J^2}
$R = (\frac{1}{2}\frac{1}{2}0)$	0.70	0.34	7.30	0.17	−0.19	2.90
$R = (100)$	2.07	0.07	10.21	−0.19	0.04	−1.69
$R = (1\frac{1}{2}\frac{1}{2})$	−0.02	−0.03	0.40	0.04	−0.06	−0.01

while the coulomb exchange mediated interactions overall dominate the magnetic behavior for the heavier, more localized, 4f systems, the opposite is true for the lighter, more delocalized, systems where (in the absence of CF effects) the hybridization mediated interactions dominate the magnetic behavior. This change of behavior of the interatomic 4f–4f interactions is a result of the sensitivity of the hybridization and coulomb exchange to the degree of 4f localization. Equally important, is that while both first- and second-nearest-neighbor 4f–4f interactions are ferromagnetic (FM) for CeSb, there is an interplay between ferromagnetic first-nearest-neighbor and antiferromagnetic (AF) second-nearest-neighbor interactions for CeTe. This results in a saturated moment for CeSb and in the ordered magnetic moment collapse for CeTe (see Table 3).

To determine whether the magnetic moment collapse might be of Kondo origin, we have evaluated the single-impurity Kondo temperature, $k_B T_K = D(D/\xi)^{4/3}(D/\Delta_{CF}^*)^2 e^{-1/2\rho(E_F)|J(E_F)|}$, across the series, for the case of a Γ_7 ground-state [25]. Here, D is the conduction-electron bandwidth, $\rho(E_F)$ is the density of states of the conduction electrons at the Fermi energy, E_F , ξ is the spin–orbit coupling, and $J(E_F)$ is the conduction electron–f effective exchange interaction at E_F , which has contributions both from the coulomb exchange interaction in Eq. (2), provided that it is negative, and the

Table 3

Calculated (from the first, ab initio based, method) and experimental [6–10] values of the zero-temperature ordered moment μ and the ordering temperature T_N with and without the CF interaction across the series. Also listed are the experimental values [10,17] of the CF splitting, Δ_{CF}^*

	Δ_{CF}^* (K)	μ (μ_B)			T_N (K)		
		No CF	CF	Exp	No CF	CF	Exp
CeS	140	1.80	0.73	0.57	1.0	11.0	8.4
CeSe	116	1.10	0.79	0.57	2.5	14.0	5.7
CeTe	32	0.60	0.46	0.30	8.0	5.0	2.2
CeP	150	2.10	0.73	0.81	14	11	8
CeAs	137	2.10	0.74	0.85	16	13	8
CeSb	37	2.10	1.80	2.06	20	18	17
CeBi	8	2.10	2.10	2.10	40	40	26

hybridization-induced interaction $J_{\text{hyb}}(E_F) = -V^2(E_F)U/|E_f - E_F|(|E_f - E_F| + U)$. The coulomb exchange interaction at E_F is positive across the entire series and hence cannot give rise to the Kondo effect. Thus, only $J_{\text{hyb}}(E_F)$, can give rise to the Kondo effect [25]. Using the ab initio values of the parameters entering the expression for T_K , we find that $T_K \ll T_{\text{ord}}$ across the series ($T_K < 10^{-4}$ K). These results show that the moment collapse from CeSb to CeTe is of non-Kondo origin. Rather, it results from an interplay of FM and AF interatomic 4f–4f interactions which arises purely from differences in the underlying electronic structure.

Listed in Table 3 are the calculated zero-temperature ordered moment and ordering temperature, T_N , from the first, ab initio based, method, with and without the CF interaction. It is clear that for the heavier systems (CeBi, CeSb, CeTe) the effect of the CF interaction on the magnetic moments is small, and it is slightly more pronounced on the ordering temperatures. This is due to the fact that for the more localized systems the CF interaction is smaller than the two-ion interactions. This is the reason that the previous calculations [4,5], neglecting the CF interaction, gave results in excellent agreement with experiment. On the other hand, for the lighter more delocalized systems the CF interactions are much larger than the interatomic 4f–4f interactions,

and hence dominate the magnetic behavior. Overall, the first, *ab initio* based, approach which takes into account all three pertinent interactions (hybridization, coulomb exchange, and CF interactions) on an equal footing, yields results for both the zero-temperature moment and the ordered temperature (a more stringent test for the theory) in excellent agreement with experiment.

A final corroboration of the success of the first *ab initio*-based method is that it predicts the experimentally observed change of the ground-state magnetic structure from the $\langle 001 \rangle$ AF-IA in CeBi and CeSb to the $\langle 001 \rangle$ AF-I in CeAs and CeP [7,15]. The sign (FM or AF) of the $|\pm 5/2\rangle$ matrix elements of the 6×6 exchange matrix determines the interplanar interaction between successive (001) Ce planes. We find, that for the heavier compounds (CeBi and CeSb) the $|\pm 5/2\rangle$ matrix elements of the coulomb exchange matrix are FM and hence favor the $\uparrow\uparrow\downarrow\downarrow$ type, while in the lighter systems (CeAs and CeP) the $|\pm 5/2\rangle$ matrix elements of the hybridization-induced two-ion matrix are AF, and hence they favor the $\uparrow\downarrow$ type.

In conclusion, we have applied two different, viz., *ab initio* based and *ab initio* LDA methods to study the dramatic change of magnetic properties across a series of strongly correlated electron systems which offer the opportunity to chemically tailor the different type of interactions (band-f hybridization, band-f coulomb exchange, and CF interactions), pertinent to the magnetic behavior. The first, *ab initio* based, approach which explicitly takes into account the interplay of the three pertinent interactions, gives results in excellent agreement with experiment for all compounds in the series, including the *moment collapse* from CeSb to CeTe and the trend of moments and ordering temperatures across the series. On the other hand, the second, *ab initio* LDA, method gives good results for the lighter chalcogenides, but it entirely fails to give, even qualitatively, the trend of the unusual magnetic behavior.

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