Modeling the actinides with disordered local moments

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A first-principles disordered local moment (DLM) picture within the local-spin-density and coherent potential approximations of the actinides is presented. The parameter-free theory gives an accurate description of bond lengths and bulk modulus. The case of δ-Pu is studied in particular, and the calculated density of states is compared to data from photoelectron spectroscopy. The relation between the DLM description, the dynamical mean-field approach, and spin-polarized magnetically ordered modeling is discussed.

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I. INTRODUCTION

The elemental actinide metals, Pu in particular, exhibit several unique features. They are among the most complex elements in nature, with a rich set of allotropes,[1] of which several have complex low-symmetry crystal structures.[2] Pu, for example, is the only element with seven condensed matter phases at zero pressure of which one (the δ phase) demonstrates negative thermal expansion. The understanding of these anomalous properties is a serious challenge. Several of the main features of the actinides can be understood in terms of the progressive filling of the $5f$ shell. In the light actinides Th–Np, the $5f$ electrons are itinerant and participate in the bonding, whereas in the heavier actinides Am–Cf, the $5f$ electrons are localized and exhibit behavior more similar to the lanthanides. Plutonium takes a particular place between these extremes. The low-temperature α phase has been shown to be well described with an itinerant bonding $5f$ electrons whereas the high-temperature phases with their increased volumes suggests a localized or partly localized configuration. This behavior indicates a Mott-like transition of the f electrons similar to the α-γ transition in cerium.[3,4] In fact, Katsnelson *et al.*[5] identified this Mott transition with the α-δ transition in Pu.

There have been several first-principles approaches to calculating the properties of the actinides.[2,5–16] Although the light actinides are well described within density functional theory, the local density approximation (LDA) fails in general to describe the $5f$ localization which occurs in actinide compounds, elemental Pu at high temperature, and in the actinides past Pu. A number of techniques have therefore been developed to include correlation effects beyond the LDA in order to describe the partially localized $5f$ electronic structure. These include LDA+U,[17,18] orbital polarization,[16] and the mixed-level model.[13] Of particular relevance to the work presented here are recent attempts to combine the LDA and dynamical mean-field theory (DMFT). DMFT has been shown to be a very useful approximation for the consideration of strongly correlated electron systems (for a review, see Ref. 19). The LDA combined with the DMFT may provide a first-principles technique to study correlated electron materials, and there have been several attempts to apply implementations of LDA+DMFT (Refs. 20 and 21); for a review, see Refs. 22 and 23. Recently this LDA+DMFT approach has been applied to the Pu problem.[24] The LDA +DMFT approach gives an opportunity to describe correlation effects on the electronic structure and properties of *d*- and *f*-electron systems. However, the technique is cumbersome and it is not *completely ab initio* because of the problem with the choice of U (see, e.g., Ref. 22). In addition, implementations of DMFT are computationally intensive which makes the calculation of complex structures difficult. Sometimes, because of the complexity of the calculations, uncontrollable approximations are made, e.g., using a single U parameter instead of a complete interaction matrix.[24,25,26]

It is commonly accepted that accounting for Hubbard correlation effects is of crucial importance for *f*-electron systems. On the other hand, some of these effects can be taken into account, in an approximate way, in the framework of more traditional density functional techniques. This is the approach taken in the present study where we have modeled the actinides by means of disordered local moments[27] (DLM's) within the local spin density approximation and the coherent potential approximation[28] (LSDA+CPA).

The purpose of the present work is to investigate if correlation effects of the actinides can be simulated by means of a parameter-free first-principles DLM approach, based on the LDA. In some way our present work may be seen as a natural extension of the early work by Skriver *et al.*,[6] where the electron-electron interactions that are responsible for the localization of the $5f$ shell of Am were sucessfully modeled by a spin-polarized LDA calculation. Here we consider a somewhat more general picture where the stability of a DLM configuration is also considered. The DLM picture, even if it is insufficient for a complete description, might lead to some insights for the understanding of the electronic structure of the actinides.

Consider, first, the status of the DLM approach in the many-body lattice models like the Hubbard or *s*-*f* exchange (''Kondo lattice'') model. The key point is an equivalence

between a many-body interacting system with Coulomb on-site interactions and a one-electron system in fluctuating charge and spin fields. This equivalence, which can be proved by the Hubbard-Stratonovich transformation, is a base of spin-fluctuation theories of itinerant-electron magnetism.[29] In a complete theory, the charge and spin fields are dynamically fluctuating both in space and time. However, a ''static approximation,'' where we neglect the dynamics of the fluctuations,[30,31] captures an important part of the correlations, while greatly simplifying the formalism, and may be sufficient for many problems of interest. In this case the correlated system is described in terms of a DLM alloy and a CPA for this alloy becomes equivalent to the ''Hubbard III'' approximation[32] for the original many-body problem (see Ref. 33). The Hubbard III approximation gives qualitatively the correct picture of the electronic structure both in atomic and broadband limits and can describe the metal-insulator (Mott) transition for half-filled bands when U is of the order of the bandwidth.[32]

The spatial fluctuations of the exchange on-site field can lead to a splitting of the energy spectra (provided the fluctuations are larger than the bandwidth) which corresponds, in the Hubbard model, to the Hubbard band splitting. The self-energy in the DLM picture is energy dependent and has an imaginary part describing the damping of the electrons on spin fluctuations. This distinguishes the DLM approach not only from magnetically ordered LSDA calculations but also from LDA+U, self-interaction correction (SIC), and the Hartree-Fock approximation. In this sense, the DLM-CPA approach can be considered as a particular case of the ''LDA ++'' (LDA+U+Σ) approach[21] with a local, energy-dependent, complex self-energy. However, in contrast to schemes taking into account Hubbard correlations, it is completely *ab initio*. A shortcoming of this approximation is an incorrect description of electron damping near the Fermi level—i.e., the absence of the Kondo resonance—which is a consequence of the *quantum* character of spin, as well as problems describing localization in systems that do not have half-filled (or completely filled) electron shells. However, this shortcoming may be of minor importance for the description of the electron energy spectrum at large energy scales as well as for calculations of the total energy and related characteristics such as the equilibrium volume and elastic moduli. Note also that this finite damping, because of electron scattering by spin fluctuations, is a physically correct picture for high enough temperatures.

Comparing the many-body lattice models with the density functional approach one is faced with the well-known ''Hubbard U versus Stoner I'' problem—i.e., with the inadequacy of the LDA approach near the atomic limit.[17,21] On the other hand, for *moderately* correlated systems such as, e.g., 3d metals, the main correlation effects are connected with spin degrees of freedom and can be described, in principle, based on the LSDA electronic structure. Of course, it is difficult to say *a priori* where the boundary is between ''moderately correlated'' and ''strongly correlated'' systems. We will demonstrate that, at least for early actinides, a LSDA-DLM description of the electronic structure turns out to be rather successful.

Due to the localized character of the spin moments, any ordered magnetic structure will resemble the result of the DLM description. It has often been noted that localization effects could partly be accounted for by way of exchange spin splitting of the 5f band, and despite an unphysical long-range magnetic ordering (absent in the DLM approach), several spin-polarized ferromagnetic (FM) and antiferromagnetic (AFM) calculations have been performed.[5,6,8,14,16] The presented DLM model gives a natural generalization to the paramagnetic state.

First we discuss some calculational details and then present the calculated volumes and bulk moduli for the actinide series. We then look at the results for δ-Pu in detail, and the results are compared with different alternative approaches and experiments.

II. CALCULATIONAL DETAILS

All total energies and densities have been calculated self-consistently within the framework of density functional theory,[35,36] in the LDA in the nonmagnetic cases and within the LSDA for the spin-polarized systems,[37–39] with the local exchange-correlation functional by Perdew *et al.*[40]

We used the basis set of the *s*, *p*, *d*, and *f* linear muffin-tin orbitals (LMTO's) in the tight-binding representation and the atomic sphere approximation (ASA) for the crystal potential.[41–44] The method was implemented within the scalar relativistic Green's function technique.[45–48] Spin-orbit coupling was not included, and all calculations are at $T=0$. The disorder of local spin moments was treated within the CPA, and other details relevant for the present calculation can be found in Refs. 47 and 49.

Since the interatomic distance is known to be the most important factor that determines the energetic of an actinide and since we are mainly interested in trends rather than in a detailed quantitative description of all the different phases of the actinides, calculations were performed for the fcc crystal structure only.

III. DISORDERED LOCAL SPIN MOMENT PICTURE OF THE ACTINIDES

Figure 1 shows a comparison between experimental and calculated Wigner-Seitz radii for the actinide metals. For the nonmagnetic LDA calculation, we find a parabolic behavior typical of bonding through a series such as the transition metals. This is in full agreement with the pioneering calculations of Skriver *et al.*,[6] but fails do describe the volumes of the heavy actinides. Within the DLM picture, on the other hand, we find a substantial improvement. For the light actinides Th–U, results are identical to the nonmagnetic LDA calculation, though for Np we find a slightly increased volume. For the later actinides we find an abrupt volume increase in close agreement with the experimental values with the transition taking place at Pu, which has an intermediate volume close to the value of the high-temperature δ phase in the fcc structure. The results in Fig. 1 are, as mentioned, quite close to the FM data presented by Skriver *et al.*[6] In this work the localization of the 5f state of Am was shown to result from the equivalence between a localized Wannier rep-

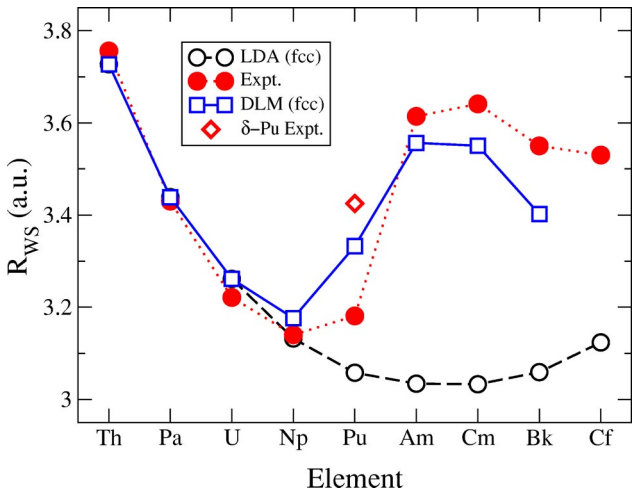

FIG. 1. Comparison between the experimental (Ref. 7) and calculated atomic Wigner-Seitz radius R_{WS} for the actinide metals.

resentation and an itinerant Bloch representation for systems with a completely filled band, which is the case for spin-polarized Am.

We find similar results for the bulk moduli. In Fig. 2 we display a comparison between the experimental bulk modulus for the ground-state structures and the calculated bulk modulus in the fcc structure. The LDA calculation gives a fairly good description of the early actinides but fails completely for the later actinides. The DLM picture, on the other hand, gives a significantly improved result where, for example, the bulk modulus of Pu is reduced by a factor of 2, though still somewhat higher than the experimental result for δ-Pu.

Given the fact that the results are from parameter free *ab initio* calculations without considering the exact crystal structures and spin-orbit coupling the agreement between the calculated equilibrium volumes and bulk moduli with experimental values is remarkably good and the results clearly indicate the ability of the LSDA+CPA approach within the

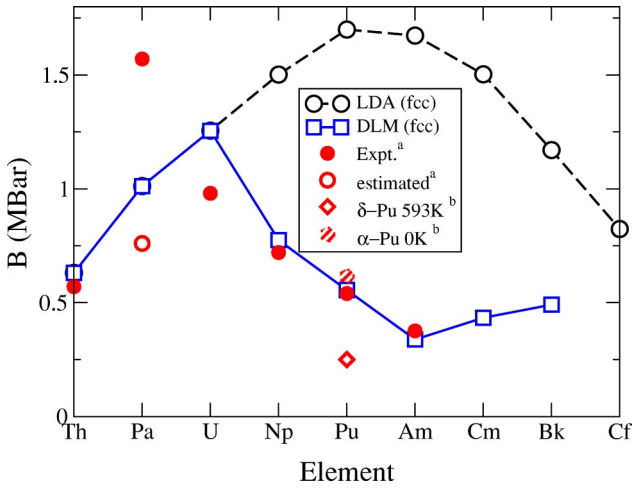

FIG. 2. Comparison between the experimental and calculated bulk modulus for the actinide metals. The experimental data are given in (a) Ref. 7 and (b) Ref. 56.

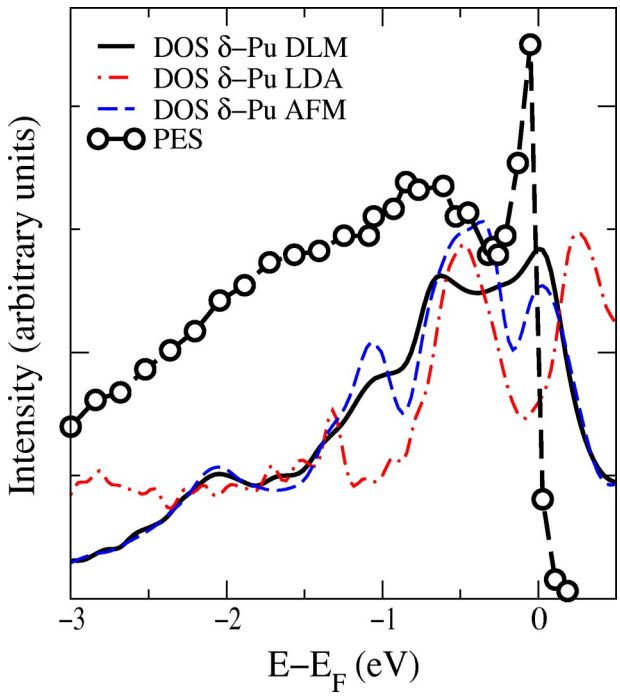

FIG. 3. Comparison between the calculated DOS within the DLM description, nonmagnetic LDA, an antiferromagnetic (AFM) structure, and the photoemission spectra (PES) (Ref. 50) for δ-Pu.

DLM picture to model important correlation effects beyond LDA in the $5f$ band, without incorporating long-ranged magnetic ordering.

The mechanism behind the improved description of the equilibrium volume and bulk modulus is the formation of local disordered moments. This gives rise to a band splitting and partial localization of the $5f$ electrons which reduces the bonding resulting in an increased lattice constant and reduced bulk modulus. For Th and Pa local spin moments are still quenched, and for U only a negligible moment of about $0.07\mu_B$ is formed. Within our DLM scheme, neptunium has a moment of $1.69\mu_B$. Though this has little effect on the equilibrium lattice constant, the bulk modulus is reduced by a factor of 2. For Pu a spin moment of $4.76\mu_B$ is found in the DLM calculation, which corresponds to an almost complete spin polarization of the $5f$ electrons. For Am and Cm a moment of $6.57\mu_B$ and $6.90\mu_B$ is formed, respectively. For Bk the disordered local moment is slightly reduced to $5.61\mu_B$. Notice that fully relativistic calculations, including the spin-orbit interaction, would reduce the moments. In the case of δ-Pu from about $5\mu_B$ to less than $2\mu_B$ (Ref. 8) and for Am the total moment can be expected to be $\sim 5\mu_B$ (Ref. 9). However, the formation of a $J=0$ atomic ground state comes natural from a completely localized $5f$ shell[7] and is consistent with experimental data.

IV. δ-PU

Figure 3 shows the calculated density of states (DOS) for Pu in comparison with the results of photoelectron spectroscopy.[50] The LDA curve has qualitatively a very different behavior compared to experiments. For example, the

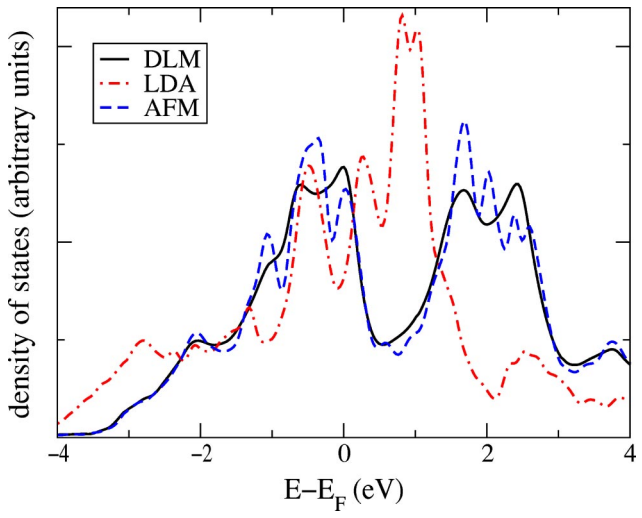

FIG. 4. Calculated DOS for δ-Pu within the DLM description in comparison with the nonmagnetic LDA DOS and an antiferromagnetic (AFM) LSDA DOS.

peak at the Fermi level seen in the photoemission spectra is absent. The DLM DOS, on the other hand, is in qualitative agreement with experimental data. The DOS is similar to the LDA-DMFT spectra by Savrasov *et al.*[24] (calculated at 600 K), but the quantitative agreement for the DLM picture is better.

The electronic structure is strongly modified in the DLM picture compared to the LDA calculation. The $5f$ band is split, as shown in Fig. 4, due to the formation of local disordered moments, leading to an effective energy lowering of the occupied $5f$ band mass. The same effect is found also for the AFM calculation. This leads to a decreased bonding, increased equilibrium lattice constant, and a reduced bulk modulus. The effect is similar to the results of LDA+U, LDA++, and LDA-DMFT. In contrast to some of these models we here have an improved agreement with the photoelectron spectra and the result is similar to what was found in the mixed-level model by Eriksson *et al.*[13] Although a direct full comparison between the Kohn-Sham eigenspectra and the photoemission data may not strictly be possible, the data clearly indicate a resonance at the Fermi level which is not present in the LDA description.

In Fig. 3 we also display the density of states for an antiferromagnetic (AFM-LSDA) calculation. Though, resembling the general DLM $5f$ band split, the DOS is in less agreement with photoemission data. The antiferromagnetic solution is about 3 mRy lower in energy compared to the DLM calculation. However, at finite temperatures this energy difference is compensated by the magnetic entropy contribution in the disordered case. This is an important feature of the DLM model that differs from magnetically ordered descriptions.

V. DISCUSSION

There are two principal approaches for describing the α-γ transition in Ce and the α-δ transition in Pu: the Mott transition model by Johansson[3–5] and the Kondo-collapse model of Allen and Martin.[51] An important question is thus what is more important for the energetics of the transitions: the appearance of the Hubbard gap or the formation of the Kondo resonance? The first feature is taken into account in the DLM scheme whereas the second one is not. Note that the Kondo resonance has small spectral weight, so it is not obvious that ignoring it is an essential shortcoming. Moreover, for both Ce and Pu there are some arguments connecting the Mott transition to the peculiarities of the atomic electronic structure (atomic collapse[52]). These peculiarities can obviously be taken into account in the local spin-density approach and thus in the DLM description. Note that this collapse phenomenon, leading to a sharp dependence on the bandwidth and lattice constant, leads to a first-order phase transition. Therefore the difference between the description of the Mott transition in the DLM or the Hubbard III approximation (continuous transition[30,34]) and DMFT (first-order transition; see Ref. 53 and references therein), which is very essential for the Hubbard model, does not play a serious role for real actinide systems where the transition is essentially of first order for ''quasi-one-electron'' reasons.

As for the description of magnetic properties at high temperatures T, the static approximation gives a qualitatively correct picture. The magnetic susceptibility χ is proportional to $\langle \epsilon^2 \rangle / T$, where ϵ is the exchange on-site field. The susceptibility corresponds to the paramagnetic Pauli spin susceptibility, provided that the exchange splitting fluctuations are Gaussian near the point $\epsilon = 0$, and to the Curie-Weiss susceptibility, provided that spontaneous spin splitting exists.[54] The description of finite-temperature magnetism of transition metals in the DLM-CPA approach[27] is different from the DMFT treatment[55] only by the consideration of spins in a classical way; in the Heisenberg model, it corresponds to the appearance of the multiplier S^2 instead of the correct factor $S(S+1)$ in the Curie constant.

The DLM picture leads to an expected Curie-Weiss behavior of the magnetic susceptibility for δ-Pu. However, recent experiments with Al- and Ga-stabilized δ-Pu show only a vanishingly small temperature dependence of the magnetic susceptibility (see Fig. 2 in Ref. 57). This is also consistent with other susceptibility measurements,[58,59] though Curie-Weiss behavior has sometimes been claimed.[57,60] The reason, explaining the absent Curie-Weiss behavior, could either be due to crystal field splitting and the formation of a nonmagnetic multiplet[13] or because of the occurrence of a Kondo resonance that may diminish the temperature dependence of the susceptibility provided that the resonance width (''Kondo temperature'') is larger than T. At least the first explanation could possibly be included separately in the DLM picture, but the second one can be described only within the framework of DMFT. At the same time, it is important to realize that the intention with the DLM picture is to model some of the main characteristics of the energetics of the actinides, and it does not necessarily describe the magnetic properties correctly.

VI. SUMMARY

In summary we have presented a first-principles disordered local moment method within the local density approxi-

mation with the disorder treated within the coherent potential approximation. The DLM picture gives an reasonably good description of bond lengths and bulk modulus for the actinide series. The equivalence between the DLM picture and the Hubbard III approximation and their relation to the DMFT description was discussed, and it was argued that the DLM picture is related to DMFT through a static approximation. The DLM density of states compares well with photoemission on δ-Pu, in contrast to that obtained from the LDA or the magnetically ordered AFM configuration. In general, it is found that the DLM picture gives a considerable improvement over the LDA results and quantitatively good agreement with experiments.

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