Dynamical mean-field theory investigation of specific heat and electronic structure of α- and δ-plutonium

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We have carried out a comparative study of the electronic specific heat and electronic structure of α- and δ-plutonium using dynamical mean-field theory. We use the perturbative T-matrix and fluctuating exchange as a quantum impurity solver. We considered two different physical pictures of plutonium. In the first, $5f^5$+, the perturbative treatment of electronic correlations has been carried out around the nonmagnetic [local-density approximation (LDA)] Hamiltonian, which results in an f occupation around a bit above $n_f=5$. In the second, $5f^6$−, plutonium is viewed as being close to a $5f^6$ configuration, and perturbation theory is carried out around the (LDA+U) starting point bit below $n_f=6$. In the latter case, the electronic specific-heat coefficient γ attains a smaller value in δ-Pu than in α-Pu, in contradiction to experiment, while in the former case, our calculations reproduce the experimentally observed large increase of γ in δ-Pu as compared to the α phase. This enhancement of the electronic specific-heat coefficient in δ-Pu is due to strong electronic correlations present in this phase, which cause a substantial increase of the electronic effective mass, and high density of states at E_F. The densities of states of α- and δ-plutonium obtained starting from the open-shell configuration are also in good agreement with the experimental photoemission spectra.

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I. INTRODUCTION

Plutonium metal is arguably the most complex elemental solid. It exhibits a large number of allotropes, and in all the phases its Pauli-like magnetic susceptibility and resistivity are an order of magnitude larger than for simple metals. The transformations between different phases are sometimes accompanied by very large discontinuities in volume.[1] There is a generalized suspicion that the origin of the unique properties of Pu must be connected to its unique position in the actinide series lying at the boundary between the early actinides where the f electrons are bandlike and the late actinides where they are more localized and hence strongly correlated. However, there is currently no consensus on the underlying electronic structure of Pu and the precise mechanism underlying the anomalous behavior of plutonium and the late actinides, and several efforts in developing realistic approaches to this class of problems are currently being pursued.

The traditional electronic structure techniques have been unable to account for the unusual properties of Pu. If one assumes an itinerant nature for the Pu $5f$ electrons, *the volume* of both the low-temperature α phase and that of the fcc high-temperature δ phase can be described reasonably well.[2] However, a significant spin polarization then results in the local spin-density approximation calculations,[3–7] which is opposite to a number of experimental investigations that have led to conclusion that Pu is nonmagnetic (for review, see Refs. 8 and 9).

The strongly localized limit for the $5f$ shell has been studied by means of the LDA+U technique.[10–13] Depending on the type of the "double-counting" correction employed and on the relative strength of the multiplets and the spin-orbit coupling and the strength of the local Coulomb interaction between $5f$ electrons, one obtains either strongly magnetic f^5 or a nonmagnetic f^6 configuration for the localized f shell.[11,12] In the latter case, one obtains the equilibrium volume of the δ phase in good agreement with the experiment.[11] That has led to the conclusion that the ground state of δ-Pu should be essentially in the f^6 nonmagnetic configuration, with the $5f$ shell being split due to the spin-orbit coupling into the completely filled $f^{5/2}$ and empty $f^{7/2}$ states, with the local Coulomb interaction U further increasing this splitting. Therefore, one predicts the ground state of δ-Pu to be fairly similar to that of Am, though with a substantially smaller degree of localization of the f electrons.

However, in this picture, one expects to have almost no f electrons in the vicinity of the Fermi level, in sharp contradiction to the experimental photoemission spectra (PES),[14] where the high peak attributed to f states is clearly observed at the Fermi level. That deficiency has been addressed in Ref. 15, where the dynamical fluctuations around f^6 ground state have been added by means of the dynamical mean-field theory[16] (DMFT) in conjunction with the perturbative treatment of the local quantum fluctuations by the fluctuating exchange and T-matrix technique (T-matrix FLEX).[17–19] The dynamical fluctuations have not changed the f shell occupancy; however, they led to essential modification of the density of states (DOS), producing a peak which now is closer to (but still separated by a finite energy from) the Fermi level, substantially improving the overall agreement between the theoretical DOS and experimental PES for δ-Pu. Similar results have been obtained recently by Shick *et al.*[20] by means of LDA+U+DMFT using Hubbard I as the impurity solver.

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Another school of thought dating back to Johansson and Rosengren[21] suggests that in the solid, plutonium is close to a $5f^5$ configuration. These ideas were supported by the first LDA+DMFT computations in this material by Savrasov *et al.*[22] At the reasonable value of the Coulomb interaction $U=4$ eV, Savrasov *et al.* have obtained a double-minima shape of the total energy versus volume curve, with positions of the minima corresponding well to the experimental equilibrium volumes of the α and δ phases of Pu, respectively. The minima have been assigned to the itinerant and localized state of the $5f$ shell; thus, the $\alpha \rightarrow \delta$ phase transition is due to the Mott localization of the Pu f electrons. The same explanation for the $\alpha \rightarrow \delta$ phase transformation had been put forward by Katsnelson *et al.*[23] The physical picture underlying this approach is that the actinides provide a complex generalization of the localization-delocalization DMFT phase diagram obtained in simple model Hamiltonians,[16,24] obtained by incorporating the realistic band structure, the realistic electronic structure of the f electrons, and most importantly, by relaxing the position of the atomic coordinates that were kept fixed in the model Hamiltonian approach. The LDA+DMFT DOS reported in Ref. 22 did not include realistic multiplet structure. Its recent incorporation has led to rather good agreement with the experimental PES, and in addition has shown that the fully self-consistent DMFT solution is nonmagnetic,[25] by allowing the possibility of ordered states. The ground-state configuration of both the α- and δ-Pu was found to be close to the "open-shell" f^5 configuration in the sense that the f occupation in the ground state is slightly bigger than $n_f=5$.

At this point, we have, within the electronic structure method +DMFT framework, two rather different pictures of the ground state of Pu. In the "near" $5f^6$ of Refs. 11, 12, and 15 one has essentially the $5f^6$ "closed-shell" nonmagnetic configuration (resulting from a strongly interacting one-body Hamiltonian obtained in LDA+U) with dynamical fluctuations reducing the f occupancy by inducing virtual fluctuations into the $5f^5$ manifold (and all other f occupancies). Another approach of Ref. 22 can be described as starting from an f^5 open-shell configuration, which is then screened by the *spd* conduction electrons, what results in a Kondo resonance being formed at the Fermi level. The one-electron Hamiltonian in this case is obtained from the nonmagnetic weakly correlated local-density approximation (LDA). These two physical pictures are not orthogonal. In a solid, the occupation is noninteger, and the theory of the Anderson impurity model teaches us that at noninteger occupancy, the ground state of the model can be adiabatically continued from *both* the f^5 and f^6 limits. Calculations based on both physical pictures produce a ground state and density of states of δ-Pu in reasonable agreement to experiment. Still, these two pictures are substantially different in content, and in order to choose which of the two approaches (and which one of the physical pictures) provides the best description of the actual plutonium, it is necessary to further compare their predictions for other physical quantities sensitive to the electronic structure. In fact, the experimental studies of the $5d$-$5f$ core-valence transition in α- and δ-Pu (Refs. 26–29) by means of the electron-energy-loss spectroscopy (EELS) and x-ray-absorption spectroscopy (XAS) rather lend support to the f^5 configuration of Pu. One may probe as well the electronic specific-heat coefficient γ as it is directly linked to strength of the electronic correlations. Moreover, it has been measured in both α- and δ-Pu, and the value of γ in the δ phase (42 and 64 mJ K^{-2} mol^{-1} in δ-Pu, stabilized by Ga and Al, respectively;[8,30] in the range of 35–55 mJ K^{-2} mol^{-1} in the $Pu_{92}Am_8$ alloy[31]) is substantially larger than in α-Pu [17 mJ K^{-2} mol^{-1} (Ref. 30)]. The specific heat is a measure of the number of degrees of freedom available to the system at a given temperature. It is much larger in the case of an open-shell configuration screened by *spd* electrons, because the degrees of freedom of the f configuration are transferred to the low-energy quasiparticle of the system. Hence, in the present work, we compare and analyze predictions of the two pictures (f^5+ and f^6−) implemented within LDA+DMFT regarding values of the γ coefficient in the α- and δ-Pu.

II. COMPUTATIONAL METHOD

We have employed the LDA+DMFT technique on the basis of the full-potential linear muffin-tin orbital[32] (FPLMTO) method and in conjunction with the spin-orbital T-matrix FLEX quantum impurity solver.[19] The details of our technique are described in Ref. 19. We start with the LDA or LDA+U calculations of α- and δ-Pu by means of the FPLMTO method. The calculations of the fcc δ-Pu phase were carried out at experimental lattice parameter ($a=4.64$ Å, $V=25$ Å^3/at.). The complex structure of the α phase has been mimicked by an orthorhombically distorted diamond structure (which has been proved to have almost the same DOS and total energy as the actual α-Pu structure[33]) at experimental atomic volume ($a=3.63$ Å, $b/a=1.61$, $c/a=2.09$, $V=20$ Å^3/at.). We have employed 242 and 150 k points in the irreducible Brillouin zone for the cubic and orthorhombic structures, respectively. In both the LDA+U and LDA+DMFT, we have taken the values of 3 and 0.55 eV for parameters U and J of the local Coulomb interaction, respectively. In the LDA+U calculations, we have employed the "around mean-field" expression for the double-counting term.[11]

The one-particle Hamiltonian $H_t(\mathbf{k})$ was obtained by Löwdin orthogonalization (using the square root of the overlap matrix) of the converged LDA or LDA+U calculations. Below we designate as LDA+FLEX or LDA+U+FLEX the cases where the LDA or LDA+U Hamiltonian, respectively, has been employed in the LDA+DMFT calculations in conjunction with the spin-orbit T-matrix FLEX quantum impurity solver. First, the local Green's function is obtained by means of the Brillouin-zone integration

$$G(i\omega) = \sum_{\mathbf{k}} [(i\omega + \mu)\mathbf{1} - H_t(\mathbf{k}) - \Sigma^{dc}(i\omega)]^{-1}, \qquad (1)$$

where $\omega=(2n+1)\pi T$ are the fermionic Matsubara frequencies for a given temperature T, μ is the chemical potential, and $\Sigma^{dc}(i\omega)$ is the local self-energy with a double-counting term subtracted, viewed as a functional of the local Green's function $G(i\omega)$ which is solved for self-consistently $\Sigma=\Sigma_{imp}-E_{dc}$.

Then, within the DMFT scheme, the local self-energy is obtained by the solution of the many-body problem for a single quantum impurity coupled to an effective electronic "bath" through the Weiss field function[16]

$$\mathcal{G}^{-1}(i\omega) = G_{ff}^{-1}(i\omega) + \Sigma^{dc}(i\omega). \tag{2}$$

G_{ff} denotes the ff block of G in Eq. (1). In the spin-orbit T-matrix FLEX quantum impurity solver, the local self-energy is obtained as a sum of three contributions:

$$\Sigma = \Sigma^{(TH)} + \Sigma^{(TF)} + \Sigma^{(PH)}, \tag{3}$$

where $\Sigma^{(TH)}$ and $\Sigma^{(TF)}$ are the T-matrix "Hartree" and "Fock" contributions, respectively, $\Sigma^{(PH)}$ is the particle-hole contribution, and $\Sigma^{(TH)}$ and $\Sigma^{(TF)}$ are obtained by substitution in the corresponding Hartree and Fock diagrams the bare Coulomb interaction with the frequency-dependent T matrix; the latter is given by summation of the ladder diagrams in the particle-particle channel. $\Sigma^{(PH)}$ is obtained by the RPA-type summation in the particle-hole channel with the bare vertex being substituted by static limit of the T matrix.[18,19]

For the double-counting term in the DMFT computations, we have used the static limit of the self-energy[18,34] for the LDA Hamiltonian and the Hartree-Fock term for the LDA+U Hamiltonian.[19] The DMFT calculations have been carried out using the 512-point Matsubara frequencies corresponding to a temperature of 950 K. We carried out DMFT iterations until convergence in both the chemical potential μ and the local self-energy was achieved. Then, the Padé approximant was used[35] for analytical continuation of the local self-energy to the real axis in order to obtain the DOS $n(E) = -1/\pi \,\mathrm{Tr}\, \Im[G(E)]$. The electronic specific-heat coefficient γ was computed as $\frac{\pi^2}{3} k_B^2 \,\mathrm{tr}[N(E_F)Z^{-1}]$, where $N(E_F)$ is the DOS matrix at the Fermi level (which for rather low temperature used here can be approximated to μ) and Z^{-1} is the quasiparticle residue matrix, $Z^{-1} = I - d\Im[\Sigma(E)]/dE|_{E=0}$, where I is the identity matrix, and sigma is zero outside the f block. The average mass enhancement $\frac{m^*}{m}$ is defined by $\frac{\mathrm{tr}[Z^{-1}N_f]}{\mathrm{tr}[N_f]}$, where N_f is the f spectral function matrix at the Fermi level.

III. RESULTS

The calculated total and partial f-state LDA and LDA+U DOSs are presented in Fig. 1. Already in the case of LDA, one may clearly distinct the filled $f^{5/2}$ and empty $f^{7/2}$ states on the DOS of δ-Pu. For α-Pu, the separation between the $f^{5/2}$ and $f^{7/2}$ states is somewhat smeared out, as has also been observed in Ref. 12. However, in both the α and δ phases, there is still substantial density of the f states at the Fermi level $N_f(E_F)$; therefore, within LDA, one obtains an open-shell configuration of the f band. The LDA+U calculations of δ-Pu lead to a familiar picture[11,12,15] of nonmagnetic configuration with the filled $f^{5/2}$ and empty $f^{7/2}$ states, well separated in energy by value of U, negligible $N_f(E_F)$ and the f shell occupancy close to 6. In α-Pu, substantial broadening and intermixing of the $f^{5/2}$ and $f^{7/2}$ states persist in the LDA+U, retaining appreciable $N_f(E_F)$.

The values of the electronic specific-heat coefficient γ and effective mass m^* calculated within the LDA+FLEX and LDA+U+FLEX techniques are listed in Table I. One may notice that moderate values of the effective mass m^* in the case of LDA+U+FLEX indicate rather weak correlations present in the system. In fact, the effective mass m^* in δ-Pu appears to be somewhat smaller than in α-Pu. Similarly, in LDA+U+FLEX, the γ coefficient of specific heat in the δ phase is nearly two times smaller as compared to α-Pu, contrary to experimental measurements, which shows γ bigger than two times and sometimes almost three times *larger* in δ-Pu. Almost order of magnitude difference between experimental and theoretical γ in the case of δ-Pu means that in the closed-shell configuration of δ-Pu, electronic correlations appear to be much weaker than one would expect on the basis of experimental evidences. This should be contrasted with the LDA+FLEX calculations which predict effective mass in δ-Pu to be quite large (4.02) and somewhat larger than in α-Pu. The LDA+FLEX technique also reproduces well ex-

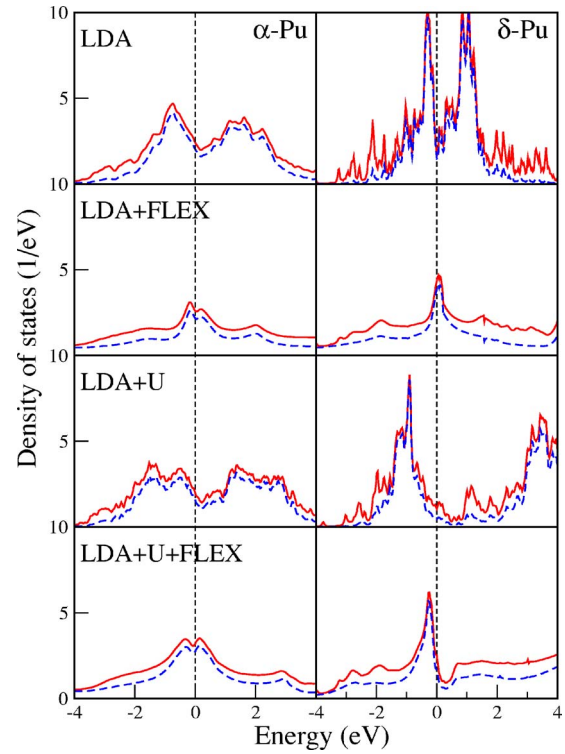

FIG. 1. (Color online) The total (solid line) and partial f state (dashed line) densities of states of α (left panel) and δ (right panel) plutonium in the LDA, LDA+FLEX, LDA+U, and LDA+U+FLEX approaches, respectively.

TABLE I. Effective mass m^*/m and the electronic specific-heat coefficient γ.

	Effective mass		γ (mJ K^{-2} K^{-2} mol^{-1})	
	α-Pu	δ-Pu	α-Pu	δ-Pu
LDA+FLEX	3.85	4.02	20.7	37.9
LDA+U+FLEX	2.22	1.68	15.6	8.6
Expt.[a]			17	42, 64, 35–55

[a]References 8, 30, and 31.

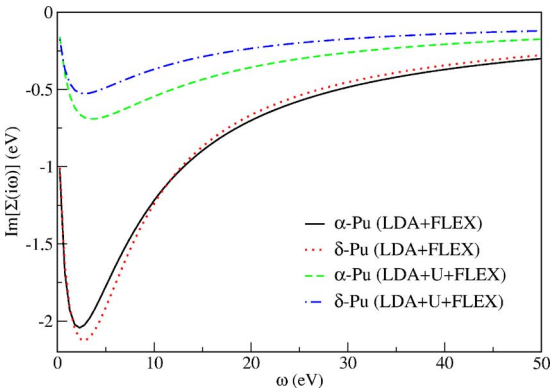

FIG. 2. (Color online) The imaginary part of self-energy $\Sigma_{mm}(i\omega)$ for $m=-3$ on the Matsubara axis, computed for α- and δ-Pu within the LDA+FLEX and LDA+U+FLEX techniques.

perimental tendency of enhancement of the value of γ in the δ phase as compared to α-Pu. Actual values of γ obtained by means of the LDA+FLEX technique are rather close to experimental results in both the α and γ phases.

In Fig. 2, we display the self-energy $\Sigma_{mm}(i\omega)$ (for $m=-3$) computed on the Matsubara axis within the LDA+FLEX and LDA+U+FLEX techniques for α- and δ-Pu. One may notice that $\Im\Sigma(i\omega)$ obtained by LDA+U+FLEX is about four times smaller than the one calculated within LDA+FLEX. That should be expected on the basis of already observed tendency for m^*. We stress again that in both descriptions (LDA+FLEX and LDA+U+FLEX), we have a quasiparticle feature in the spectra. This feature becomes the famous Kondo resonance as U increases. However, the values of the many-body renormalizations, namely, the value of the slope of $\Im\Sigma(i\omega)$ obtained in the LDA+U+FLEX calculations of δ-Pu, are relatively small and closer to the noninteracting system (see Fig. 2) while the peak at E_F that is present in the LDA+FLEX DOS is closer to the Fermi level and more enhanced.

Finally, in Fig. 3, we compare the α- and δ-Pu DOSs obtained within the open-shell LDA+FLEX approach to the experimental photoemission spectra, collected at a photon energy of 40.8 eV, where the band $6d$ and $5f$ cross sections are nearly equal.[14] In order to produce the theoretical spectra,

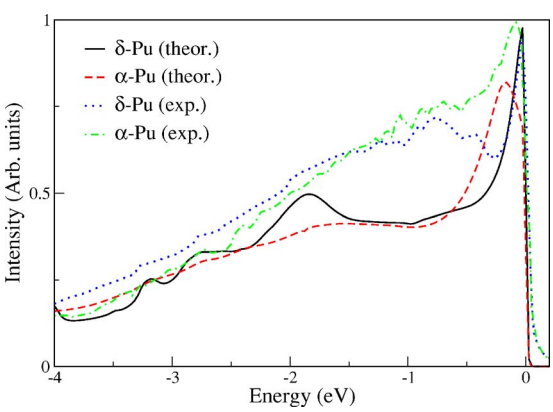

FIG. 3. (Color online) The theoretical LDA+FLEX and experimental PES (Ref. 14) for α- and δ-Pu.

we have multiplied the total DOS by the Fermi function, corresponding to the experimental temperature of 80 K and normalized it to the equal spectral weight between −4 and 0 eV for α- and δ-Pu, as was done in the analysis of the experimental PES in Ref. 14. As a result, one has very good agreement between experimental and theoretical PESs in the vicinity of the Fermi level. For lower energies below −0.5 eV, the agreement is less satisfactory, but there the d states should give appreciated contribution to PES; therefore, the accurate evaluation of the corresponding $6d$ and $5f$ matrix elements may become necessary for a faithful representation of PES. Moreover, the multiplet effects in the $5f$ shell should be taken into account and these are beyond our simple T-matrix FLEX impurity solver.

In conclusion, we have carried out comparative analysis of the specific heat and electronic structure in α- and δ-plutonium by means of the LDA+DMFT technique in conjunction with the perturbative T-matrix and fluctuating exchange quantum impurity solver. We have shown that the "closed" f^6 configuration of the Pu f shell cannot explain high value of the electronic specific-heat coefficient γ in δ-Pu as well as substantial enhancement of γ in the δ phase as compared to $\alpha-$Pu, even in the case when the dynamical fluctuations are properly taken into account. At the same time, by assuming rather the open-shell configuration, which is closer to f^5, one may obtain the observed enhancement of γ in the δ phase and actual values of γ in rather good agreement with the experiment. The experimental PES is also well reproduced by the LDA+DMFT DOS in the open-shell configuration. This suggests that the actual[7] ground state of the f shell in Pu should be rather closer to the open-shell f^5 configuration than f^6. This picture is consistent with the results of a series of EELS and XAS studies of Refs. 26–29 and in good agreement with the results of recent LDA+DMFT (Ref. 25) calculations, where more sophisticated solvers were used to access the strong correlation regime. The good agreement with respect to experiments achieved by our work suggests the possibility of exploring the paramagnetic state of inhomogeneous alloys and interfaces of actinides using DMFT LDA+FLEX. Notice in the context that simplified solvers such as the iterated perturbation theory were very useful for the study of the paramagnetic phase of the Hubbard model, but fared worse in the description of magnetically ordered phases. For this reason, we have not addressed in this paper the issue of magnetic long-range order. This issue is very delicate because as is well known in the context of the Anderson impurity model, approximate perturbative treatments that signal the onset of magnetism can indicate the need to include explicitly Kondo screening rather than the occurrence of a magnetic instability.

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