

PDF hosted at the Radboud Repository of the Radboud University Nijmegen

The following full text is a preprint version which may differ from the publisher's version.

For additional information about this publication click this link.

<http://hdl.handle.net/2066/111456>

Please be advised that this information was generated on 2019-11-17 and may be subject to change.

Unified character of correlation effects in unconventional Pu-based superconductors and δ -Pu

A. B. Shick,^{1,2} J. Kolorenc,² J. Ruzs,^{3,2} P. M. Oppeneer,³
A. I. Lichtenstein,⁴ M. I. Katsnelson,⁵ and R. Caciuffo¹

¹*European Commission, Joint Research Centre,*

Institute for Transuranium Elements, Postfach 2340, D-76125 Karlsruhe, Germany

²*Institute of Physics, ASCR, Na Slovance 2, CZ-18221 Prague, Czech Republic*

³*Dept. of Physics and Astronomy, Uppsala University, Box 516, S-751 20 Uppsala, Sweden*

⁴*University of Hamburg, Jungiusstrasse 9, 20355 Hamburg, Germany*

⁵*Radboud University Nijmegen, Heyendaalseweg 135, 6525 AJ Nijmegen, The Netherlands*

(Dated: January 17, 2013)

Electronic structure calculations combining the local-density approximation with an exact diagonalization of the Anderson impurity model show an intermediate $5f^5$ - $5f^6$ -valence ground state and delocalization of the $5f^5$ multiplet of the Pu atom $5f$ -shell in PuCoIn₅, PuCoGa₅, and δ -Pu. The $5f$ -local magnetic moment is compensated by a moment formed in the surrounding cloud of conduction electrons. For PuCoGa₅ and δ -Pu the compensation is complete and the Anderson impurity ground state is a singlet. For PuCoIn₅ the compensation is partial and the Pu ground state is magnetic. We suggest that the unconventional d -wave superconductivity is likely mediated by the $5f$ -states antiferromagnetic fluctuations in PuCoIn₅, and by valence fluctuations in PuCoGa₅.

PACS numbers: 74.70.Tx, 74.45.+c, 74.20.Mn, 74.20.Pq

Providing a consistent description of correlation effects in the electronic structure of elemental actinides and their compounds is a complex problem due to the interplay between the localized and the itinerant nature of the $5f$ electrons. It is commonly accepted that $5f$ -electrons in light actinides form rather broad conduction bands whereas for the heavy actinides the $5f$ states are atomic-like. Johansson [1] described this situation as a “Mott transition in the $5f$ -electron subsystem” taking place between Pu and Am when moving along the Periodic Table. Katsnelson *et al.* [2] linked the broadening of the $5f$ band to the “atomic collapse” characterizing the transformation from the high-temperature expanded and the low-temperature compressed phases of Pu.

A quantitative description of the Mott transition in actinides [3] was obtained by the dynamical mean-field theory (DMFT) [4] more than 20 years after the concept was formulated. Further DMFT studies suggested an intermediate-valence nature of the Pu-atom $5f$ shell [5] and provided justification for the experimentally proved absence of magnetism in δ -Pu [6].

The intermediate-valence and nonmagnetic character of the $5f$ shell can play an important role in stabilizing the superconducting state exhibited by PuCoGa₅ below a critical temperature T_c of 18.5 K. [7–9]. The unconventional character of superconductivity in this compound is now generally accepted but the microscopic mechanism responsible for electron pairing remains unknown. The d -wave symmetry of the superconducting gap in PuCoGa₅ has been proven by point-contact spectroscopy experiments [10] that also provided the first spectroscopic measure-

ments of the gap amplitude and its temperature dependence.

Recently, superconductivity has been discovered also in PuCoIn₅ [11], with $T_c = 2.5$ K. The experimental studies of this compound were immediately followed by conventional density functional theory (DFT) calculations in the local-density generalized-gradient approximation (LDA/GGA) [12, 13]. Keeping in mind a well known failure of DFT in the case of δ -Pu [6], it can be expected that LDA/GGA does not provide an accurate description of the electronic structure for this strongly correlated material. A few static mean-field correlated band theory calculations were also performed [12, 14], making use of different flavors of the LDA/GGA plus Coulomb’s U (LDA+ U) method. While being an improvement over the conventional band theory, the LDA(GGA)+ U falls short in describing the itinerant-to-localized crossover of the $5f$ manifold in δ -Pu [5] and PuCoGa₅ [10].

Here, we report electronic structure calculations of PuCoIn₅, PuCoGa₅ and δ -Pu performed by combining LDA with the exact diagonalization (ED) [15] of a discretized single-impurity Anderson model [16]. In this approach, the band structure obtained by the relativistic version of the full-potential linearized augmented plane wave method (FP-LAPW) [17] is consistently extended to account for the full structure of the $5f$ -orbital atomic multiplets and their hybridization with the conduction bands [18].

The starting point of our approach is the multi-band Hubbard Hamiltonian [19] $H = H^0 + H^{\text{int}}$. $H^0 = \sum_{i,j,\gamma} H_{i\gamma_1,j\gamma_2}^0 c_{i\gamma_1}^\dagger c_{j\gamma_2}$, where i, j label lattice sites and $\gamma = (lm\sigma)$ mark spinorbitals $\{\phi_\gamma\}$, is the

one-particle Hamiltonian found from *ab initio* electronic structure calculations of a periodic crystal; H^{int} is the on-site Coulomb interaction [19] describing the f -electron correlation. We assume that electron interactions in the s , p , and d shells are well approximated in DFT.

The effects of the interaction Hamiltonian H^{int} on the electronic structure are described by a \mathbf{k} -independent one-particle selfenergy $\Sigma(z)$, where z is a (complex) energy. The selfenergy is constructed with the aid of an auxiliary impurity model describing the complete seven-orbital $5f$ shell. This multi-orbital impurity model includes the full spherically symmetric Coulomb interaction, the spin-orbit coupling (SOC), and the crystal field (CF). The corresponding Hamiltonian can be written as [16]

$$\begin{aligned}
H_{\text{imp}} = & \sum_{\substack{kmm' \\ \sigma\sigma'}} [\epsilon^k]_{mm'}^{\sigma\sigma'} b_{km\sigma}^\dagger b_{km'\sigma'} + \sum_{m\sigma} \epsilon_f f_{m\sigma}^\dagger f_{m\sigma} \\
& + \sum_{mm'\sigma\sigma'} [\xi \mathbf{1} \cdot \mathbf{s} + \Delta_{\text{CF}}]_{mm'}^{\sigma\sigma'} f_{m\sigma}^\dagger f_{m'\sigma'} \\
& + \sum_{\substack{kmm' \\ \sigma\sigma'}} \left([V^k]_{mm'}^{\sigma\sigma'} f_{m\sigma}^\dagger b_{km'\sigma'} + \text{h.c.} \right) \quad (1) \\
& + \frac{1}{2} \sum_{\substack{mm'm'' \\ m'''\sigma\sigma'}} U_{mm'm''m'''} f_{m\sigma}^\dagger f_{m'\sigma'}^\dagger f_{m''\sigma''} f_{m'''\sigma''}
\end{aligned}$$

where $f_{m\sigma}^\dagger$ creates an electron in the $5f$ shell and $b_{m\sigma}^\dagger$ creates an electron in the “bath” that consists of those host-band states that hybridize with the impurity $5f$ shell. The energy position ϵ_f of the impurity level, and the bath energies ϵ^k are measured from the chemical potential μ . The parameter ξ specifies the strength of the SOC and Δ_{CF} is the crystal-field potential at the impurity. The parameter matrices V^k describe the hybridization between the $5f$ states and the bath orbitals at energy ϵ^k .

The band Lanczos method [15] is employed to find the lowest-lying eigenstates of the many-body Hamiltonian H_{imp} and to calculate the one-particle Green’s function $[G_{\text{imp}}(z)]_{mm'}^{\sigma\sigma'}$ in the subspace of the f orbitals at low temperature ($k_{\text{B}}T = 1/500$ eV). The self-energy $[\Sigma(z)]_{mm'}^{\sigma\sigma'}$ is then obtained from the inverse of the Green’s-function matrix $[G_{\text{imp}}]$.

Once the self-energy is known, the local Green’s function $G(z)$ for the electrons in the solid,

$$[G(z)]_{\gamma_1\gamma_2} = \frac{1}{V_{\text{BZ}}} \int_{\text{BZ}} d^3k [z + \mu - H_{\text{LDA}}(\mathbf{k}) - \Sigma(z)]_{\gamma_1\gamma_2}^{-1}, \quad (2)$$

is calculated in a single-site approximation as given in [18]. Then, with the aid of the local Green’s function $G(z)$, we evaluate the occupation matrix $n_{\gamma_1\gamma_2} = -\frac{1}{\pi} \text{Im} \int_{-\infty}^{E_{\text{F}}} dz [G(z)]_{\gamma_1\gamma_2}$. The matrix $n_{\gamma_1\gamma_2}$

is used to construct an effective LDA+ U potential V_U , which is inserted into Kohn–Sham-like equations:

$$[-\nabla^2 + V_{\text{LDA}}(\mathbf{r}) + V_U + \xi(\mathbf{1} \cdot \mathbf{s})] \Phi_{\mathbf{k}}^b(\mathbf{r}) = \epsilon_{\mathbf{k}}^b \Phi_{\mathbf{k}}^b(\mathbf{r}). \quad (3)$$

These equations are iteratively solved until self-consistency over the charge density is reached. In each iteration, a new Green’s function $G_{\text{LDA}}(z)$ [which corresponds to $G(z)$ from Eq.(2) with the self-energy Σ set to zero], and a new value of the $5f$ -shell occupation are obtained from the solution of Eq. (3). Subsequently, a new self-energy $\Sigma(z)$ corresponding to the updated $5f$ -shell occupation is constructed. Finally, the next iteration is started by evaluating the new local Green’s function, Eq.(2).

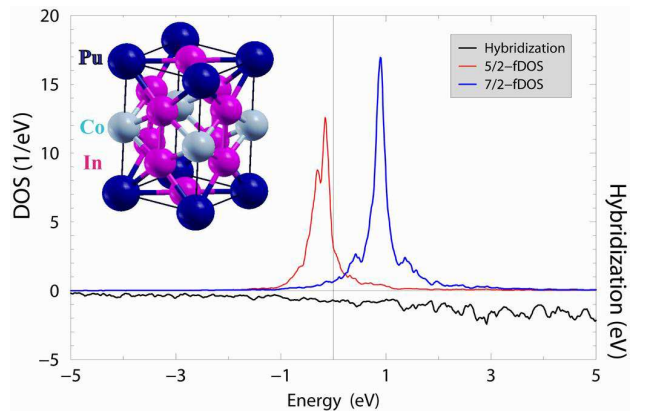


FIG. 1. (Color online) The Pu atom LDA $j = 5/2, 7/2$ projected DOS, and LDA hybridization function $\Delta(\epsilon) = -\frac{1}{\pi} \text{Im} \text{Tr}[G^{-1}(\epsilon + i\delta)]$. The inset shows the PuCoIn₅ crystal structure.

In order to determine the bath parameters V^k and ϵ^k , we assume that the LDA represents the non-interacting model. We then associate the LDA Green’s function $G_{\text{LDA}}(z)$ with the Hamiltonian of Eq. (1) when the coefficients of the Coulomb interaction matrix are set to zero ($U_{mm'm''m'''} = 0$). The hybridization function $\Delta(\epsilon)$ is then estimated as $\Delta(\epsilon) = -\frac{1}{\pi} \text{Im} \text{Tr}[G_{\text{LDA}}^{-1}(\epsilon + i\delta)]$. The curve obtained for $\Delta(\epsilon)$ is shown in Fig. 1, together with the $j = 5/2, 7/2$ -projected LDA densities of the f -states. The results also show that the hybridization matrix is, to a good approximation, diagonal in the $\{j, j_z\}$ representation. Thus, we assume the first and fourth terms in the impurity model, Eq. (1), to be diagonal in $\{j, j_z\}$, so that we only need to specify one bath state (six orbitals) with $\epsilon_{j=5/2}^{k=1}$ and $V_{j=5/2}^{k=1}$, and another bath state (eight orbitals) with $\epsilon_{j=7/2}^{k=1}$ and $V_{j=7/2}^{k=1}$. Assuming that the most important hybridization is the one occurring in the vicinity of E_{F} , the numerical values of the bath parameters $V_{5/2,7/2}^{k=1}$ are found from the relation [20] $\sum_k |V_k^j|^2 \delta(\epsilon_k^j - \epsilon) = -\Delta(\epsilon)/N_f$ integrated over the

energy interval, $E_F - 0.5 \text{ eV} \leq \epsilon \leq E_F + 0.5 \text{ eV}$, with $N_f = 6$ for $j = 5/2$ and $N_f = 8$ for $j = 7/2$. The bath-state energies $\epsilon_{5/2,7/2}^{k=1}$ shown in Table I are adjusted to approximately reproduce the LDA $5f$ -state occupations $n_f^{5/2}$ and $n_f^{7/2}$.

TABLE I. $5f$ -states occupations $n_f^{5/2}$ and $n_f^{7/2}$, and bath state parameters $\epsilon_{5/2,7/2}^1$ (eV), $V_{5/2,7/2}^1$ (eV) for Pu-atom in PuCoIn₅, PuCoGa₅, and δ -Pu from LDA calculations.

Material	$n_f^{5/2}$	$n_f^{7/2}$	$\epsilon_1^{5/2}$	$V_1^{5/2}$	$\epsilon_1^{7/2}$	$V_1^{7/2}$
PuCoIn ₅	4.78	0.39	0.36	0.21	-0.25	0.25
PuCoGa ₅	4.38	0.76	0.25	0.29	-0.07	0.34
δ -Pu	4.16	0.85	0.33	0.27	-0.01	0.36

In the calculations we used an in-house implementation [21, 22] of the FP-LAPW method that includes both scalar-relativistic and spin-orbit coupling effects. The calculations were carried out assuming a paramagnetic state with crystal structure parameters for PuCoIn₅, PuCoGa₅, and δ -Pu taken from Refs. [11, 23, 24], respectively. The Slater integrals were chosen as $F_0 = 4.0 \text{ eV}$, and $F_2 = 7.76 \text{ eV}$, $F_4 = 5.05 \text{ eV}$, and $F_6 = 3.07 \text{ eV}$ [25]. They corresponds to commonly accepted values for Coulomb's $U = 4.0 \text{ eV}$ and exchange $J = 0.64 \text{ eV}$. The SOC parameters $\xi = 0.28 \text{ eV}$ for PuCoIn₅ and PuCoGa₅ and 0.29 eV for δ -Pu were determined from LDA calculations. CF effects were found to be negligible and Δ_{CF} was set to zero. For the double-counting term entering the definition of the LDA+ U potential, V_U , we have adopted the fully-localized (or atomic-like) limit (FLL) $V_{dc} = U(n_f - 1/2) - J(n_f - 1)/2$. Furthermore, we set the radii of the atomic spheres to 3.1 a.u. (Pu), 2.3 a.u. (Co), 2.3 a.u. (Ga), and 2.5 a.u. (In). The parameter $R_{\text{Pu}} \times K_{\text{max}} = 10.54$ determined the basis set size, and the Brillouin zone (BZ) sampling was performed with 1152 k points. The self-consistent procedure defined by Eqs. (1)–(3) was repeated until the convergence of the $5f$ -manifold occupation n_f was better than 0.01.

We are now ready to discuss the solution of Eq.(1). For PuCoIn₅, the ground state of the cluster formed by the $5f$ shell and the bath is given by a superposition of a magnetic sextet (23%) and a non-magnetic singlet (77%), with occupation numbers $\langle n_f \rangle = 5.40$ in the f shell and $\langle n_{\text{bath}} \rangle = 8.40$ in the bath states. This ground state is not a singlet and carries a non-zero magnetic moment. For the $5f$ shell alone, the expectation values of the spin (S_f), orbital (L_f) and total (J_f) angular moments can be calculated as $\langle \hat{X}_f^2 \rangle = X_f(X_f + 1)$ ($X_f = S_f, L_f, J_f$), giving $S_f = 2.27$, $L_f = 3.90$, and $J_f = 2.09$. The individual components of the moments vanish, $\langle \hat{S}_f^z \rangle = \langle \hat{L}_f^z \rangle = 0$, unless the symmetry is broken by an external magnetic field.

In the case of PuCoGa₅, on the other hand, the hybridized ground state of the impurity is a non-magnetic singlet with all angular moments of the $5f$ -bath cluster equal to zero ($S = L = J = 0$). It consists of $\langle n_f \rangle = 5.30$ f states and $\langle n_{\text{bath}} \rangle = 8.70$ bath states. In a pictorial way, we can imagine that the magnetic moment of the $5f$ shell (for which we get $S_f = 2.18$, $L_f = 4.05$, $J_f = 2.43$) is completely compensated by the moment carried by the electrons in the conduction band. As the value of the $5f$ magnetic moment fluctuates in time, because of the intermediate-valence electronic configuration, this compensation must be understood as dynamical in nature. The same situation is realized in δ -Pu ($S_f = 2.11$, $L_f = 4.21$, $J_f = 2.62$), whose ground state is found to be a nonmagnetic singlet with $\langle n_f \rangle = 5.21$ and $\langle n_{\text{bath}} \rangle = 8.79$.

The $5f$ -orbital density of states (DOS) obtained from Eq. (2) for the three investigated compounds is shown in Fig. 2. Below the Fermi energy E_F the DOS exhibits the three-peak structure typical for Pu and for a number of its compounds, and its shape is in good agreement with experimental photoemission spectra. It can be noticed that the multiplets for the atomic f^6 configuration ($f^6 \rightarrow f^5$ transition, lying closer to E_F) are better resolved than for the f^5 part of the spectrum ($f^5 \rightarrow f^4$ transition).

Comparison with previous LDA+Hubbard-I (HIA) calculation for δ -Pu [18], and PuCoGa₅ [26] shows that the three-peak manifold lying above 2 eV binding energy has a slight upright shift towards E_F . At binding energies around 4 eV, the LDA+HIA peaks are substantially modified, and in the LDA+ED calculations they are spread over a $\sim 3 \text{ eV}$ energy interval. These changes in the DOS are induced by the hybridization and suggest partial delocalization of the f^5 multiplet. This is a situation suggested first by Hanzawa [27] in intermediate-valence rare-earth compounds such as SmS or SmB₆, where fluctuations occur between two atomic-like $4f$ configurations. Here, the $5f$ states remain localized for the f^6 configuration but become itinerant for the f^5 one.

As the many-body resonances lying closer to the Fermi energy are produced by $f^6 \rightarrow f^5$ multiplet transitions, they are in a way analogs to the *Racah* peaks, specific transitions between Racah multiplets [28] of f^n and $f^{n\pm 1}$. On the other hand, these structures determine the metallic character of the investigated materials that can therefore be considered as a realization of a *Racah* metal, situated between the two limiting cases represented by fully localized intermediate-valence rare-earth compounds and metallic systems (e.g., nickel) with a non-integer number of d electrons.

Both PuCoGa₅ and δ -Pu display a temperature-independent magnetic susceptibility at low temperatures [6, 29]. Analogous to the intermediate-valence rare-earth compounds [30], the magnetic susceptibil-

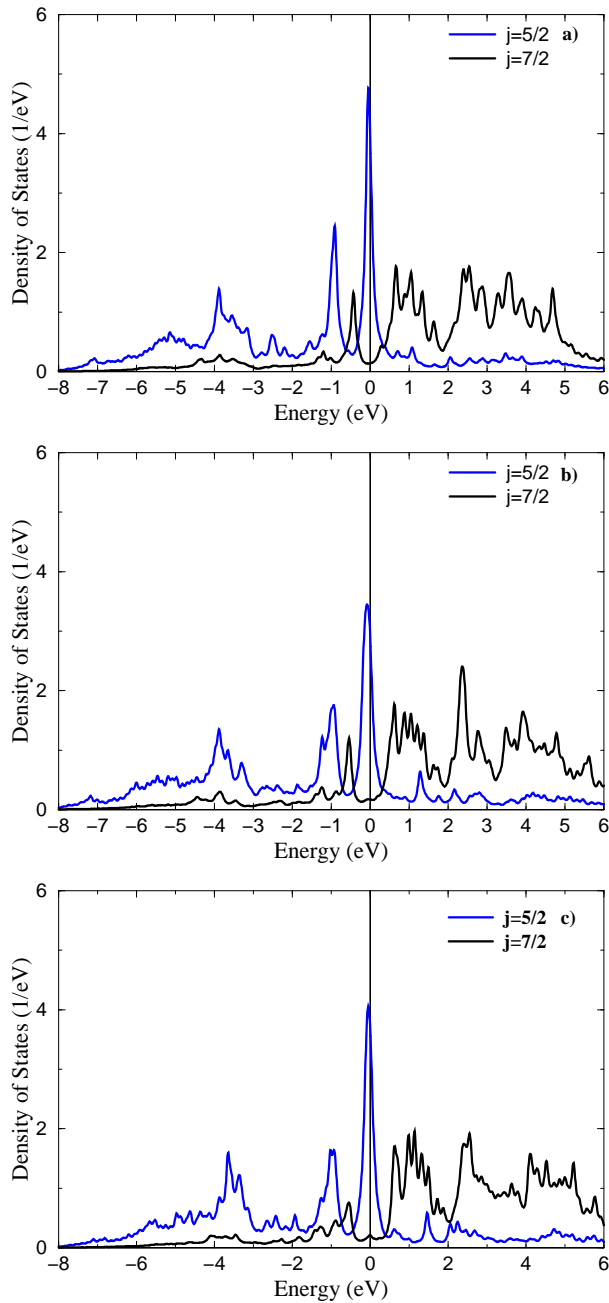


FIG. 2. (Color online) f -electron density of states (DOS, $j = 5/2, 7/2$ projected) for the Pu atom in PuCoIn₅ (a), PuCoGa₅ (b) and δ -Pu (c).

ity is anticipated to behave as $\chi \sim 1/(T + T_{fc})$, where the temperature T_{fc} describes fluctuations between the $5f$ and conduction band electron states. T_{fc} corresponds indeed to the broadening of the quasiparticle resonance near E_F due to valence fluctuations [31]. As the ground state of the impurity is a singlet, we estimate T_{fc} using a renormalized perturbation theory of the Anderson model [16], $T_{fc} = -\frac{\pi^2}{4} Z [\Delta(E_F)/N_f]$, where $[\Delta(E_F)/N_f]$ is the hybridization per orbital

at E_F , and Z is a quasiparticle weight, $Z = (\text{Tr}[N(E_F)(1 - \frac{d\Sigma(\epsilon)}{d\epsilon})|_{\epsilon=E_F}]/\text{Tr}[N(E_F)])^{-1}$. We get $T_{fc} = 72$ meV (~ 850 K) for PuCoGa₅ and $T_{fc} = 63$ meV (~ 750 K) for δ -Pu. Since T_{fc} is high, χ remains constant for $T \ll T_{fc}$, as observed experimentally for PuCoGa₅ and δ -Pu. The situation is different in the case of PuCoIn₅ where the ground state of the impurity is not a pure singlet due to weaker hybridization. Consequently, the temperature dependence of χ is expected to be more pronounced.

The electronic specific-heat coefficient can be estimated as $\gamma = \frac{\pi^2}{3} k_B^2 \text{Tr}[N(E_F)(1 - \frac{d\Sigma(\omega)}{d\omega})|_{\omega=0}]$. For δ -Pu, we get ≈ 44 mJ K⁻² mol⁻¹, in very good agreement with experimental data. For PuCoGa₅, we get ≈ 43 mJ K⁻² mol⁻¹ which is smaller than the experimental value of 80–100 mJ K⁻² mol⁻¹. For PuCoIn₅, the estimated γ value of ≈ 52 mJ K⁻² mol⁻¹ is even further away from the experimental value of ≈ 180 mJ K⁻² mol⁻¹. In this case, it is difficult to obtain an accurate value for γ due to the sharp DOS peak in the vicinity of E_F (see Fig. 2). When taken right at the DOS peak position, the γ value of 95 mJ K⁻² mol⁻¹ is obtained. Also, note that a possible enhancement of

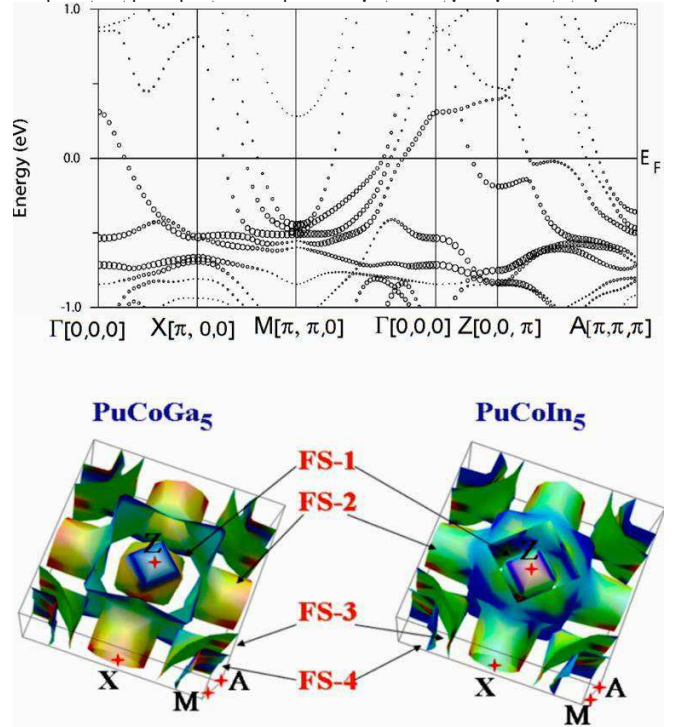


FIG. 3. (Color online)(Top) The band structure with f -weight fatbands for PuCoIn₅, and (bottom) the Fermi surface of PuCoGa₅ and PuCoIn₅ obtained from LDA+ED calculations. The shade of colors encodes the size of the energy gradient.

Figure 3 shows the band structure and the corre-

sponding Fermi Surface (FS) for PuCoIn₅, calculated from the solutions of Eq. (3), which represents an extended LDA+*U* static-mean-field band structure with the 5*f*-states occupation matrix obtained from the local impurity Greens function Eq.(2). For comparison, Fig. 3 shows also the FS for PuCoGa₅ (Fig. S2 of Ref. [10]). Close similarities in the band structure of the two compounds are immediately apparent. Both are compensated multiband metals, as the Fe-based superconductors, and for both materials the *f* bands move away from the Fermi level when the Coulomb-*U* is included, as can be seen by examining the *f*-weighted fatbands. The Fermi surfaces are composed by four sheets (1–4), one that is hole-like (FS-1) and three that are electron-like (FS-2,3,4). The Fermi velocities ratio $\langle v_{x,y}^2 \rangle^{1/2} / \langle v_z^2 \rangle^{1/2}$ of 1.54 for PuCoIn₅, and 1.55 for PuCoGa₅ are calculated in reasonable agreement with the experimental anisotropy ratio of the critical field H_{c2} , 2 – 2.3 for PuCoIn₅, and indicate a two-dimensional character of the electronic structure.

DFT electronic structure calculations for Pu-based 115 material have recently been reported by Ronning *et al.* [13] and Zhu *et al.* [12] Their analysis of the DFT band structure and FS (see, e.g., Figs. 3 and 4 of Ref. [12]) indicated two possible superconducting gap symmetries, the so-called $s\pm$ and $d_{x^2-y^2}$, which correspond to a pairing potential peaked at the $(\pi, \pi, 0)$ reciprocal lattice position. The conclusion was drawn that for Pu-based “115” superconductors, the $s\pm$ order parameter is more likely than the $d_{x^2-y^2}$ one. This is in contradiction with point-contact spectroscopy results [10] showing a zero-bias conductance anomaly that is not expected for $s\pm$ gap symmetry [32].

The presence of a 5*f* local moment dynamically compensated by the surrounding conduction electrons together with the f^5 - f^6 intermediate-valence ground state in PuCoGa₅ and PuCoIn₅ opens various possibilities for unconventional superconductivity. In PuCoIn₅ the Pu *f*-shell local moment is not fully compensated and superconductivity could be related to an antiferromagnetic quantum critical point [11, 33]. On the other hand, in PuCoGa₅ the ground state is a singlet and it seems more plausible that superconductivity results from a valence instability, as in heavy-fermion superconductors [34].

We are grateful to D. Daghero and L. Havela for helpful comments and discussion. We acknowledge financial support from Czech Republic Grants No. GACR P204/10/0330 and No. GAAV IAA100100912 and from DFG Grant No. 436 TSE 113/53/0-1.

-
- [1] B. Johansson, Phys. Rev. B **11**, 2740 (1975).
 - [2] M. I. Katsnelson, I. V. Solovyev, and A. V. Trefilov, JETP Letters **56**, 272 (1992).
 - [3] S. Y. Savrasov, G. Kotliar, and E. Abrahams, Nature **410**, 793 (2001).
 - [4] A. Georges, G. Kotliar, W. Krauth, and M. Rozenberg, Rev. Mod. Phys. **68**, 13 (1996).
 - [5] J. H. Shim, K. Haule, and G. Kotliar, Nature **446**, 513 (2007).
 - [6] J. C. Lashley, A. Lawson, R. J. McQueeney, and G. H. Lander, Phys. Rev. B **72**, 054416 (2005).
 - [7] J. Sarrao *et al.*, Nature **420**, 297 (2002).
 - [8] N. J. Curro *et al.*, Nature **434**, 622 (2005).
 - [9] F. Jutier *et al.*, Phys. Rev. B **77**, 024521 (2008).
 - [10] D. Daghero *et al.*, Nat. Commun. **3**, 786 (2012).
 - [11] E. Bauer *et al.*, J. Phys. Condens. Matter **24**, 052206 (2012).
 - [12] J.-X. Zhu *et al.*, Europhys. Lett. **97**, 57001 (2012).
 - [13] F. Ronning *et al.*, J. Phys. Condens. Matter **24**, 294206 (2012).
 - [14] J. Ruz and P. M. Oppeneer, unpublished (2012).
 - [15] J. Kolorenč, A. I. Poteryaev, and A. I. Lichtenstein, Phys. Rev. B **85**, 235136 (2012).
 - [16] A. Hewson, *The Kondo Problem to Heavy Fermions* (Cambridge University Press, 1993).
 - [17] E. Wimmer, H. Krakauer, M. Weinert, and A. J. Freeman, Phys. Rev. B. **24**, 864 (1981).
 - [18] A. B. Shick, J. Kolorenč, A. I. Lichtenstein, and L. Havela, Phys. Rev. B **80**, 085106 (2009).
 - [19] A. I. Lichtenstein and M. I. Katsnelson, Phys. Rev. B **57**, 6884 (1998).
 - [20] O. Gunnarsson, O. K. Andersen, O. Jepsen, and J. Zaanen, Phys. Rev. B **39**, 1708 (1989).
 - [21] A. B. Shick, A. I. Lichtenstein, and W. E. Pickett, Phys. Rev. B **60**, 10763 (1999).
 - [22] A. B. Shick and W. E. Pickett, Phys. Rev. Lett. **86**, 300 (2001).
 - [23] I. Opahle and P. M. Oppeneer, Phys. Rev. Lett. **90**, 157001 (2003).
 - [24] H. M. Ledbetter and R. L. Moment, Acta Metall. **24**, 891 (1976).
 - [25] K. Moore and G. van der Laan, Rev. Mod. Phys. **81**, 235 (2009).
 - [26] A. B. Shick, J. Ruz, J. Kolorenč, P. M. Oppeneer, and L. Havela, Phys. Rev. B **83**, 155105 (2011).
 - [27] K. Hanzawa, J. Phys. Soc. Jpn. **67**, 3151 (1998).
 - [28] G. Racah, Phys. Rev. **76**, 1352 (1949).
 - [29] A. Hiess *et al.*, Phys. Rev. Lett. **100**, 076403 (2008).
 - [30] D. Khomskii, Sov. Phys. Usp. **129**, 443 (1979).
 - [31] C. M. Varma and Y. Yafet, Phys. Rev. B **13**, 2950 (1976).
 - [32] D. Daghero, M. Tortello, G. Ummarino, and R. Gonnelli, Rep. Prog. Phys. **74**, 124509 (2011).
 - [33] T. Das, J.-X. Zhu, and M. J. Graf, Phys. Rev. Lett. **108**, 017001 (2012).
 - [34] K. Miyake, J. Phys. Condens. Matter **19**, 125201 (2007).