Direct observation of coexisting Kondo hybridization and antiferromagnetic state in UAs₂

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In *f*-electron heavy fermion systems, a wide variety of fascinating magnetic and electronic properties arise, and they are often thought to be related to a crossover behavior between localized and itinerant regimes for *f* electrons. Uranium-based compounds with partially occupied 5*f* orbitals provide an ideal platform to elucidate the outstanding issue of the competition between magnetic order and Kondo entanglement. Using angle-resolved photoemission spectroscopy, complemented by density functional theory simulations, we probe the temperature-dependent evolution of the low-energy electronic structure of UAs₂ and observe two nearly flat bands of different origin in the antiferromagnetic (AFM) state. A nearly flat band which behaves with quasi-two-dimensional character has been observed and contributed to the heavy spectral weight at the Γ point around *E*_F. This flat band reveals typical Kondo hybridization. Another flat band around the *M* point is closely related to paramagnetic (PM)-AFM phase transition, which opens an energy gap below the transition temperature ~273 K. Our results provide direct spectral demonstration of the electronic structure evolution across the *f*-*c* hybridization and PM-AFM transition in UAs₂.

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I. INTRODUCTION

Heavy fermion (HF) materials [1], as one of the most complex systems in condensed matter physics, can feature a fascinating interplay of strongly correlated and itinerant electronic physics, setting a stage for emergent phenomena such as quantum criticality, magnetic ordered states, HF superconductivity [2-6], and elusive hidden order states [7]. In the case of f-electron HF systems, possessing the dual nature of felectrons, these mysterious physical properties are believed to have a close connection with the *f*-electron behavior. At high temperature, f electrons are essentially localized as magnetic moments. With lowering temperature, f electrons tend to be itinerant and hybridize with the broadbands of conduction electrons through the Kondo process, which weakens the magnetic orders of the materials [8,9]. The ground state completely depends on the competition between the Kondo effect and the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction [10,11]. Unlike the Kondo effect, the RKKY interaction tends to stabilize long-range magnetic order. Theoretically, there are two scenarios to picture the zero-temperature phase diagram of HFs. The first one describes that the onset of long-range magnetic order and the destruction of the Kondo lattice both vanish simultaneously at a single quantum critical point (QCP). In the second scenario, there are two separate QCPs for them [11–15]. Many theoretical and experimental efforts have been made to elucidate this question of which scenario is more accurate to describe the phase diagram of the different HF materials. In YbRh₂Si₂, the Kondo destruction happens at the magnetic QCP [16,17], while recently in CeSb [18] and USb₂ [19], these two states can coexist at low temperature. Considering the quantum phase transitions like unconventional superconductivity or hidden orders also exist in an extended phase space near the QCP, it is very important to get more experimental and theoretical results of HF compounds to reveal the microscopic physics.

As one of the antiferromagnetic (AFM) UX_2 (X = As, Sb, Bi) series compounds, UAs₂ has the highest Néel temperature $(T_{\rm N} = 273 \,{\rm K})$ among uranium compounds [20]. Below $T_{\rm N}$, the magnetic moments order ferromagnetically in the (001) plane and stack AFM along the [001] direction. It is a moderately correlated electron system with a quasi-two-dimensional (quasi-2D) electronic structure which makes it an ideal platform for electronic structure research of HF system [20,21]. However, there is still no direct observation of its detailed electronic structure like with angle-resolved photoemission spectroscopy (ARPES) or scanning tunneling microscopy (STM) results. Whether the Kondo resonance coexists with the magnetic order is an interesting topic. In addition to that, the coordinating element As has many more exotic electronic states [22] than the other two elements Sb and Bi. A detailed electronic structure investigation of UAs₂ can help to understand the microscopic physics diagram between the Kondo effect and the RKKY interaction in an AFM ordered state.

In this paper, we report the clear Fermi surface topology and complete band structures of UAs₂ by ARPES and density functional theory (DFT) calculation. Two nearly flat bands α , β and conduction bands γ , ε can be observed at different high-symmetry points at low temperature by ARPES, which are very consistent with DFT calculations. Photon energydependent measurements reveal that the flat band around the Γ point exhibits a quasi-2D property. Temperature-dependent

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ARPES results further show that the heavy quasiparticle bands near $E_{\rm F}$ have different temperature behavior at the Γ and M points. The flat band around the Γ point is due to the hybridization between the 5f electrons and conduction electrons. It is a typical phenomenon of the Kondo hybridization. Meanwhile, the flat band around the M point has a clear broadening across the AFM transition, and we observe a gap opening below $T_{\rm N}$ (273 K), which indicates that this band has a close connection with the AFM transition. Our results reveal that the Kondo resonance and magnetic order can coexist with each other at low temperature, and they are related to different flat bands near $E_{\rm F}$ at a specific momentum space location.

II. METHODS

High-quality UAs₂ samples have been synthesized by the vapor transport method with a 3–5 mg/cm³ iodine carrier. A U block (3 N 99.9%) and an As granule (4 N 99.99%) with atomic ratio 1:2.02 were put into a quartz tube under argon atmosphere then sealed after evacuated to 10^{-3} Pa. The quartz tubes were heated for a week in a two-zone furnace in which hot- and cold-zone temperatures were kept at 900 and 750 °C, respectively. The chemicals were placed in the hot zone, and the grown single crystals were found in the middle of the tubes.

Electronic structure calculations were performed with a plane-wave basis projected augmented wave method within the DFT framework, as implemented in the Vienna Ab initio Simulation Package [23–26]. The 5f electrons were treated as itinerant valence electrons, and the spin-orbit coupling (SOC) effect was considered using a second variational step. The Perdew-Burke-Ernzerhof flavor [27] of the generalized gradient approximation was adopted to describe the exchange-correlation of the valence electrons. Based on the experimentally determined bulk AFM unit cell [28], a symmetric (001) slab model with As 2-terminated atomic planes was constructed to interpret the ARPES results. The As 2-terminated slab model consists of 10 atomic layers with 18 Å vacuum layer. An energy cutoff of 600 eV and 11 imes 11×1 k-mesh in the Monkhorst-Pack scheme were employed to converge the structure optimization and static self-consistence calculations to better than 1 meV/atom.

III. RESULTS

At 10 K, UAs₂ is in a complex and interesting mixing state in which Kondo resonance and AFM state coexist. The crystal structure, three-dimensional Brillouin zone, conductivitytemperature (ρ -T) curve, and detailed electronic structures are shown in Fig. 1. Here, UAs₂ crystallizes in the tetragonal structure in the anti-Cu₂Sb type, as shown in Fig. 1(a). There are two types of As sites in UAs₂ marked by As1 and As2. The *c/a* value exceeds 2, meaning that its easy cleavage surface is along the [001] direction. For UAs₂, there are several possible surface terminations when the crystal is cleaved. However, in this paper, several single crystals were cleaved *in situ*, and we only observed one kind of electronic structure. Only the As 2-terminated cleavage surface can lead to a symmetric cut between the As planes. In addition to that, the cleavage surface of the isostructural compound USb₂ has been reported to be a similar Sb 2-terminated surface [19,29]. The cleavage surface of UAs₂ supposes to be the As-2 (001) surface. The Brillouin zone is depicted in Fig. 1(b). At 273 K, UAs₂ enters the AFM phase, and the residual resistivity ratio (ρ_{300}/ρ_0) is 241 which means high sample quality as shown in Fig. 1(c).

The photoemission intensity map of UAs₂ at 10 K taken with 108 eV light horizontally-polarized photons (the onresonance photon energy of the 5f electron) is displayed in Fig. 1(d). The Fermi surface consists of a squarelike Fermi pocket and heavy spectral weight around the zone center, which can be assigned to the β and α bands, respectively. A Fermi pocket can be observed around the X point which can be assigned to the γ and ε bands. According to the calculation result, two Fermi pockets are supposed to exist, but only one is observed at the X point. This is ascribed to the high degree of degeneracy of these two conduction bands, as shown in Fig. 1(e). In addition to this, the energy resolution of the used soft x ray (16 meV) is not accurate enough to distinguish these two degenerated conduction bands. We mention that large spectral weights exist around both the Γ and M points, which is due to the formation of heavy quasiparticle bands near $E_{\rm F}$. Figures 1(f1)–1(f3) show the band structure along typical high-symmetry directions. Two nearly flat bands named α and β in the vicinity of $E_{\rm F}$ can be observed around the Γ and Mpoints, respectively. Along Γ -M in Fig. 1(f1), these two flat bands can be clearly observed. The α band hybridizes with conduction bands, forming a heavy quasiparticle band near the Γ point. Meanwhile, the nearly flat β band contributes large spectral weight near $E_{\rm F}$ around the M point. A detailed electronic structure around the X point can be clearly identified from the band structure along the Γ -X and X-M directions in Figs. 1(f2) and 1(f3), and an electronlike band can be observed crossing $E_{\rm F}$, forming a Fermi pocket around the X point. To investigate the electronic structure in detail, we have performed energy band structure calculations for the As (2)-terminated surface in Fig. 1(e). Both the Fermi surface and band structure are in good accordance with experimental results: the observed α , β , γ , and ε bands near $E_{\rm F}$ can all be found in the calculation. The accordance between ARPES and DFT calculations further underlines that the cleavage surface should be the As 2-terminated surface.

Quantum oscillation experiments (dHvA) reveal that there are quasi-2D Fermi surfaces in UAs₂ around the Γ point with relatively heavy quasiparticles effective mass [20,21]. By varying the photon energy (hv; h, Planck constant; v, frequency) of ARPES, the momentum detection range in the Γ -Z direction changes, and we could obtain the band dispersions along Kz, which is normal to the (001) surface in Figs. 1(a) and 1(b). The ARPES data collected with several photon energies along the Γ -M direction are shown in Fig. 2. Unlike the 4f electron materials which can only be identified at specific photon energy, 5f bands in UAs₂ can be observed in a rather large photon energy range. The nearly flat α band and conduction band around the Γ point can be clearly observed under 60 eV photons. With hv = 60, 96, and 104 eV, the heavy quasiparticle flat band α at the Γ point can be distinguished with a clearly similar in-plane momentum extent. To further probe its in-plane contour, the momentum distribution curves at selected photon energies are shown in Fig. 2(b). The K z-dependent ARPES measurements of the α band indicate



FIG. 1. The electronic structure of UAs₂ taken with 108 eV light at 10 K. (a) The crystal structure of tetragonal UAs₂. (b) The first Brillouin zone of UAs₂. (c) Temperature dependence of electric resistivity data in zero magnetic field with electric current applied in the *a-b* plane. (d) Photoemission intensity map of UAs₂ at E_F . The intensity is integrated over a window of $(E_F - 4 \text{ meV}, E_F + 4 \text{ meV})$ at the (001) crystal face. The Brillouin zone is marked by red dashed line. (e) Calculated band structure of the As 2-terminated surface. The main energy bands around E_F are marked by respective colors. Photoemission intensity distributions along (f1) Γ -*M*, (f2) Γ -*X*, and (f3) *X*-*M*. Here, 108 eV energy photons are used, and both the *f* bands and conduction bands can be clearly resolved.

quasi-2D Fermi surfaces exist in UAs₂ around the Γ point. It is very consistent with the dHvA results, as a nesting warped cylindrical quasi-2D Fermi surface exists around the Γ point.

To reveal the origins of these two nearly flat bands and the electronic structure evolution across f-c hybridization and phase transition, we performed detailed temperaturedependent measurements with 21.2 eV photons around the Γ and M points. Figure 3 displays the temperature evolution of the electronic structure around the Γ point. In Fig. 3(a6), one conduction band with fast dispersion and a very weak nearly flat band can be observed at 290 K. The 5f electrons behave mainly like an atomic local moment at such high temperature, and only a small part of the 5f electrons exhibit an itinerant character as f-c hybridization already existing at 290 K. Upon decreasing temperature, the atomic 5f electrons exhibit much more itinerant character, and the hybridization intensity of 5f-c electrons is enhanced, which form heavy quasiparticle flat band with indirect hybridization gap around E_F . This temperature-dependent evolution can be further illustrated by the energy distribution curves (EDCs) in Fig. 3(b). The integrated window has been marked by a black dashed block in Fig. 3(a1). The temperature-dependent evolution of the α band is shown in the inset of Fig. 3(b), and in this heavy-electron Kondo liquid, it follows a logarithmic increase in density of states with decreasing temperature. This logarithmic relation is universal in heavy-electron materials [30].

In a wide temperature range, an obvious f-electron feature can be observed as a flat band around E_F , which is due to the hybridization between the f band and the conduction electrons. This results in the redistribution of the f spectral



FIG. 2. Angle-resolved photoemission spectroscopy (ARPES) K_z dependence cut sets along Γ -M under light vertically polarization at several photon energies. (a) ARPES data taken along Γ -M under several photon energies. (b) The momentum distribution curves along Γ -M from 60 to 108 eV photon energies with the E- E_F range in [0, -0.2 eV].

weight and forms the weakly dispersive band near $E_{\rm F}$. This hybridization process can be described under the periodic Anderson model (PAM), as illustrated in Fig. 3(c). Here, we use 60 eV photons with ultrahigh angle resolution to better probe the electronic structure around the Γ point. The f states develop with decreasing temperature, forming the f-c hybridization band with heavy spectral weight in Fig. 3(c)around E_F. Such a process starts from a much higher temperature, and there is an onset temperature T^* to mark the formation of this f-electron heavy quasiparticle band [31]. In previous research on USb₂, the localized-to-itinerant transition of f electrons is a crossover behavior, and the f band almost disappears at 130 K. Meanwhile, in UAs₂, the felectron flat band can still be observed at 290 K, which means the T^* may be higher than room temperature. In USb₂, the maximum T value of the ρ -T curve with current along the c axis is marked as $T_{\rm coh}$ which represents the Kondo resonance and is usually close to T^* [32]. In this paper, there is still no ρ -T curve report with current along the c axis because the ultrathin flake-shaped samples make it difficult to get c-axis conductivity data. The detailed PAM analysis is displayed in a later section to discuss the high T^* from the aspect of Kondo hybridization strength. This direct visualization of the hybridization between the f bands and conduction bands at high temperature signifies the onset of Kondo correlations between the 5f local moments with conduction electrons.

Here, UAs₂ enters the AFM phase below a high Néel temperature of 273 K. To study the electronic structure evolution across the AFM transition, we performed temperaturedependent measurements around the *M* point from 11 up to 275 K and found the β band around the *M* point changes dramatically. At 275 K in Fig. 4(a8), above the transition temperature T_N , some spectral weight can be observed at E_F , which was enhanced and shifted away from E_F with temperature decreasing <273 K, resulting in an energy gap opened at E_F in Fig. 4(a1). When the temperature returns to 11 K after one cycle, the center of the spectral weight is shifted to 30 meV below $E_{\rm F}$ again, which means this gap opening is intrinsic. This trace is much clearer in the symmetrized EDCs of the β band around the *M* point in Fig. 4(b). We can track the gap opening behavior, and it opens right between 270 and 275 K. The gap size gradually increases with decreasing temperature and saturates at low temperature. The quantitative evolution of the gap size with temperature is shown in Fig. 4(c). The largest gap size is ~30 meV at 11 K. The opening temperature of the gap is in line with the AFM transition temperature (273 K), indicating that the formation of the nearly flat β band around $E_{\rm F}$ is related to the magnetic phase transition.

IV. DISCUSSION AND CONCLUSIONS

In this paper, our ARPES study unveils two nearly flat bands (α, β) exhibiting different temperature-dependent behavior in the low-energy electronic structure of UAs₂. The α band around the Γ point shows a typical Kondo effect; the spectral weight of this quasiparticle band is gradually enhanced with decreasing temperature. The characteristic temperature T^* is the coherence temperature marking the onset of the f-c hybridization [31], and we could see that the heavy quasiparticle bands emerge gradually as temperature falls below T^* . In UAs₂, the *f*-*c* hybridization band already exist at 290 K, which is much higher than other HF materials such as CeCoIn₅ (120 K) [33] or USb₂ (130 K) [19]. The lattice constants exceed the Hill limit (\sim 3.4 Å), and the crystal volume of USb₂ is 27.18% larger than UAs₂. Hence, the overlaps between 5f electrons and conduction electrons of orbitals are larger, which lead to a more itinerant character of 5f electrons in UAs₂. This significant difference in characteristic temperature may originate from the different extent of 5f localization or itinerancy in these two isostructural compounds.



FIG. 3. Temperature evolution of the electronic structure around the Γ point of UAs₂. (a1)–(a6) Photoemission intensity plots around the Γ point at the temperatures indicated. (b) Temperature dependence of the quasiparticle spectral weight in the vicinity of Γ . Integrated window has been marked by the black dashed block in (a). The inset shows the temperature evolution of the intensity of α band in (b), which perfectly follows logarithmic fitting. (c) Angle-resolved photoemission spectroscopy (ARPES) data taken with 60 eV photons at 10 K along the Γ -*M* direction and a schematic diagram of the hybridization process under a periodic Anderson model (PAM). The blue dashed line is the conduction band. The orange curve represents the hybridization band, and the red dashed line denotes the position of *f* band.

In addition to that, we used PAM [33-35] to fit the hybridization band in Fig. 3(c):

$$E^{\pm} = \frac{\varepsilon_0 + \varepsilon(k) \pm \sqrt{[\varepsilon_0 - \varepsilon(k)]^2 + 4|V_k|^2}}{2}, \qquad (1)$$

where ε_0 is the renormalized *f*-level energy (the crystal electric field ground state here), ε_k is the conduction-band dispersion at high temperature, and V_k is the renormalized hybridization strength. Within this simplified approach, the non-5*f* conduction bands hybridize with the renormalized 5*f* quasiparticle peaks (the Kondo resonances), leading to a redistribution of quasiparticle band dispersion and a direct energy gap (≈ 2 V) around E_F . By setting the hybridization parameter $V_k = 55 \pm 7$ meV, PAM can perfectly reproduce the hybridization bands around the Γ point of UAs₂. We notice that the direct energy gap of a similar hybridization flat band around the Γ point in USb₂ is 17 meV [19], which is much

smaller than UAs₂ ($\approx 100 \text{ meV}$). The PAM simulation can reasonably explain the discrepancy of the characteristic temperature, as the hybridization intensity of UAs₂ is relatively strong.

The spectral weight of the β flat band clearly shifts away from $E_{\rm F}$ across the AFM transition, which leads to an AFM gap opening. We mention that the AFM gap size of UAs₂ is 29.8 meV, which is slightly larger than USb₂ (28 meV) at 11 K. Meanwhile, the AFM transition temperature of UAs₂ (273 K) is also higher than USb₂ (203 K). Interestingly, a similar tendency between the Néel temperature and the AFM gap has been discussed in URu₂Si₂ [36,37], as the higher the $T_{\rm N}$, the larger the size of the AFM energy gap. It basically follows the Bardeen-Cooper-Schrieffer (BCS) model in URu₂Si₂ [38,39]. The trend of $T_{\rm N}$ and the AFM gap in the UX₂ series ($X = {\rm As}$, Sb, Bi) is like the BCS fitting in URu₂Si₂ and still needs more experimental and theory study. The similarity



FIG. 4. The evolution of electronic structure with antiferromagnetic phase transition along the Γ -*M* direction in UAs₂. (a1)–(a9) Temperature dependence of the band structure around the *M* point at temperature indicated. (b) Temperature dependence of the symmetrized energy distribution curves (EDCs) around the *M* point. The integrated window has been marked by the black dashed block in (a). (c) The evolution of the gap size with temperature. The gap size is extracted from the peak position of the symmetrized gap in (b).

to the URu₂Si₂ indicates the itinerant AFM property. The magnetic ordered states have two different scenario originations in metals: a spin-density wave instability in a Fermi liquid of itinerant electrons and an instability in a liquid of local magnetic moments interacting through conduction electrons [40]. Here, UAs₂ harbors itinerant-electron magnetic characteristics below T_N that grow out of a high-temperature local moment state, which bridges the extremes. Investigations about the detailed connection between magnetic property and electronic structure of other AFM HF materials are highly desired.

In conclusion, the detailed electronic structure and Fermi surface of the HF AFM material UAs₂ are investigated by ARPES. Our experiments and calculations directly reveal two nearly flat bands around E_F at the Γ and M points, respectively, as well as the conduction bands at the X point. The photon energy- and temperature-dependent measurements show that the flat band α around the Γ point has a quasi-2D property and is originated from the hybridization between the 5f electrons and conduction electrons, while another flat band β around the M point has a close connection with the AFM transition. The α flat band reveals the typical picture of the localized-to-itinerant crossover behavior in actinide compounds, and the β flat band exhibits the electronic structure evolution across the AFM transition. Our results give a clear coexisting scenario of the Kondo effect and RKKY

interaction and how the electronic structure changes in this phase, which provides a comprehensive understanding about the 5f-electron behavior and magnetic ordered states in HF materials.

V. PHOTOEMISSION EXPERIMENT

ARPES data of UAs₂ from Figs. 1 and 2 were obtained at BL09U and BL03U at the Shanghai Radiation Facility with a Scienta DA30 analyzer, and the vacuum was always kept $<5 \times 10^{-11}$ mbar. The samples were cooled using a closedcycle He refrigerator. The overall energy resolution is 16 meV, and the samples were cleaved in situ along the [001] direction at 10 K. We did the temperature evolution study on the nearly flat bands around $E_{\rm F}$ by in-house ARPES (21.2 eV He-II), as shown in Figs. 3 and 4. The energy and angular resolutions are 5 meV and 0.2°, respectively. The position of the Fermi level was determined by the position of that of in situ evaporated gold film. The measured positions were determined with a free-electron final state model by taking the photon momentum into consideration. The momentum of the electron perpendicular to the surface with the free-electron final-state model is given by

$$k_{\perp} = \sqrt{\frac{2m}{\hbar^2}} (E_{\rm kin} \cos^2\theta + V_0) - k_{\perp \rm photon},$$

where *m* is the electron mass, E_{kin} is the kinetic energy of the photoelectron, θ is the emission angle of the photoelectron relative to the surface normal, V_0 is the inner potential, and $k_{\perp photon}$ is the momentum of the incident photon perpendicular to the surface. By varying the photon energy and the Kz map, we get the inner potential $V_0 = 16 \text{ eV}$ which is close to the typical value for HF compounds [41]. To ensure the validity of the temperature dependencies of the ARPES spectra, we used several UAs₂ single crystals for ARPES scanning and confirmed that the temperature dependence of the ARPES spectra is reproducible.

- [1] G. R. Stewart, Rev. Mod. Phys. 56, 755 (1984).
- [2] F. Steglich, J. Aarts, C. D. Bredl, W. Lieke, D. Meschede, W. Franz, and H. Schafer, Phys. Rev. Lett. 43, 1892 (1979).
- [3] J. J. M. Franse, P. H. Frings, A. Devisser, A. Menovsky, T. T. M. Palstra, P. H. Kes, and J. A. Mydosh, Physica B 126, 116 (1984).
- [4] T. T. M. Palstra, A. A. Menovsky, J. Vandenberg, A. J. Dirkmaat, P. H. Kes, G. J. Nieuwenhuys, and J. A. Mydosh, Phys. Rev. Lett. 55, 2727 (1985).
- [5] C. Geibel, C. Schank, S. Thies, H. Kitazawa, C. D. Bredl, A. Bohm, M. Rau, A. Grauel, R. Caspary, R. Helfrich *et al.*, Z. Phys. B 84, 1 (1991).
- [6] H. Q. Yuan, F. M. Grosche, M. Deppe, C. Geibel, G. Sparn, and F. Steglich, Science 302, 2104 (2003).
- [7] S. Elgazzar, J. Rusz, M. Amft, P. M. Oppeneer, and J. A. Mydosh, Nat. Mater. 8, 337 (2009).
- [8] P. Nozieres and A. Blandin, J. Phys. 41, 193 (1980).
- [9] Y. F. Yang, Rep. Prog. Phys. 79, 074501 (2016).
- [10] J. C. Xavier, R. G. Pereira, E. Miranda, and I. Affleck, Phys. Rev. Lett. 90, 247204 (2003).
- [11] Q. M. Si, S. Rabello, K. Ingersent, and J. L. Smith, Nature 413, 804 (2001).
- [12] P. Coleman, C. Pepin, Q. M. Si, and R. Ramazashvili, J. Phys.: Condens. Matter 13, R723 (2001).
- [13] J. A. Hertz, Phys. Rev. B 14, 1165 (1976).
- [14] A. Millis, Phys. Rev. B 48, 7183 (1993).
- [15] W. Knafo, S. Raymond, P. Lejay, and J. Flouquet, Nat. Phys. 5, 753 (2009).
- [16] S. Friedemann, T. Westerkamp, M. Brando, N. Oeschler, S. Wirth, P. Gegenwart, C. Krellner, C. Geibel, and F. Steglich, Nat. Phys. 5, 465 (2009).
- [17] S. Paschen, S. Friedemann, S. Wirth, F. Steglich, S. Kirchner, and Q. Si, J. Magn. Magn. Mater. 400, 17 (2016).
- [18] S. Jang, R. Kealhofer, C. John, S. Doyle, J. S. Hong, J. H. Shim, Q. Si, O. Erten, J. D. Denlinger, and J. G. Analytis, Sci. Adv. 5, eaat7158 (2019).
- [19] Q. Y. Chen, X. B. Luo, D. H. Xie, M. L. Li, X. Y. Ji, R. Zhou, Y. B. Huang, W. Zhang, W. Feng, and Y. Zhang, Phys. Rev. Lett. 123, 106402 (2019).
- [20] P. Wisniewski, D. Aoki, K. Miyake, N. Watanabe, Y. Inada, R. Settai, Y. Haga, E. Yamamoto, and Y. Onuki, Physica B 281, 769 (2000).
- [21] P. Wisniewski, D. Aoki, N. Watanabe, K. Miyake, R. Settai, Y. Onuki, Y. Haga, E. Yamamoto, and Z. Henkie, J. Phys.: Condens. Matter 12, 1971 (2000).

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- [22] P. Zhang, J. Z. Ma, Y. Ishida, L. X. Zhao, Q. N. Xu, B. Q. Lv, K. Yaji, G. F. Chen, H. M. Weng, X. Dai *et al.*, Phys. Rev. Lett. **118**, 046802 (2017).
- [23] G. Kresse and J. Furthmuller, Comput. Mater. Sci. 6, 15 (1996).
- [24] G. Kresse and J. Furthmuller, Phys. Rev. B 54, 11169 (1996).
- [25] G. Kresse and J. Hafner, Phys. Rev. B 49, 14251 (1994).
- [26] G. Kresse and J. Hafner, Phys. Rev. B 47, 558 (1993).
- [27] J. P. Perdew, K. Burke, and M. Ernzerhof, Phys. Rev. Lett. 77, 3865 (1996).
- [28] G. Amoretti, A. Blaise, and J. Mulak, J. Magn. Magn. Mater. 42, 65 (1984).
- [29] W. Feng, D. H. Xie, X. B. Luo, S. Y. Tan, Y. Liu, Q. Liu, Q. Q. Hao, X. G. Zhu, Q. Zhang, Y. Zhang *et al.*, Phys. Rev. B 104, 235103 (2021).
- [30] Y. F. Yang and D. Pines, Phys. Rev. Lett. 100, 096404 (2008).
- [31] S. Nakatsuji, D. Pines, and Z. Fisk, Phys. Rev. Lett. 92, 016401 (2004).
- [32] D. H. Xie, M. L. Li, W. Zhang, L. Huang, W. Feng, Y. Fang, Y. Zhang, Q. Y. Chen, X. G. Zhu, Q. Liu, B. K. Yuan, L. Z. Luo, P. Zhang, X. C. Lai, and S. Y. Tan, arXiv:1611.08059.
- [33] Q. Y. Chen, D. F. Xu, X. H. Niu, J. Jiang, R. Peng, H. C. Xu, C. H. P. Wen, Z. F. Ding, K. Huang, L. Shu *et al.*, Phys. Rev. B 96, 045107 (2017).
- [34] S. Fujimori, Y. Takeda, T. Okane, Y. Saitoh, A. Fujimori, H. Yamagami, Y. Haga, E. Yamamoto, and Y. Onuki, J. Phys. Soc. Jpn. 85, 062001 (2016).
- [35] H. J. Im, T. Ito, H. D. Kim, S. Kimura, K. E. Lee, J. B. Hong, Y. S. Kwon, A. Yasui, and H. Yamagami, Phys. Rev. Lett. 100, 176402 (2008).
- [36] K. Hasselbach, J. R. Kirtley, and P. Lejay, Phys. Rev. B 46, 5826 (1992).
- [37] R. Escudero, F. Morales, and P. Lejay, Phys. Rev. B 49, 15271 (1994).
- [38] W. A. Roshen, Phys. Rev. B 31, 7296 (1985).
- [39] P. Fulde, J. Keller, and G. Zwicknagl, Solid State Phys. 41, 1 (1988).
- [40] H. v. Löhneysen, A. Rosch, M. Vojta, and P. Wölfle, Rev. Mod. Phys. 79, 1015 (2007).
- [41] J. D. Denlinger, G. H. Gweon, J. W. Allen, C. G. Olson, M. B. Maple, J. L. Sarrao, P. E. Armstrong, Z. Fisk, and H. Yamagami, J. Electron Spectrosc. Relat. Phenom. 117, 347 (2001).