Exploring the exotic f states of prototype compounds CeSb and USb

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Abstract

To unravel the interplay between the strong electronic correlation and itinerant-localized dual nature in typical f electron systems, we employed the density functional theory in combination with the single-site dynamical mean-field theory to systematically investigate the electronic structures of CeSb and USb. We find that the 4f states in CeSb are mostly localized with a weak quasi-particle resonance peak near the Fermi level. Conversely, the 5f electrons in USb display partially itinerant features, accompanied by mixed-valence behavior and prominent valence state fluctuations. Particularly, the 4f electronic correlations in CeSb are orbital-selective with strikingly renormalized $4f^{5/2}$ states, according to the low-energy behaviors of 4f self-energy functions. It is believed that the strong electronic correlation and fantastic bonding of f states contribute to elucidating the magnetism.

Keywords: dynamical mean-field theory, electronic correlation, itinerant-localized dual nature, valence state fluctuation

(Some figures may appear in colour only in the online journal)

1. Introduction

Lanthanides and actinides with partially filled 4f and 5f shells exhibit abundant physical behaviors including heavy-fermion behavior [1], quantum criticality [2], magnetic ordering [3–6], unconventional superconductivity [7, 8] and mixed-valence state [9]. It is generally believed that the properties are closely associated with electronic structure which arises from strong electronic correlation, large spin-orbital coupling and intricate crystal field splitting. Usually, the 4f electrons of the rare earths are considered to be localized and unlikely to involve in bonding. On the other hand, the early actinides (from Ac to Np) with successive filled 5f shell incline to be itinerant. Consequently, 5f electrons tend to locate near the Fermi level and strongly participate in bonding, generating a plethora of interesting and unique physics [9].

Special interests have been drawn to cerium antimonide (CeSb) and uranium antimonide (USb), which stabilize in the rock-salt (NaCl) type of crystal structure (see figure 1) with lattice constant 6.388 Å [10] and 6.191 Å [4], respectively. It is reported that CeSb is a semimetal with a small overlapping of Ce-5d and Sb-5p states, and 4f states are mostly localized far away from the Fermi level. It orders antiferromagnetically below $T_N = 16$ K and undergoes further phase transitions with decreasing temperature. Meanwhile, USb develops antiferromagnetic phase just below $T_N = 213$ K [6, 11, 12]. It is guessed that the extraordinary properties mainly stem from Ce-4f and U-5f electrons.

The magnetic phases of CeSb have been extensively studied using transport, thermodynamic, neutron scattering and spectroscopic experiments [3, 13–21] for half a century. In the cubic crystal field, $4f^{5/2}$ state of Ce atom splits into doublet $\Gamma_2$ and quartet $\Gamma_8$ states with a small energy gap around 19 K ~ 26 K [22], which enables the random distribution of spins and the formation of complicated antiferromagnetic ordering. Moreover, the photoemission spectroscopy (PES), angle-resolved photoemission spectroscopy (ARPES), optical conductivity and dHvA quantum oscillation shed light on the evolution of the electronic structure through paramagnetic to antiferromagnetic phase transition [23–26]. On the theoretical
The red Ising model [12] and exchange model [47] have been successively explored [5, 6, 11, 12, 38–46]. Theoretically, the magnetic phase transition and spin dynamics have been intensively explored [39]. The magnetic phase diagram tuned by temperature and pressure, magnetic phase transition and spin dynamics have been intensively explored [5, 6, 11, 12, 38–46]. Theoretically, the layered Ising model [12] and exchange model [47] have been used to explicate the multi-k antiferromagnetic structures. However, the somewhat simplified model can not be generalized to treat other magnetic phases. Besides, the traditional p–f mixing model based on c–f hybridization fails to adequately seize the essence of the magnetic phase [27, 48, 49], which reveals a probable novel mechanism. Furthermore, previous relativistic spin-density-functional theory [50] has been adopted to survey the band structure and magnetism of USb. They not only calculated the spin and orbital moment, but adopted to survey the band structure and magnetism of USb. It is established that the traditional density functional theory (DFT) combined with DMFT is a non-perturbative many-body approach to treat the local interactions between electrons [61]. This method has been successfully utilized to study many lanthanides and actinides materials [62–64]. In the present paper, we employ the DFT + DMFT method to carry out charge fully self-consistent calculations to examine the electronic structure in detail.

Generally, the DFT + DMFT approach maps the lattice model to a quantum impurity model self-consistently and solves the obtained quantum impurity model by using various quantum impurity solvers. The calculation is divided into the DFT and DMFT parts. The DFT calculation is conducted by using the WIEN2k [65] code which implements a full-potential linear augmented plane wave (FP-LAPW) formalism. The Perdew–Burke–Ernzerhof (PBE) functional [66] was chosen to express the exchange–correlation potential. The k-points mesh was 21 × 21 × 21. Besides, RMTKMAX = 7.0. In addition, the spin–orbital coupling was explicitly included. The convergence criteria for charge and energy reach 10−4 e and 10−4 Ry, respectively. The experimental crystal structures for CeSb [10] and USb [4] were used. Since the inverse temperature β = 40 (T ≈ 298.0 K), it was reasonable to retain only the paramagnetic solutions.

We employed the EDMFT code [67], which implements the DFT + DMFT computational engine and the corresponding quantum impurity solvers, to study the obtained DFT + DMFT Hamiltonian. The constructed multi-orbital character of 5f states. For example, the detected 5f2 atomic multiplets imply the localized behavior of 5f electrons [49]. The optical measurement manifests the existence of a wide U-6d and U-5f hybridization band around the Fermi level, demonstrating the itinerant 5f states [57]. Thus it is hard to depict the partially itinerant 5f electrons regarding the oversimplified assumption of the completely localized or itinerant 5f states. Previous electronic structure calculations within local-density approximation [58–60] are inadequate to capture the strong correlation among the 5f electrons. Until now, the credible theoretical investigation of electronic structure is still lacking.

The present paper aims to address the following issues. First of all, the localized 4f electrons and itinerant-localized 5f electrons remain long-standing issues. Second, the impact of strong correlation among f electrons on electronic structure is not yet fully understood. Third, the underlying physics behind the magnetic phase transition is still unclear. To answer the questions above, it is crucial to examine the detailed electronic structures of CeSb and USb to explore the itinerant-localized dual nature and electronic correlation of f states. It is believed that these results will enrich our understanding about the f electron systems and serve for further studies.

2. Methods

The strong correlation of Ce-4f states and U-5f states should be taken into account to accurately describe the electronic structure of CeSb and USb. It is established that the traditional density functional theory (DFT) combined with DMFT is a non-perturbative many-body approach to treat the local interactions between electrons [61]. This method has been successfully utilized to study many lanthanides and actinides materials [62–64]. In the present paper, we employ the DFT + DMFT method to carry out charge fully self-consistent calculations to examine the electronic structure in detail.

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quantum impurity models were solved using the hybridization expansion continuous-time quantum Monte Carlo impurity solver (dubbed as CT-HYB) [68, 69]. The Coulomb interaction strength $U$ and the Hund’s exchange parameter $J$ are $6.0 \text{ eV}$ and $0.7 \text{ eV}$ [70–73] via the Slater integrals [74], respectively. In order to simplify the calculations, we not only utilized the good quantum numbers $N$ and $J$, to reduce the sizes of matrix blocks of the local Hamiltonian, but also made a truncation for the local Hilbert space. It is emphasized that the atomic eigenstates were set with $N \in [0, 3]$ for Ce and with $N \in [0, 4]$ for U. Lastly, the lazy trace evaluation trick was applied to accelerate the Monte Carlo sampling further.

We performed charge fully self-consistent DFT + DMFT calculations, i.e., the correlation-corrected density matrix $\rho$ was built in the DMFT part, and then fed back to the DFT part to generate a new Kohn–Sham Hamiltonian $\hat{H}_{KS}$. Of the order of 60 DFT + DMFT iterations were required to obtain good convergence for the chemical potential $\mu$, charge density $\rho$, and total energy $E_{\text{DFT+DMFT}}$. The Matsubara self-energy functions $\Sigma(i\omega_n)$ generated in the last 10 DFT + DMFT iterations were collected and stored for further postprocessing. We utilized the maximum entropy method [75] to do the analytical continuation to extract the real-frequency self-energy $\Sigma(\omega)$ from the Matsubara self-energy $\Sigma(i\omega_n)$. $\Sigma(\omega)$ is an essential input for the calculation of the density of states $A(\omega)$, momentum-resolved spectral functions $A(k, \omega)$, and quasi-particle weight $Z$.

3. Results

3.1. Photoemission spectroscopy

To verify the reliability of our results, we first examine the calculated total density of states by referring to available experimental data. Figure 2 shows our calculated results and experimental density of states for CeSb [see figure 2(a)] and USB [see figure 2(b)]. It is apparent that almost no spectral weight exists near the Fermi level, revealing the localized $4f$ states. Furthermore, the calculated total density of states with a two-peak structure distribute around $-4 \text{ eV} \sim 0 \text{ eV}$, which are consistent with ultraviolet photoemission spectra (UPS) data [76]. For USB, the most prominent feature is the significant quasi-particle resonance peak near the Fermi level, which indicates the itinerant behavior of $5f$ electrons. Apart from that, a small shoulder peak about $-2 \text{ eV}$ is exactly reproduced, which agrees with UPS data [77, 78]. The consistency between our computed density of states and available experiment data confirms the correctness and reasonability of our DFT + DMFT calculated results.

3.2. Density of states and hybridization functions

Here we discuss about the integrated spectral functions and hybridization functions of CeSb and USB. Figures 3(a1) and (a2) present total density of states $A(\omega)$ of CeSb and USB, respectively. It is evident that CeSb exhibits very weak quasi-particle resonance peak in the Fermi level, with one main peak centered at $-2 \text{ eV}$, followed by the unoccupied $4f^2$ multiplets around $2 \text{ eV} \sim 6 \text{ eV}$. Notice that the occupied states around the Fermi level are ascribed to $4f^{3/2}$ states. The upper Hubbard band above the Fermi level is contributed by $4f^{3/2}$ states. Combined with the partial density of states in figures 3(b1) and (b2), it is suggested that the low-lying $4f^{5/2}$ states and high-lying $4f^{7/2}$ states are split by the spin–orbit coupling with energy separation about $300 \text{ meV}$, which agrees with those observed in the other cerium-based heavy fermion compounds [79, 80]. In figure 3(a2), a remarkable quasi-particle resonance peak emerges at the Fermi level, which comes from $5f^{3/2}$ states of USB. Meanwhile, a pronounced peak centered at $-2 \text{ eV}$ roots from the hybridization between U-$5f$ bands and U-$6d$ bands. Moreover, the upper Hubbard band around $0 \text{ eV} \sim 6 \text{ eV}$ from the unoccupied $5f^{7/2}$ states forms a ‘hump’. Then the hybridization strength between $f$ states and ligand $c$ bands are clearly characterized by the hybridization functions for $f^{5/2}$ and $f^{7/2}$ states [see figures 3(c1) and (c2)]. Obviously, $c – f$ hybridization of USB is much stronger than that of CeSb, demonstrating the localized $4f$ states and partially itinerant $5f$ states.

3.3. Momentum-resolved spectral functions

In this section, we analyze the momentum-resolved spectral functions $A(k, \omega)$ of CeSb and USB [see figure 4] along the high-symmetry line $X – \Gamma – X$ in the irreducible Brillouin zone [see figure 1(b)]. As expected, the computed band structures reproduce the typical traits of experimental ARPES spectra [24, 27, 48, 49]. Figure 4(a) plots the band structure of CeSb, which demonstrates missing $4f$ bands and the prominent Sb-$5p$ states about $-3 \text{ eV} \sim 0 \text{ eV}$. It is found that hole pockets at the $\Gamma$-point corresponding to Sb-$5p$ bands, and electron pockets at the X-point belonging to Ce-$5d$ states [23]. On the other hand, the band structure of USB [see figure 4(b)] displays two flat $5f$ bands just above the Fermi level, hybridizing with conduction bands, which are in line with the itinerant-localized nature of $5f$ states. It is discovered that an electron pocket just below the Fermi level at the $\Gamma$-point is attributed to U-$6d$ states and hole pockets around $-3 \text{ eV} \sim -1 \text{ eV}$ originate from Sb-$5p$ states. Beyond the previous theoretical studies [58–60],
Figure 3. Electronic density of states of CeSb and USb obtained by DFT + DMFT calculations. Total density of states (thick solid lines) and partial f density of states (color-filled regions) for CeSb (a1) and USb (a2), respectively. \( f_{5/2} \) (thick solid lines) and \( f_{7/2} \) (color-filled regions) for CeSb (b1) and USb (b2), respectively. The data presented in this figure are rescaled for a better view. Hybridization functions of \( f_{5/2} \) (thick solid lines) and \( f_{7/2} \) states (color-filled regions) for CeSb (c1) and USb (c2), respectively. The data presented in this figure are also rescaled. The vertical dashed lines denote the Fermi level.

Figure 4. Momentum-resolved spectral functions \( A(\mathbf{k}, \omega) \) of CeSb (a) and USb (b) under ambient pressure. The horizontal lines denote the Fermi level.

our calculation nicely captures the archetypical bands, further demonstrating the reliability of the DFT + DMFT method.

It is instructive to emphasize the representative band structures of CeSb and USb. (i) The 4f bands of CeSb are nearly invisible, in contrast, the 5f bands of USb are clearly detected adjacent to the Fermi level. It is commonly accepted that the position of f bands relative to the Fermi level plays an important role in determining bonding and related physical properties. (ii) The significant Sb-5p states at the \( \Gamma \)-point hybridize with the partially occupied 4f states, or totally occupied 5f bands. Additionally, the band width of Sb-5p states seems a bit smaller in CeSb than USb. (iii) The hybridization of U-5f and U-6d states right above the Fermi level manifests the itinerant 5f states, embodying the itinerant-localized dual nature of USb. It is proposed that the correlation and localized degree of f electrons are tightly related to the magnetism.

3.4. Self-energy functions

Generally speaking, electronic correlations could be enclosed by self-energy functions. Self-energy functions are the direct outputs of quantum impurity solver by solving the quantum impurity models. Figure 5 shows the Matsubara self-energy functions of CeSb and USb derived by DFT + DMFT calculations. (a) \( f_{5/2} \) components. (b) \( f_{7/2} \) components.

Figure 5. Imaginary parts of Matsubara self-energy functions of CeSb and USb derived by DFT + DMFT calculations. (a) \( f_{5/2} \) components. (b) \( f_{7/2} \) components.
the value of 4f\(_{5/2}\) state. Thirdly, the low-energy scattering rate of 5f states remains finite. Fourthly, 5f\(_{5/2}\) state in Usb deviates from the description of the Landau Fermi-liquid theory. As a consequence, it is concluded that the system resembles the non-Fermi-liquid state.

Then the quasi-particle weight \(Z\) and effective electron mass \(m^*\) are evaluated via the following equation [61] (table 1):

\[
Z = \frac{m^*}{m_e} = 1 - \frac{\partial}{\partial \omega} \text{Re} \Sigma(\omega)|_{\omega=0}.
\] (1)

Table 1 lists the computed effective electron mass \(m^*\) and quasi-particle weight \(Z\) of \(f_{5/2}\) and \(f_{7/2}\) states for CeSb and Usb. Evidently, the quasi-particle weight \(Z\) of 4f\(_{7/2}\) states for CeSb is close to one, producing relatively small effective electron mass and suggesting the weakly correlated 4f\(_{7/2}\) states. Instead, the 4f\(_{5/2}\) bands are much more renormalized than the 4f\(_{7/2}\) bands with a large effective electron mass (\(\approx 43.425 m_e\)). Therefore the orbital differentiation of 4f orbitals is notable in CeSb compared with the weakly renormalized 5f bands in Usb. Consequently, the 4f electronic correlations are strongly orbital-selective and commonly exist in the other cerium-based heavy fermion compounds [72].

### 3.5. Valence state fluctuations

Next let us concentrate on f electronic configurations and valence state fluctuations for CeSb and Usb. The calculated valence state histogram (or equivalently atomic eigenstate probability) \(p_{1}\) for f electrons is the direct output of the CTHYB quantum impurity solver, which stands for the probability to find out an f valence electron in a given atomic eigenstate \(\langle \psi_T \rangle\) (labeled by perfect quantum numbers \(N, J\) and the rest of atomic quantum numbers \(\gamma\) as mentioned in section 2) [81]. If valence electrons only favor one or two dominant atomic eigenstates, it implies that the valence state fluctuation in such a system is weak or restricted. On the contrary, if valence electrons incline to wander in a large number of atomic eigenstates, the valence state fluctuation could be very strong.

Figures 6(a) and (b) illustrate the calculated f valence state histograms for CeSb and Usb, respectively. For CeSb, the leading atomic eigenstate is \(|N = 1, J = 2.5, \gamma = 0\rangle\) with the atomic eigenstate probability accounting for 93%. At the same time, the atomic eigenstates probabilities for \(|N = 0, J = 0.0, \gamma = 0\rangle\) and \(|N = 1, J = 3.5, \gamma = 0\rangle\) are less than 1%, which are nearly indiscernible [see figure 6(a)]. It confirms the localized 4f electrons in CeSb with valence state confined to the primary atomic eigenstate \(|N = 1, J = 2.5, \gamma = 0\rangle\). Meanwhile, the corresponding valence state fluctuations are very weak. By summing up the atomic eigenstates probabilities \(p_{1}\) with respect to \(N\), we can derive the distribution of f electronic configurations. It will provide further information about the f valence state fluctuations and mixed-valence behaviors. In CeSb, the 4f\(^1\) configuration is predominant with its probability larger than 90%, while those of the 4f\(^0\) and 4f\(^2\) configurations decline to less than 5%. Consequently, the mixed-valence behavior is suppressed. In comparison with CeSb, Usb expresses two competing atomic eigenstates \(|N = 2, J = 4.0, \gamma = 0\rangle\) and \(|N = 3, J = 4.5, \gamma = 0\rangle\) with the atomic eigenstate probabilities being 63% and 19%, respectively. In the meantime, the probabilities for the other atomic eigenstates are less than 3%, which reveals that the 5f electrons would fluctuate between the two principle atomic eigenstates and hybridize with conduction bands. Furthermore, the probabilities for the 5f\(^1\) and 5f\(^2\) configurations reach 69% and 26%, respectively, whereas those of 5f\(^0\) and 5f\(^3\) configurations are less than 4%. Thus 5f states are partially itinerant and valence state fluctuations become noticeable.

### 4. Discussions

**Similarities and differences between CeSb and Usb.** First of all, they crystalize in NaCl type of structure and their ground states are antiferromagnetic. Secondly, the electronic correlation of 4f states is strongly orbital-dependent, while the 5f states are moderately correlated. Thirdly, 4f states tend to be localized with a small quasi-particle resonance peak near the Fermi level and show weak valence state fluctuations. In contrast, 5f states display mixed-valence behavior with non-integer 5f occupations. Lastly, the hybridization between 4f states and partially occupied Sb-5p states pushes the Sb-5p band toward the Fermi level, changing the band structure and Fermi surface during the magnetic phase transition.

**Unveiling the electronic correlation and magnetism.** It is mentioned that the physical mechanism behind the ground
states of CeSb and USB seem quite different. For CeSb, localized 4f states are likely to form local moments, and the small crystal field splitting polarizes the spin along various directions to generate various magnetic phases [22]. It is anticipated that the hybridization between 4f electrons and Sb-5p states, as well as 4f electronic correlations play a vital role in magnetic transition. However, it is another story for USB. The itinerant 5f electrons locating above Sb-5p states produce the extended spatial wave function and prefer to hybridize with totally occupied Sb-5p states, which are pushed away from the Fermi level. Thus the p – f mixing effect could not balance the energy cost during the magnetic transition [27]. Therefore a credible model regarding the electronic correlation and crystal field splitting should be formulated to resolve such an interesting problem. The present work is undertaken to interpret the long-standing issue.

5. Conclusion

In summary, the subtle electronic structures of CeSb and USB have been comprehensively investigated using the established DFT + DMFT method. The momentum-resolved spectral functions A(k, ω), total and f partial density of states A(ω) and A_f(ω), hybridization functions, Matsubara self-energy functions, and f valence state fluctuations are exhaustively studied. The calculated results not only accord with the available experimental data but also serve as critical predictions for future research. It is identified that the 4f electrons in CeSb are generally localized while the 5f states in USB exhibit itinerant-localized dual nature. Hence, tiny spectral weights near the Fermi level and weak valence state fluctuations are observed in CeSb. Instead a significant quasi-particle resonance peak appears around the Fermi level and mixed-valence behavior is remarkable in USB. Especially, it is suggested that 4f states show orbital-dependent correlation, which is absent in 5f states. Consequently, it is expected that the intrinsic electronic structure might lift the veil of the mysterious magnetism, which deserves further experimental and theoretical attention.

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