Electronic correlations in cerium’s high-pressure phases

Haiyan Lu and Li Huang

Science and Technology on Surface Physics and Chemistry Laboratory, PO Box 9-35, Jiangyou 621908, People’s Republic of China

E-mail: lihuang.dmft@gmail.com

Received 16 May 2018, revised 21 August 2018
Accepted for publication 23 August 2018
Published 7 September 2018

Abstract

Under high pressure, cerium exhibits three distinct phases, namely $\alpha'$, $\alpha''$, and $\epsilon$-cerium. It is unclear whether the $4f$ electronic correlations will play a vital role in these phases or not. By utilizing the combination of traditional density functional theory and single-site dynamical mean-field theory, we tried to calculate the electronic structures of cerium’s high-pressure phases. Their momentum-resolved spectral functions, total and $4f$ partial density of states, local self-energy functions, and $4f$ electronic configurations were exhaustively studied. The calculated results show that the correlated $4f$ bands strongly hybridize with the conducting $spd$ bands around the Fermi level. The Matsubara self-energy functions exhibit Fermi-liquid like characteristic in the low-frequency regime. In addition, the fluctuations among the $4f$ atomic eigenstates are somewhat prominent (especially for the $\epsilon$ phase), which lead to slight modification of the $4f$ occupancy. It is suggested that the $4f$ electrons in these phases tend to be itinerant.

Keywords: strongly correlated electron systems, rare earth metals, dynamical mean-field theory

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

1. Introduction

Cerium (Ce) is one of the most fantastic elements in the periodic table because of its unusual electronic structures, which manifest in its multiple allotropic phases. Ce may posses four allotropes ($\alpha$, $\beta$, $\gamma$, and $\delta$ phases) under ambient pressure, and undergo three successive solid phase transitions before reaching its liquid state [1]. When $P \sim 0.8$ GPa and at room temperature, strikingly, an iso-structural phase transition would take place between the $\alpha$ and $\gamma$ phases (both phases are in face-centered-cubic structure). Though the crystal structure is preserved during the transition, the atomic volume changes by $\sim 15\%$, which has not been observed in any other simple metals. The underlying physics and driving force of the $\alpha - \gamma$ phase transition have been, and are being to this day, warmly debated. Particularly, concerning the role played by the correlated $4f$ electrons in the transition, it is still a matter of dispute and ongoing research [2–15].

Under moderate pressure and temperature cerium will exhibit another three distinct phases, namely the $\alpha'$, $\alpha''$, and $\epsilon$ phases, which result in an extremely complicated $P - T$ phase diagram [16]. These high-pressure phases stabilize in low-symmetry crystal structures (see figure 1). The $\alpha'$ phase is orthorhombic, while the $\alpha''$ phase is monoclinic. The $\alpha$ phase will transform into the $\alpha'$ and $\alpha''$ phases in the pressure range from 5 to 12 GPa, but which phase transition (i.e. $\alpha - \alpha'$ or $\alpha - \alpha''$ transition) could take place in a cerium sample strongly depends on the method of sample preparation [17, 18]. Beyond 12 GPa, both the $\alpha'$ and $\alpha''$ phases will transform into the body-centered tetragonal $\epsilon$ phase [19].

It is very difficult to prepare and identify pure high-pressure phases of Ce, which requires precise controls of pressure and thermal process [20, 21]. As a result, it is not easy to conduct extensively experimental researches. Up to now most of the available experiments have been contributed to study the high-pressure equation of states, electron-phonon coupling, lattice instability, and superconductivity of Ce [19, 22, 23]. On the other hand, low-symmetry crystal structures, strong spin-orbit coupling, and notable electronic correlations in $4f$ electrons also pose great challenges to the theoretical calculations.
We observe some [30–36], the low-temperature hidden order phase of URu$_2$Si$_2$ are $Cmcm$, $Cmmm$, $I_{4}mmnm$, respectively.

Though numerous efforts have been made to explore the fundamental properties of cerium’s high-pressure phases, actually we know a little about their electronic structures. There are a lot of puzzles and questions that need to be solved. For instance, do the 4f electrons remain itinerant or localized state [29]? What’s the consequence of the interplay between spin–orbit coupling and electronic correlation in 4f electronic structures? Is there strong hybridization between the 4f and spd bands as predicted by the Kondo volume collapse scenario [4, 5]? Last, but by no means least, are the 4f electronic configurations for these high-pressure phases the same, and are they similar to or different from those for the other phases under ambient pressure [30–36]? In order to answer the above questions, more experimental investigations and theoretical calculations are highly desired.

2. Methods

In the present work, we attempt to sketch an unified picture for the electronic structures of cerium’s high-pressure phases by utilizing the state-of-the-art ab initio many-body approach, specifically, the density functional theory in combination with the single-site dynamical mean-field theory (dubbed as DFT + DMFT). This approach can treat the strong 4f electronic correlations, spin–orbit coupling, as well as on-site Kondo screening on the same footing, and incorporate them into realistic band structures based on DFT calculations. It has been successfully applied to study many interesting problems emerged in 4f and 5f strongly correlated electron systems, such as the best known $\alpha - \gamma$ phase transition in Ce [30–36], the low-temperature hidden order phase of URu$_2$Si$_2$ [37], and the valence state fluctuations in Yb [38] and Pu [39, 40]. As for the basic principles and technical details of the DFT + DMFT method, please refer to the good reviews (see [41, 42]) and references therein.

We performed charge fully self-consistent DFT + DMFT calculations by using the EDMFT software package [43]. The experimental crystal structures [16] were used. Within the DFT part, the WIEN2K code which implements a full-potential linear augmented plane-wave formalism [44], was employed to solve the Kohn–Sham equation. We selected the generalized gradient approximation (Perdew–Burke–Ernzerhof functional) [45] to represent the exchange-correlation potential. The spin–orbit coupling was always included in the calculations. The cutoff parameter $R_{MTK_{MAX}}$ was set to 7.0. A $17 \times 17 \times 17$ uniform $k$-mesh was adopted for the Brillouin zone integration. Within the DMFT part, the hybridization expansion version continuous-time quantum Monte Carlo impurity solver (dubbed as CT-HYB) [46–48] was used to solve the quantum impurity model (inverse temperature $\beta = 40.0 \, eV^{-1}$, $T \approx 290 \, K$). Undoubtedly, the 4f bands were treated as correlated orbitals. The corresponding interaction parameters were on-site Coulomb interaction $U = 6.0 \, eV$ and Hund’s exchange coupling $J = 0.7 \, eV$, which were in accord with the values used in the literatures [32, 33, 49]. For the double counting term, we chose the fully localized limit scheme [50]. After the DFT + DMFT calculations were fully converged, we carried out analytical continuations for the Matsubara self-energy functions $\Sigma(i\omega_n)$ by the maximum entropy method [51], and then used the real-frequency self-energy functions $\Sigma(\omega)$ to evaluate the other physical observables, such as the momentum-resolved spectral functions and density of states.

3. Results

3.1. Momentum-resolved spectral functions $A(k, \omega)$

The calculated spectral functions of the three high-pressure phases are displayed in figures 2(a)–(c). Since most of the 4f bands in Ce are unoccupied, their positions are well above the Fermi level. As $E_F < \omega < 1.5 \, eV$, we observe some intense and stripe-like features, which are mainly associated with the 4f bands. Their bandwidths are approximately 0.8–1.2eV, which are much smaller than the Coulomb interaction strength (i.e. $W \ll U$). It is a direct evidence to support the statement that the 4f bands in cerium’s high-pressure phases are still correlated [42]. In addition, we also observe heavy $e - f$ hybridizations between the 4f and the spd conduction bands in this energy window. As $\omega > 1.5 \, eV$ and $\omega < E_F$, the general features become somewhat blurry. The bands in this energy range exhibit remarkable dispersions and large bandwidths. Apparently, they belong to the spd itinerant bands to a large extent. It has come to our notice that a few years ago Eriksson et al. had employed a linear muffin-tin orbital code by using the local density approximation to study the electronic structures of $\alpha'$, $\alpha''$, and $\epsilon$-Ce [26, 27]. In their study, the 4f bands were treated as fully delocalized and the electronic correlations were ignored completely, so that the obtained band structures differ from ours. Compared to our results, their 4f bands exhibit larger bandwidth (~2.0eV) and stronger dispersion. In order to reproduce their results, we also performed conventional DFT calculations for the three high-pressure phases. The fat band structures obtained by DFT calculations are shown in figures 2(f)–(h). Clearly, the DFT + DMFT band structures near and above the Fermi level are strongly renormalized, as compared to the DFT ones. Consequently, the effective masses of 4f electrons predicted by our DFT + DMFT calculations must be heavier than theirs.
Figure 2. (a)–(c) Momentum-resolved spectral functions $A(k, \omega)$ of $\alpha'$, $\alpha''$, and $\epsilon$-Ce obtained by the DFT + DMFT method. The horizontal dashed lines represent the Fermi level. (d) Total density of states $A(\omega)$ (solid thick lines) and $4f$ partial density of states $A_{4f}(\omega)$ (color-filled regions) of $\alpha'$, $\alpha''$, and $\epsilon$-Ce obtained by the DFT + DMFT method. (e) $4f$ hybridization functions $\tilde{\Delta}(\omega) = -\text{Im}\Delta(\omega)/\pi$ of $\alpha'$, $\alpha''$, and $\epsilon$-Ce obtained by the DFT + DMFT method. The spectra for the $4f_{5/2}$ and $4f_{7/2}$ components are plotted as solid thick lines and color-filled regions, respectively. (f)–(h) Fat band structures of $\alpha'$, $\alpha''$, and $\epsilon$-Ce obtained by the DFT method. Here, green dots indicate the contribution of cerium’s $4f$ orbitals. (i) Total density of states $A(\omega)$ (solid thick lines) and $4f$ partial density of states $A_{4f}(\omega)$ (color-filled regions) of $\alpha'$, $\alpha''$, and $\epsilon$-Ce obtained by the DFT method. In panels (d), (e) and (i), the original data are rescaled and shifted vertically for a better view. The vertical dashed lines represent the Fermi level.

Now let us concentrate on the similarities and differences in the band structures of the three phases. As for the $\alpha'$ and $\alpha''$ phases, since their lattice volumes are very close and their crystal structures are tightly related, the corresponding band structures are quite similar and share some common features, such as the positions of the $4f$ and valence bands. However, for the $\epsilon$ phase, which exists under higher pressure and thus has a smaller lattice volume [16], the center of the correlated $4f$ bands shifts upwards slightly and the itinerant $spd$ bands exhibit much more significant dispersions. Finally from figures 2(a) and (b), we can speculate that the Fermi surfaces that enclose the $\Gamma$ point are probably hole-type and electron-type in the $\alpha'$ and $\alpha''$ phases, respectively.

3.2. Density of states $A(\omega)$

The total density of states $A(\omega)$ are shown in figure 2(d). In the vicinity of the Fermi level, there is the so-called Kondo resonance peak with sharp two-peaks structure. This splitting is owing to the spin–orbit coupling effect. Away from the Fermi level, the spectrum spreads out and becomes almost featureless. Just as discussed above, the spectra for the $\alpha'$ and $\alpha''$ phases are very similar, including the magnitude of the Kondo resonance peak, the two satellite peaks between $-2$ eV and $E_F$, and the total bandwidth. While for the $\epsilon$ phase, its spectrum turns broader and has a stronger Kondo resonance peak. In the previous DFT calculations [26], the two satellite peaks below the Fermi level were also observed. They were associated with the $s$ and $p$ itinerant bands. In addition, obvious ‘pseudogap’ structures were identified for the three high-pressure phases, which were then used to elaborate why distorted and low-symmetry crystal structures (see figure 1) were favored in Ce at lower volumes. However, in our calculated results, the so-called ‘pseudogap’ feature is absent. In this regard, the ‘pseudogap’ mechanism for the phase stability of distorted phases of Ce under pressure requires further theoretical and experimental validations.

The $4f$ partial density of states $A_{4f}(\omega)$ are shown in figure 2(d) as well (see color-filled regions). According to the difference between $A(\omega)$ and $A_{4f}(\omega)$, it is clear that the contributions from the $4f$ bands are predominant near the Fermi level. They compose the Kondo resonance peak. On the other hand, below the Fermi level, the itinerant $spd$ bands are the most important (the $4f$ spectral weight approaches zero). Due to the spin–orbit coupling, the $4f$ bands are split into two components, namely $4f_{5/2}$ and $4f_{7/2}$. The $4f_{5/2}$ component has a lower energy and is closer to the Fermi level. The lower Hubbard bands are almost invisible since the $4f$ occupancy is small. The upper Hubbard bands look like broad ‘humps’, and they locate roughly from 2 eV to 8 eV. All of these features are comparable to those already found in the $\alpha$ phase by using the DFT + DMFT method [31–34] and photoemission spectroscopy [53, 54]. Compared to the $\alpha'$ and $\alpha''$ phases, the $A_{4f}(\omega)$ of the $\epsilon$ phase is a bit different. The peaks ascribed to
the 4f$_{5/2}$ and 4f$_{7/2}$ components (and the upper Hubbard bands) have larger intensity, and their positions are shifted to high-energy regime marginally.

In figure 2(i), the total density of states $A(\omega)$ and 4f partial density of states $A_{4f}(\omega)$ obtained by the DFT method are shown for comparison. Both of them exhibit larger band width near the Fermi level. The spin–orbit coupling splitting effect is less pronounced. Furthermore, the upper and lower Hubbard bands are absent.

3.3. Hybridization functions $\Delta(\omega)$

In figure 2(e), we visualize the imaginary parts of the real-frequency hybridization functions $\Delta(\omega)$, which are approximately proportional to the strength of hybridization effect between the strongly correlated 4f bands and the weakly correlated (or non-correlated) spd bands. We can see that the hybridization effect is very strong, especially near the Fermi level. It indicates that the Kondo volume collapse scenario not only can be used to explain cerium’s $\alpha - \gamma$ phase transition [4, 5], but also is useful for understanding the underlying electronic structures of cerium’s high-pressure phases. Notice that the hybridization function of the $\epsilon$ phase is somewhat higher than the others, which implies that its 4f electrons should be more itinerant. Naturally, we conclude that the valence state fluctuation in the $\epsilon$ phase must be the most pronounced among cerium’s allotropes. We will discuss this issue later.

3.4. Local self-energy functions

Within the framework of the DFT + DMFT approach, the electronic self-energy function should be local. We can utilize it to analyze the 4f electronic correlations in cerium’s high-pressure phases. In figure 3(a), we plot the imaginary parts of Matsubara self-energy functions $-\text{Im}\Sigma(\imath\omega_n)$ for the 4f$_{5/2}$ and 4f$_{7/2}$ components, respectively. In low-frequency regime, the data display conspicuous quasi-linear behavior, and they can be extrapolated to zero at $\omega_n \to 0$. And then we use the empirical formula:

$$-\text{Im}\Sigma(\imath\omega_n) = c(\imath\omega_n)^\alpha + b, \quad (1)$$

to fit the data (only the first five data points are used). The fitting parameters $c$, $b$, and $\alpha$ are collected in table 1. For the three high-pressure phases, we find that the values for the fitting parameter $\alpha$ (b) are very close to 1.0 (0.0), indicating that these local self-energy functions could be understood with the Landau Fermi-liquid theory [42].

By using the maximum entropy method [51], we can extract the real-frequency self-energy function $\Sigma(\omega)$ from the Matsubara self-energy function $\Sigma(\imath\omega_n)$. The final results (only the real parts) are shown in figures 3(b) and (c). $\text{Re}\Sigma(\omega)$ is approximately linear around the Fermi level (i.e. $\omega = 0$). We can evaluate the quasi-particle weight $Z$ and effective electron mass $m^*$ via the following equation [42]:

$$Z^{-1} = \frac{m^*}{m_e} = 1 - \frac{\partial}{\partial \omega}\text{Re}\Sigma(\omega)\big|_{\omega=0}, \quad (2)$$

The calculated $Z$ is about 0.44–0.63 (see table 1), which reveals that the 4f electrons in cerium’s high-pressure phases are moderate correlated. Among the three phases, the $\alpha'$ phase has the smallest $Z$, thus in principle it will manifest the strongest electronic correlation and have the largest $m^*$ ($m^* = 2.28m_e$ and 1.92$m_e$ for the 4f$_{5/2}$ and 4f$_{7/2}$ components, respectively). As a comparison, the effective electron mass for the $\alpha$ phase is about 15$m_e$–20$m_e$ [30, 55].

3.5. Distribution of atomic eigenstates

The CT-HYB quantum impurity solver is capable of computing the valence state histogram $p_{\alpha}$, which means the probability to find a valence state electron (such as cerium’s 4f electrons) in a given atomic eigenstate $|\psi\rangle$ (labelled by $\Gamma$) [47]. It provides us with a powerful lens to learn the subtle electronic structures of strongly correlated systems directly [39, 40, 56]. Here, we would like to utilize it to unveil whether the 4f electrons in cerium’s high-pressure phases are localized or not. In the presence of spin–orbit coupling, the 4f atomic eigenstates can be classified by using the good quantum numbers $N$ (total occupancy), $J$ (total angular momentum), and $\gamma$ ($\gamma$ stands for the rest of the atomic quantum numbers, such as $J_z$).

In the present work, in order to accelerate the calculations, we made a crucial truncation that only those atomic eigenstates with $N \in [0, 3]$ were taken into considerations [47]. Next we will prove that the contributions from the atomic eigenstates with larger occupancy ($N \geq 3$) are trivial and the truncation we used is reasonable.

The obtained valence state histograms $p_{\alpha}$ are shown in figures 4(a)–(c). As is seen in this figure, the dominant atomic eigenstates are $|N = 1, J = 2.5, \gamma = 0\rangle$ and $|N = 1, J = 3.5, \gamma = 0\rangle$. Their probabilities add up to about 68%–74%. The less important atomic eigenstate is $|N = 0, J = 0.0, \gamma = 0\rangle$, which amounts to about 12%–15%. For the $N = 2$ case, the contributions from various atomic eigenstates account for about 13%–17%. They are comparable and there are no dominant ones. The probabilities for the atomic eigenstates with $N = 3$ are tiny ($<1\%$ in total), so it is difficult to see them in figures 4(a)–(c). Since the contributions from the $N \geq 3$ atomic eigenstates are unimportant, it is acceptable to discard them to improve the computational efficiency during the DFT + DMFT iterations. Actually, we repeated all of the DFT + DMFT calculations with $N \in [0, 2]$ and $N \in [0, 4]$. The benchmark results are practically identical.

---

**Table 1.** Fitting parameters for the imaginary parts of Matsubara self-energy functions. See main text for the detailed explanations.

| Phases | Types | $c$  | $b$  | $\alpha$ | $m^*/m_e$ | $Z$ |
|--------|-------|------|------|----------|-----------|-----|
| $\alpha'$ | 4f$_{5/2}$ | 0.94 | -0.0039 | 0.92 | 2.06 | 0.48 |
| $\alpha'$ | 4f$_{7/2}$ | 0.73 | -0.0020 | 0.93 | 1.78 | 0.56 |
| $\alpha''$ | 4f$_{5/2}$ | 1.09 | -0.0059 | 0.91 | 2.28 | 0.44 |
| $\alpha''$ | 4f$_{7/2}$ | 0.84 | -0.0031 | 0.94 | 1.92 | 0.52 |
| $\epsilon$ | 4f$_{5/2}$ | 0.70 | -0.0015 | 0.96 | 1.73 | 0.58 |
| $\epsilon$ | 4f$_{7/2}$ | 0.58 | -0.0013 | 0.96 | 1.58 | 0.63 |
Next, let us compare the valence state histograms of the three phases. First, in the $\alpha'$ and $\alpha''$ phases, the probability of the $|N = 1, J = 2.5, \gamma = 0\rangle$ eigenstate is nearly twice as much as the one of the $|N = 1, J = 3.5, \gamma = 0\rangle$ eigenstate. While for the $\epsilon$ phase, the probabilities for the two atomic eigenstates are close. Second, the probabilities for the $N = 0$ and $2$ cases in the $\epsilon$ phase are quite larger than those in the $\alpha'$ and $\alpha''$ phases. All these facts reveal that the $4f$ electrons in cerium’s high-pressure phases are not always bound to the $N = 1$ case, and favor to hop among a variety of atomic eigenstates with different occupancies and angular momentums. Especially for the $\epsilon$ phase, this tendency is the most noticeable.
3.6. Valence state fluctuations

From the 4f valence state histograms, we can easily assess the distributions of 4f electronic configurations, and then discuss the valence state fluctuation phenomenon which usually manifests itself in the rare earth compounds (such as the Ce-, Sm-, and Yb-based heavy fermion systems [38, 57]) and the actinides (such as Pu [39, 40]). We can use the following equation to calculate the weights (or distributions) for 4f electronic configurations:

\[ p(4f^i) = \sum_{N} \sum_{J} \sum_{\gamma} \delta(N - i) p_{\gamma}, \quad i \in [0, 3], \tag{3} \]

The calculated results are visualized in figures 4(d)–(f). Under external pressure, the unit cell volume is reduced, and the corresponding electronic structures (including the band structure, density of states, Fermi surface, valence state histogram, and distribution of electronic configuration) are tuned gradually. Here, we would like to figure out the relationship between the unit cell volume and the 4f electronic configurations. In figure 4(g), we try to plot the \( p(4f^i) \) against unit cell volume since 4f is cerium’s ground state configuration. In order to gain a clear impression about the evolution of electronic configurations, we performed additional calculations for the \( \alpha \) and \( \gamma \) phases, and supplemented their data to this figure. We find that the \( p(4f^i) - V \) curve exhibits a quasi-linear behavior. Then we used the formula \( f(x) = ax + b \) to fit the calculated data. The fitting parameters \( a \) and \( b \) are 0.0028 and 0.29, respectively. This linear behavior is easily to be understood: if the unit cell volume is expanded, the 4f electrons will be more localized and the 4f valence state fluctuation will get weaker. In consequence, the 4f electrons have a tendency to stay at the 4f ground state configuration instead of hopping to and fro, with respect to the increment of unit cell volume. On the other hand, we think that the \( p(4f^i) \) could be considered as a quantitative tool to measure the valence state fluctuation and electronic localized degree of freedom for Ce-based system.

Based on the obtained data, we reach the following conclusions. First, the electronic configurations for the \( \alpha' \) and \( \alpha'' \) phases are quite similar in all respects. Second, in cerium’s high-pressure phases, the 4f valence state fluctuations are more significant than the other phases under ambient pressure. Particularly, in the \( \epsilon \) phase, the 4f valence state fluctuation is much stronger than the other allotropes. Third, strong valence state fluctuation will modify the 4f occupancy inevitably (the nominal 4f occupancy is 1.0). Thus, we employed the following equation to evaluate the averaged 4f occupancy \( N_{4f} \) [56],

\[ N_{4f} \approx \sum_{i=0}^{3} p(4f^i) \times i \tag{4} \]

The \( N_{4f} \) values for the \( \alpha' \), \( \alpha'' \), and \( \epsilon \) phases are 0.983, 1.009, and 1.029, respectively.

4. Summary

In conclusion, we calculated the electronic structures of three high-pressure phases (\( \alpha' \), \( \alpha'' \), and \( \epsilon \)) of Ce by using the charge fully self-consistent DFT + DMFT method. Overall, the 4f electrons of the three phases are moderate correlated (the electronic correlation in the \( \alpha' \) phase is somewhat stronger than the other two phases), but they exhibit more itinerant features than the \( \alpha \) and \( \gamma \) phases. It is suggested that the Matsubara self-energy functions of the three phases at low-frequency regime should show apparent Landau Fermi-liquid like behavior, which could be validated by optical spectroscopy. Furthermore, the valence state fluctuation in these phases obey the following sequence: \( \gamma < \alpha < \alpha'' < \alpha' < \epsilon \), which is precisely described by the \( p(4f^i) - V \) curve.

To the best of our knowledge, this study presents for the first time the correlated electronic structures of \( \alpha' \), \( \alpha'' \), and \( \epsilon - Ce \) by using a first-principles many-body approach. It is also the first step to build an unified picture for the electronic structures and related physical properties of all allotropes of Ce. Unfortunately, the corresponding experiments are rare in the literature. Our results serve as critical predictions, and require further experimental examinations.

Acknowledgments

This work was supported by the Natural Science Foundation of China (No. 11504340 and No. 11704347), the Foundation of President of China Academy of Engineering Physics (No. YZ2015012), and the Science Challenge Project of China (No. TZ2016004).

ORCID iDs

Li Huang https://orcid.org/0000-0001-7504-7231

References

[1] Koskenmaki D C and Gschneidner K A Jr 1978 Handbook on the Physics and Chemistry of Rare Earths vol 1, ed K A Gschneidner Jr and L Eyring (Amsterdam: Elsevier) ch 4
[2] Johansson B 1974 Phil. Mag. 30 469
[3] Johansson B, Abrikosov I A, Aldén M, Ruban A V and Skriber H L 1995 Phys. Rev. Lett. 74 2335
[4] Allen J W and Martin R M 1982 Phys. Rev. Lett. 49 1106
[5] Allen J W and Liu L Z 1992 Phys. Rev. B 46 5047
[6] Jeong I K, Darling T W, Graf M J, Proffen T, Heffner R H, Lee Y, Vogt T and Jorgensen J D 2004 Phys. Rev. Lett. 92 105702
[7] Liu M J, Jackson D, Cynn H, Aracne C, Evans W J and McMahan A K 2008 Phys. Rev. Lett. 101 165703
[8] Jarlgård T 2014 Phys. Rev. B 89 184426
[9] Casadei M, Ren X, Rinke P, Rubio A and Scheffler M 2012 Phys. Rev. Lett. 109 146402
[10] Lanatà N, Yao Y X, Wang C Z, Ho K M, Schmalian J, Haule K and Kotliar G 2013 Phys. Rev. Lett. 111 196801
[11] Amadon B and Gersossi A 2015 Phys. Rev. B 91 161103
[12] Östlin A, Di Marco I, Locho I L M, Lashley J C and Vitos L 2016 Phys. Rev. B 93 094103
[13] Amadon B, Jollet F and Torrent M 2008 Phys. Rev. B 77 155104
[14] Svane A 1996 Phys. Rev. B 53 4275
