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Abstract
The LDA + DMFT (local density approximation combined with dynamical mean-field theory) computation scheme has been used to calculate spectral properties of LaFeAsO—the parent compound of the new high-T_c iron oxypnictides. The average Coulomb repulsion $\bar{U}$ and Hund's exchange J parameters for iron 3d electrons were calculated using the *first-principles* constrained density functional theory scheme in the Wannier functions formalism. Resulting values strongly depend on the number of states taken into account in the calculations: when the full set of O-2p, As-4p and Fe-3d orbitals and the corresponding bands are included, the interaction parameters $\bar{U} = 3$–4 eV and $J = 0.8$ eV are obtained. In contrast, when the basis set is restricted to the Fe-3d orbitals and bands only, the calculation gives much smaller values of $\bar{U} = 0.5$–0.6 eV, $J = 0.5$ eV. Nevertheless, DMFT calculations with both parameter sets and the corresponding basis sets result in a weakly correlated electronic structure that is in agreement with the experimental x-ray and photoemission spectra.

(Some figures in this article are in colour only in the electronic version)

Recent discovery of high-T_c superconductivity in iron oxypnictides LaO$_{1-x}$F$_x$FeAs [1] has stimulated intense experimental and theoretical activity. In a striking similarity with the high-T_c cuprates, the undoped LaFeAsO is not superconducting, but exhibits an antiferromagnetic commensurate spin-density wave below 150 K [2]. Only when electrons (or holes) are added to the system via doping, antiferromagnetism is suppressed and superconductivity appears. As it is generally accepted that the Coulomb correlations between the copper 3d electrons are responsible for the anomalous properties of cuprates, it is tempting to suggest that the same is true for the iron 3d electrons in LaFeAsO.

The ratio of the Coulomb interaction U and the bandwidth W determines the correlation strength. For $U/W < 1$ the system is weakly correlated and the results of density functional theory (DFT) calculations are enough to explain its electronic and magnetic properties. However, if the U value is comparable with W or even larger the system is in an intermediate or a strongly correlated regime and the Coulomb interactions must be treated explicitly in the electronic structure calculations. The partially filled bands formed by Fe-3d states in LaFeAsO have a width of ≈ 4 eV (see the shaded area in the lower panel of figure 1), so the interaction parameter U should be compared with this value.

In practice, U is often considered a free parameter to achieve the best agreement between the calculated and measured properties of the investigated system. However, the most attractive approach is to determine the Coulomb interaction parameter U from *first principles*. Two methods
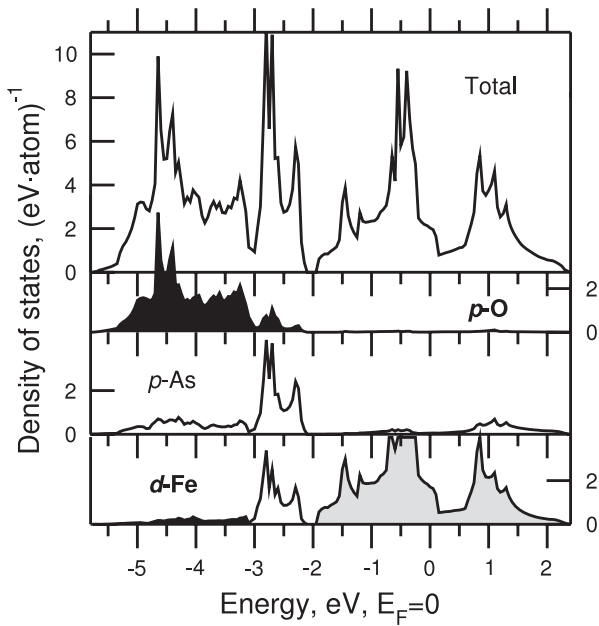
Figure 1. Total and partial densities of states for LaFeAsO obtained in DFT calculations in the framework of the LMTO method.

are generally used for this purpose: the constrained DFT scheme [3, 4], where the d-orbital occupancies in DFT calculations are fixed to certain values and U is determined as a numerical derivative of the d-orbital energy over its occupancy, and the random phase approximation (RPA) [5], where the screened Coulomb interaction between the d electrons is calculated using perturbation theory. Recently, RPA calculations of the interaction parameter U in LaFeAsO were reported [6], estimating putting the U value in the range 1.8–2.7 eV. In [7] it was proposed to use a U of 4 eV obtained in RPA calculations for metallic iron [8]. This value of the Coulomb parameter (with Hund's exchange parameter $J = 0.7$ eV) was used in dynamical mean-field theory (DMFT) [9] calculations for LaFeAsO [7, 11, 10]. These studies find the iron 3d electrons to be in an intermediate or a strongly correlated regime, as can be expected for the Coulomb parameter $U = 4$ eV and the Fe-3d bandwidth of ≈ 4 eV.

To estimate the correlation strength one can compare experimental spectra with the densities of states (DOS) obtained in DFT calculations. For strongly correlated materials additional features in the experimental photoemission, x-ray absorption and optical spectra appear that are absent in the DFT DOS. These features are interpreted as lower and upper Hubbard bands. If no Hubbard bands are observed and the DOS obtained in DFT calculations describes the experimental spectra satisfactorily the material is considered to be in a weakly correlated regime. LaFeAsO was studied by soft x-ray absorption and emission spectroscopy [12], x-ray absorption (O K-edge) spectroscopy [13] and photoemission spectroscopy [14]. All these studies conclude that DOS obtained in DFT calculations agree well with the experimental spectra and the estimated value of the Coulomb parameter is less than 1 eV [13]. Such a contradiction with the DMFT results [7, 11, 10] using $U = 4$ eV shows that the

first-principles calculation of the Coulomb parameter U for LaFeAsO is needed to assess the strength of correlations in this material. Results of such calculations using the constrained DFT methods are reported in the present work.

It is important to note that the Coulomb interaction parameter U depends on the choice of a model and, more specifically, on the choice of the orbital set that is used in the model. For example, the constrained DFT calculations for high-T_c cuprates result in a U value for the Cu d-shell between 8 and 10 eV [15]. A value of U in this range was used in cluster calculations where all Cu d-orbitals and p-orbitals of neighboring oxygens were taken into account, resulting in spectra in good agreement with the experimental data [16]. However, in a one-band model, where only the $x^2 - y^2$ orbital of copper is explicitly included [17], the U value giving a good agreement with experimental data falls into the 2.5–3.6 eV range, that is 3-4 times smaller than the constrained DFT value. The same situation occurs for titanium and vanadium oxides: the U value from constrained DFT calculations is ≈ 6 eV; the cluster calculations where all the transition metal d-orbitals and p-orbitals of neighboring oxygens were taken into account using U close to this value lead to a good agreement between the calculated and experimental spectra [18]. However, in the model where only the partially filled t_{2g} orbitals are included, a much smaller U value (corresponding to Slater integral $F^0 = 3.5$ eV) gives the results in agreement with experimental data [19]. It is interesting that such a small U value can be obtained in the constrained DFT calculations for titanates and vanadates where only t_{2g}-orbital occupancies are fixed while all the other states (e$_g$-orbitals of vanadium and p-orbitals of oxygen) are allowed to relax self-consistently [20, 19]. Thus the computational scheme used in the constrained DFT (the set of orbitals with fixed occupancies) should be consistent with the basis set of the model where the calculated U value is to be used.

Another source of uncertainty in the constrained DFT scheme is the definition of atomic orbitals whose occupancies are fixed and energies are calculated. In some DFT methods, like linearized muffin-tin orbitals (LMTO), these orbitals could be identified with LMTOs. However, for other basis sets, for example plane waves in the pseudopotential methods, one should use a more general definition of the localized atomic-like orbitals such as Wannier functions (WFs) [23]. A practical way to calculate WFs for specific materials using the projection of atomic orbitals on the Bloch functions was developed in [24].

In figure 1 the total and partial DOS for LaFeAsO obtained in the LMTO basis are shown. The crystal field splitting of the Fe-3d states in this material is rather weak ($\Delta_{cf} = 0.25$ eV) and all five d-orbitals of iron form a common band in the energy range $(-2, +2)$ eV relative to the Fermi level (see the gray region in the bottom panel of figure 1). There is a strong hybridization of the iron t_{2g} orbitals with the p-orbitals of arsenic, the effect of which becomes apparent in the energy interval $(-3, -2)$ eV (the white region in the bottom panel of figure 1) where the As-p band is situated. A weaker hybridization with the oxygen p states can be seen in the $(-5.5, -3)$ eV energy window (the black region in the bottom panel of figure 1).
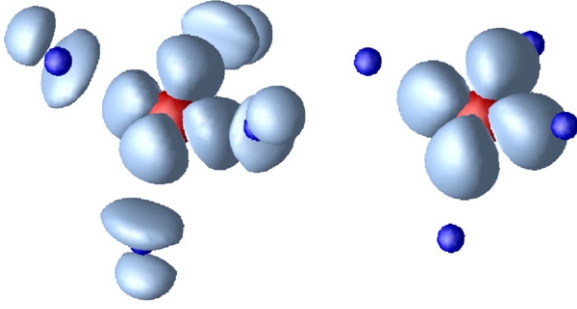
Figure 2. Modulus square of $d_{x^2-y^2}$-like Wannier function computed for Fe-3d bands only (left panel) and for a full set of O-2p, As-4p and Fe-3d bands (right panel). Big sphere in the center marks Fe ion position and four small spheres around it correspond to As neighbors.

We have calculated the average Coulomb interaction $\bar{U}$ and Hund's exchange J parameters in the WF basis using the constrained DFT procedure with fixed occupancies of WFs of d-symmetry. For this purpose we have used two computational schemes based on two different DFT methods. The first involves linearized muffin-tin orbitals produced by the TB-LMTO-ASA code [21]; the corresponding WF calculation procedure is described in detail in [25]. The second, based on the pseudopotential plane-wave method PWSCF, as implemented in the Quantum ESPRESSO package [22], is described in [26]. The difference between results obtained with the two schemes gives an estimate of the uncertainty of $\bar{U}$ and J determination.

The WFs are defined by the choice of Bloch functions' Hilbert space and by a set of trial localized orbitals that will be projected onto these Bloch functions [25]. We have performed calculations for two different choices of the Bloch functions and atomic orbitals. The first one includes only the bands of predominantly Fe-3d character in the energy window $(-2, +2)$ eV and an equal number of Fe-3d atomic orbitals to be projected on the Bloch functions for these bands. This choice corresponds to a model where only the five Fe-d orbitals are included but all the arsenic and oxygen p-orbitals are integrated out. The second choice includes all bands in the energy window $(-5.5, +2)$ eV that are formed by O-2p, As-4p and Fe-3d states and correspondingly a full set of O-2p, As-4p and Fe-3d atomic orbitals to be projected on the Bloch functions for these bands. This corresponds to an extended model where, in addition to the Fe-d orbitals, all the p-orbitals are included as well.

For both choices we have obtained Hamiltonians in the WF basis that reproduce exactly the Fe-3d bands in the energy window $(-2, +2)$ eV (figure 1), but in the second case bands formed by p-orbitals in the energy window $(-5.5, -2)$ eV will be reproduced too. However, WFs with Fe-d symmetry computed in the two cases have very different spatial distributions. In figure 2 the modulus square of a $d_{x^2-y^2}$-like WF is plotted. While in the second case in which the full set of bands and atomic orbitals was used (right panel) WF is nearly pure atomic d-orbital (iron states contribute 99%), the WF computed only using the Fe-3d bands is much more

Table 1. The constrained DFT calculated values of average Coulomb interaction $\bar{U}$ and Hund's exchange J (eV) parameters for d-symmetry Wannier functions computed with two different sets of bands and orbitals.

DFT method	Restricted to Fe-3d bands	Full bands set
TB-LMTO-ASA	$\bar{U} = 0.49, J = 0.51$	$\bar{U} = 3.10, J = 0.81$
PWSCF	$\bar{U} = 0.59, J = 0.53$	$\bar{U} = 4.00, J = 1.02$

extended (left panel). It has a significant weight on neighboring As ions with only a 67% contribution from the central iron atom. The origin of the difference is the p–d hybridization. In the case where the p bands are integrated out the p–d hybridization is reflected in the shape of the WF. The Fe-3d band in the energy window $(-2, +2)$ eV corresponds to an anti-bonding combination of Fe-3d and As-4p states which is clearly seen in the left panel of figure 2.

Different spatial distribution of the two WFs calculated with full and restricted bases can be expected to lead to different effective Coulomb interactions for electrons in these orbitals. The results of constrained DFT calculations of the average Coulomb interaction $\bar{U}$ and Hund's exchange J parameters for electrons in WFs computed with the two different sets of bands and orbitals (and using two different DFT methods: LMTO and pseudopotential) are presented in table 1. One can see that a very different Coulomb interaction is obtained for a separate Fe-3d band and the full bands. While the latter gives a value of 3–4 eV, close to that previously used [7, 11, 10], the Fe-3d band restricted calculation results in $\bar{U}$ of 0.5–0.6 eV, which is much smaller but agrees with spectroscopy estimates [13].

The main reason for such a drastic difference between the two results is a very different spatial extent of the WFs (see figure 2): nearly complete localization on the central iron atom for the 'full bands set' WF (99%) and only 67% for the 'Fe-3d band set' WF with 33% of WF on the neighboring As atoms. Another source of the strong reduction of the calculated $\bar{U}$ value when going from the 'full bands set' to the 'Fe-3d band set' WF is an additional screening due to p–d hybridization with the As-4p band, which is situated just below the Fe-3d band (see figure 1). A similar substantial decrease of the effective $\bar{U}$ value when going from the full orbital model to a restricted basis was found previously for high-T_c cuprates ($U = 8$–10 eV for full p–d-orbitals basis [15] and 2.5–3.6 eV for the one-band model [17]).

In the constrained DFT calculations an average Coulomb interaction $\bar{U}$ is obtained which can be approximated [4] as $\bar{U} = F^0 - J/2$, where F^0 is the zeroth Slater integral. Hence F^0 can be calculated as $F^0 = \bar{U} + J/2$. For the 'Fe-3d band set' WF that gives $F^0 = 0.8$ eV and $J = 0.5$ eV. The Coulomb parameters for the 'full basis' calculated in the same way using the data from the first row of table 1 give $F^0 = 3.5$ eV and $J = 0.81$ eV. With this set of parameters the Coulomb interaction matrix $U_{mm'}$ was calculated and used in LDA + DMFT [27] calculations (for a detailed description of the present computation scheme see [25]). The DFT band structure was calculated within the TB-LMTO-ASA method [21]. Crystal structure parameters of [1] were used.
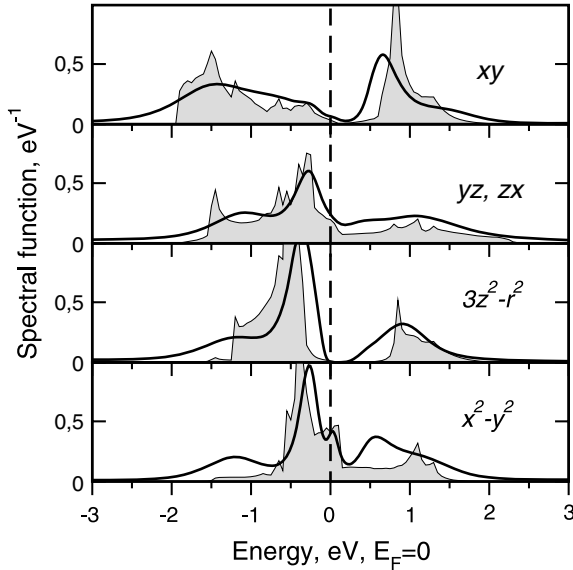
Figure 3. Partial densities of states for Fe-3d orbitals obtained within the DFT (filled areas) and LDA + DMFT orbitally resolved spectral functions for 'restricted basis' and $F^0 = 0.8$ eV, $J = 0.5$ eV (bold lines).

The LDA + DMFT calculations were performed for both models: the restricted basis and the full basis, including also the As-p and O-p states. For the latter case a double-counting term $\bar{U}(n_{\mathrm{DMFT}} - \frac{1}{2})$ was used to obtain the noninteracting Hamiltonian [26]. Here n_{DMFT} is the total number of d electrons obtained self-consistently within the LDA + DMFT scheme. The effective impurity model within the DMFT was solved by the Hirsch–Fye QMC method [28]. In the present implementation of the QMC impurity solver the Coulomb interaction between different orbitals on the same atom is limited to density–density terms, i.e. the form $\sum_{m\sigma,m'\sigma'} U_{mm'}^{\sigma\sigma'}(F^0, J)\hat{n}_{m\sigma}\hat{n}_{m'\sigma'}$. In particular, this means that the coupling between the local spins is of Ising and not Heisenberg type. Since this is a significant approximation a few comments are in order, especially concerning the question whether this approximation underestimates or overestimates the many-body renormalization of quasiparticle bands. We argue quite generally that introducing the spin–flip exchange (and other interaction terms beyond density–density) allows electrons to avoid each other more efficiently and thus the electron propagation through the crystal is inhibited less than with Ising exchange. As an example one can imagine two electrons with opposite spin in different orbitals. Allowing the spin–flip exchange the Ising-only interaction energy U' can be reduced to $U' - J$ by forming the triplet state with $S_z = 0$. This argument is also supported by recent numerical studies of two bands comparing full Coulomb and Ising-only interaction terms [29]. Therefore we expect our results rather to overestimate than underestimate the quasiparticle renormalization. Calculations for both models were performed at the inverse temperature $\beta = 10$ eV^{-1}. The interval $0 < \tau < \beta$ was divided into 100 slices. 6×10^6 QMC sweeps were used in a self-consistency loop within the LDA + DMFT scheme and 12×10^6 of QMC sweeps were used to calculate the spectral functions.
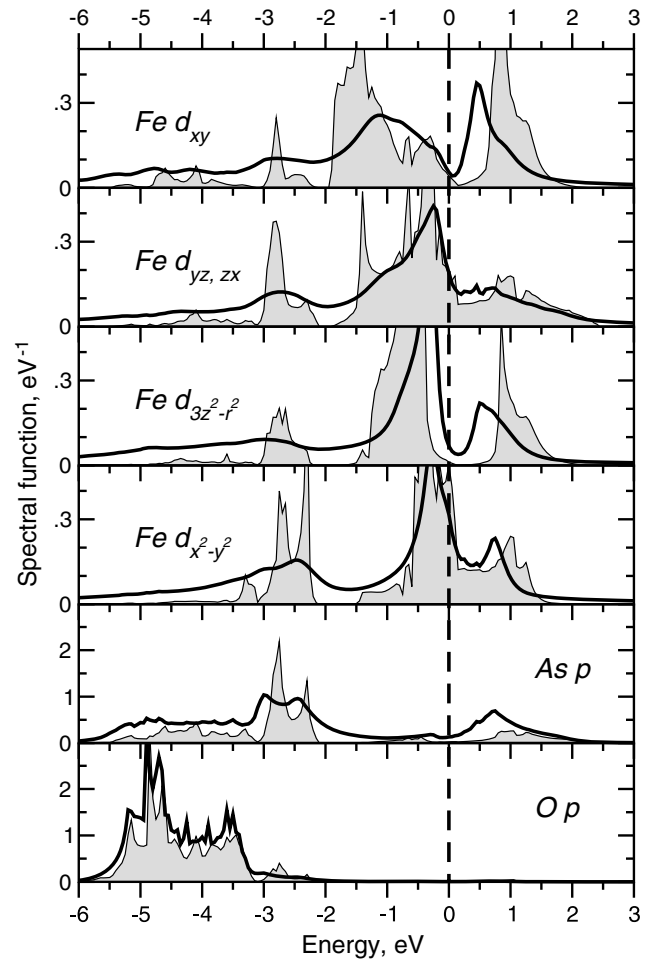

Figure 4. Partial densities of states for Fe-3d, As-4p and O-2p states obtained within the DFT (filled areas) and LDA + DMFT orbitally resolved spectral functions for 'full basis' calculations with $F^0 = 3.5$ eV and $J = 0.81$ eV (bold lines).

The iron 3d orbitally resolved spectral functions obtained within DFT and LDA + DMFT for the 'restricted basis' with $F^0 = 0.8$ eV and $J = 0.5$ eV are presented in figure 3. The effect of correlations on the electronic structure of LaFeAsO is minimal: there are relatively small changes of peak positions for $3z^2 - r^2$, xy and $x^2 - y^2$ orbitals (a shift toward the Fermi energy) and practically unchanged spectral functions for the yz, zx bands. There is no appearance of either a Kondo resonance peak on the Fermi level or Hubbard bands in the spectrum.

The results of the 'full basis' LDA + DMFT calculations are presented in figure 4. Note that, though much larger Coulomb U and J parameters ($F^0 = 3.5$ eV, $J = 0.81$ eV) were used in this calculation, the spectra around the Fermi energy are very similar to those obtained in the 'restricted basis' calculations (figure 3). The general shape of the spectra does not show either Kondo resonance at the Fermi level or Hubbard bands; the features in Fe-d spectral functions below -2 eV correspond to hybridization with As-p and O-p bands. The reason for such weak correlation effects in spite of the relatively strong Coulomb interaction is a very strong hybridization of the Fe-d orbitals with As-p states (see the
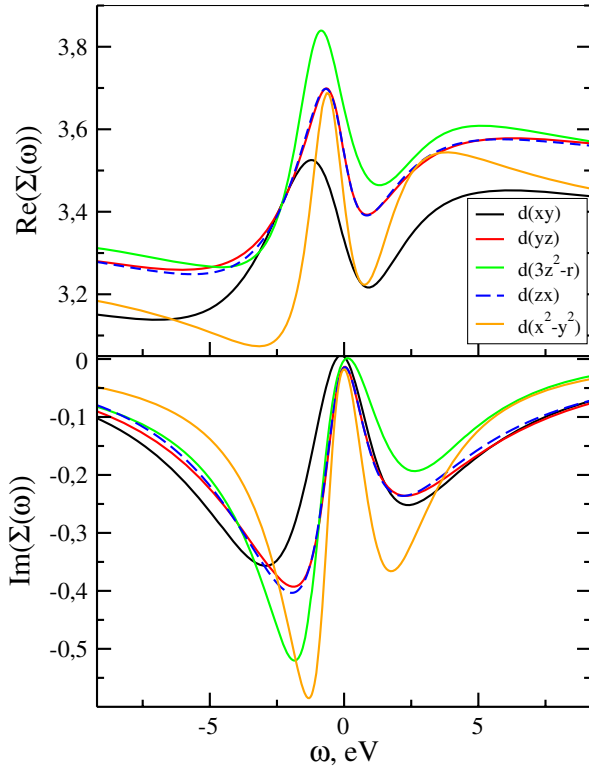
Figure 5. Real (upper panel) and imaginary (lower panel) parts of LDA + DMFT self-energy interpolated on the real axis with the use of the Padé approximant for 'restricted basis' and $F^0 = 0.8$ eV, $J = 0.5$ eV.
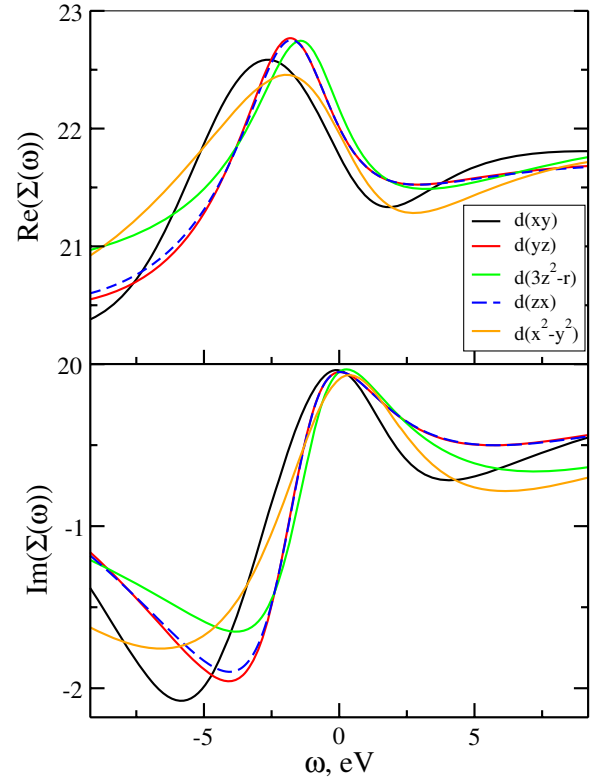
Figure 6. Real (upper panel) and imaginary (lower panel) parts of LDA + DMFT self-energy interpolated on the real axis with the use of the Padé approximant for 'full basis' and $F^0 = 3.5$ eV, $J = 0.81$ eV.

peaks in the Fe-d spectral function in the −2 to −3 eV range corresponding to mixing with As-p bands). The hybridization provides an additional very efficient channel for screening of the Coulomb interaction between Fe-d electrons.

These observations agree with the results of the soft x-ray absorption and emission spectroscopy study [12]. It was concluded there that LaFeAsO does not represent a strongly correlated system since the Fe L_3 x-ray emission spectra do not show any features that would indicate the presence of the lower Hubbard band or a quasiparticle peak that were predicted by the LDA + DMFT analysis [7, 11, 10] with the large $U = 4$ eV. The comparison of the x-ray absorption spectra (O K-edge) with the LDA calculations gave [13] an upper limit of the on-site Hubbard $U \approx 1$ eV. The photoemission study of LaFeAsO suggests [14] that the lineshapes of Fe 2p core-level spectra correspond to an itinerant character of Fe-3d electrons. It was demonstrated there that the valence-band spectra are generally consistent with the band-structure calculations except for shifts of the Fe 3d-derived peaks towards the Fermi level. Such a shift is indeed observed in our LDA + DMFT spectra (figure 3).

The behavior of the real part of self-energy near zero frequency $\Sigma(\omega)|_{\omega \to 0}$ provides important information about band narrowing and renormalization of the electron mass. The Padé approximant [30] was used to obtain the self-energy on the real frequency axis. The results for both basis sets are presented in figures 5 and 6. The calculated values of the quasiparticle renormalization factor $Z = (1 - \frac{\partial \Sigma(\omega)}{\partial \omega}|_{\omega=0})^{-1}$

are found to be 0.77, 0.63, 0.71 and 0.46 in the 'restricted basis' and 0.56, 0.54, 0.45 and 0.56 in the 'full basis' for d_{xy}, d_{yz} (or d_{zx}), $d_{3z^2-r^2}$ and $d_{x^2-y^2}$ orbitals, respectively. The values for the 'restricted basis' agree well with the effective narrowing of the LDA + DMFT spectral functions relative to LDA DOS (figure 3). Note that the quasiparticle renormalization factor $Z = (1 - \frac{\partial \Sigma(\omega)}{\partial \omega}|_{\omega=0})^{-1}$ from the 'full basis' calculations cannot be directly used to estimate the narrowing of the bands. Due to the hybridization with As-p and O-p states the actual narrowing is smaller than suggested by Z. With this, we can conclude that both models agree rather well with each other. The effective mass enhancement $m^* = Z^{-1}$ of 1.3, 1.59, 1.41 and 2.17 ('restricted basis') for d_{xy}, d_{yz} (or d_{zx}), $d_{3z^2-r^2}$ and $d_{x^2-y^2}$ orbitals, respectively, agrees well with the mass enhancement factor between 1.7 and 2.1 reported in the dHvA study [31]. The $d_{x^2-y^2}$ orbital has the largest effective mass and exhibits the most evident narrowing of the LDA spectrum (see figure 3). This orbital has its lobes directed into the empty space between nearest iron neighbors in the Fe plane. Hence it has the weakest overlap, the smallest bandwidth and the largest U/W ratio.

The small effective mass enhancement shows that LaFeAsO is a weakly correlated system, in contrast to the results of the LDA + DMFT calculation [7] by Haule *et al* where a strongly renormalized low energy band with a fraction of the original width ($Z \approx 0.2$–0.3) was found while most of the spectral weight was transferred into a broad Hubbard band
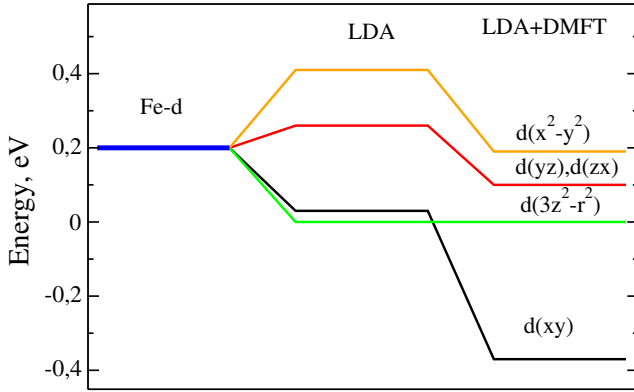
Figure 7. Splitting of Fe-d orbitals obtained in LDA and LDA + DMFT for 'full basis' and $F^0 = 3.5$ eV, $J = 0.81$ eV.

Figure 8. Calculated Fe-d LDA + DMFT ('full basis' and $F^0 = 3.5$ eV, $J = 0.81$ eV) spectral function (green solid line) and experimental Fe L_3 XES spectrum (black circles) from [12].

at the binding energy ≈ 4 eV. The authors of [7] report that 'slightly enhanced Coulomb repulsion ($U = 4.5$ eV) opens the gap' so that the system is in a strongly correlated regime on the edge of a metal–insulator transition.

In LaFeAsO the iron ion is tetrahedrally coordinated with four As ions exhibiting a slight tetragonal distortion. In the tetrahedral symmetry group T_d the five d orbitals should be split by the crystal field [5] into a low energy doublet of $3z^2 - r^2$, xy corresponding to the e_g irreducible representation and a high energy triplet of $x^2 - y^2$, xz, yz belonging to the t_{2g} representation. We have calculated the WF orbital energies and have found that the t_{2g}–e_g crystal field splitting is very small $\Delta_{cf} \approx 0.25$ eV. The slight tetragonal distortion of the tetrahedron leads to an additional splitting of the t_{2g} and e_g levels with the following orbital energies (the energy of the lowest $3z^2 - r^2$ orbital is set to zero): $\varepsilon_{3z^2-r^2} = 0.00$ eV, $\varepsilon_{xy} = 0.03$ eV, $\varepsilon_{xz,yz} = 0.26$ eV, $\varepsilon_{x^2-y^2} = 0.41$ eV. The correlation leads not only to narrowing of the bands but also to substantial shifts of the Fe-d orbitals energies. For the 'full basis' calculation, adding the $\mathrm{Re}(\Sigma(0))$ to the LDA orbital energies results in $\varepsilon_{3z^2-r^2} = 0.00$ eV, $\varepsilon_{xy} = -0.37$ eV, $\varepsilon_{xz,yz} = 0.10$ eV and $\varepsilon_{x^2-y^2} = 0.20$ eV (see figure 7). Note that the actual band shifts are smaller due to the p–d hybridization.

Comparison of the LDA + DMFT single-particle spectral functions obtained with the full basis set to various experimental spectra is presented in figures 8 and 9. Taking into account the selection rules for XES (x-ray emission spectroscopy) (neglecting the energy dependence of matrix elements) we compare the Fe L_3 XES spectrum of [12], which corresponds to $2p \rightarrow 3d$ transitions, with the calculated LDA + DMFT Fe-3d spectral function (see figure 8) to find a good agreement between the two. The shoulder in the experimental curve near -2.5 eV corresponds to the low energy peak in the calculated spectrum originating from strong hybridization between the Fe-d and As-p states (see also figure 1). Note that these features are missing in the calculations with the restricted basis (see the orbital resolved spectra in figure 3). In figure 9 we present

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[5] The coordinate axes x, y in the LaFeAsO crystal structure are rotated by 45° from the standard tetrahedral notation and so xy and $x^2 - y^2$ orbitals are interchanged.
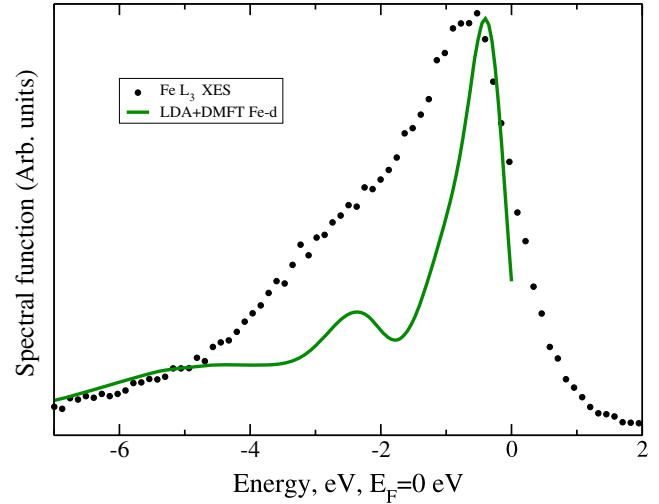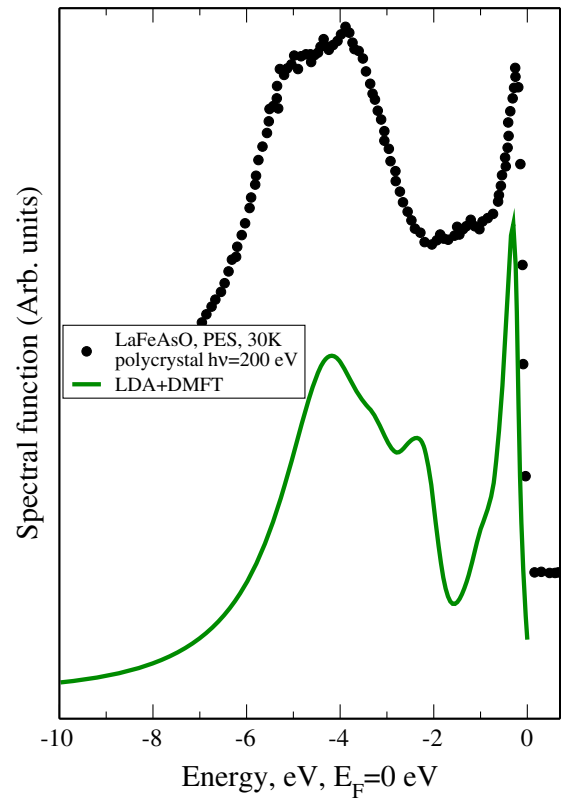
Figure 9. Calculated total LDA + DMFT ('full basis' and $F^0 = 3.5$ eV, $J = 0.81$ eV) spectral function (green solid line) and experimental LaFeAsO PES spectrum (black circles) from [32].

the total LDA + DMFT spectral function together with the experimental photoemission data of [32]. Again we find there is very good agreement between the theory and experiment. The sharp peak at the Fermi energy corresponds to a partially filled Fe-d band while the broad feature between -2 and 6 eV corresponds to the oxygen and arsenic p bands.

In conclusion, we have calculated the average Coulomb interaction U and J within the Fe d-shell in LaFeAsO using the

constrained DFT procedure in the basis of Wannier functions. For the 'restricted basis' including only the Fe-3d orbitals and bands we have obtained the Coulomb parameters $F^0 = 0.8$ eV and $J = 0.5$ eV. For the 'full basis' Coulomb parameters $F^0 = 3.5$ eV and $J = 0.8$ eV have been calculated. The LDA + DMFT calculations for both models yield weakly correlated iron d bands in this compound. This conclusion is supported by earlier spectroscopic studies of this material. As the choice of orbitals to construct an effective Hubbard model from LDA bands is, to some extent, arbitrary, demonstrating that different choices of the model leading to largely different interaction parameters yield similar physical observables provides an important consistency test of the whole procedure.

Acknowledgments

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