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# Effect of Correlations and Doping on the Spin Susceptibility of Iron Pnictides: the Case of $\text{KFe}_2\text{As}_2$ <sup>†</sup>

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The temperature dependence of the paramagnetic susceptibility of the iron pnictide superconductor  $\text{KFe}_2\text{As}_2$  and its connection with the spectral properties of that material is investigated by a combination of density functional theory (DFT) in the local density approximation and dynamical mean-field theory (DMFT). Unlike other iron pnictide parent compounds where the typical oxidation state of iron is 2, the formal valence of Fe in  $\text{KFe}_2\text{As}_2$  is 2.5, corresponding to an effective doping with 0.5 hole per iron atom compared to, for example,  $\text{BaFe}_2\text{As}_2$ . This shifts the chemical potential and thereby reduces the distance between the peaks in the spectral functions of  $\text{KFe}_2\text{As}_2$  and the Fermi energy as compared to  $\text{BaFe}_2\text{As}_2$ . The shift, which is clearly seen on the level of DFT as well as in DMFT, is further enhanced by the strong electronic correlations in  $\text{KFe}_2\text{As}_2$ . In  $\text{BaFe}_2\text{As}_2$  the presence of these peaks results (Phys. Rev. B **86**, 125124 (2012)) in a temperature increase in the susceptibility up to a maximum at  $\sim 1000$  K. While the temperature increase was observed experimentally the decrease at even higher temperatures is outside the range of experimental observability. We show that in  $\text{KFe}_2\text{As}_2$  the situation is different. Namely, the reduction of the distance between the peaks and the Fermi level due to doping shifts the maximum in the susceptibility to much lower temperatures, such that the decrease in the susceptibility becomes visible in experiment.

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## INTRODUCTION

The discovery of high-temperature superconductivity in fluorine-doped  $\text{LaFeAsO}$  in 2008 by Kamihara et al. [1] has placed the iron-arsenic systems into the center of activity of solid state physics. To date a variety of Fe-based superconductors have been found. The so-called “122” family (compounds with the common formula  $AE\text{Fe}_2\text{As}_2$ , where  $AE$ —alkaline earth element) is the most studied one. Unlike other iron-arsenic systems, undoped compounds of the “122” family superconduct under pressure, with  $T_c$  up to 29 K [2, 3]. The highest critical temperature,  $T_c = 38$  K, in this family is detected in the potassium doped compound  $\text{Ba}_{1-x}\text{Fe}_2\text{As}_2$  with  $x = 0.4$  [4–6]. Therefore  $\text{KFe}_2\text{As}_2$  is the end member of the family and can be considered a parent compound in which superconductivity emerges under chemical doping. Although the critical temperature is rather low in  $\text{KFe}_2\text{As}_2$  ( $T_c = 3.8$  K [7]) this material is a rare example of a stoichiometric pnictide superconductor.

It is widely accepted that Coulomb correlations are crucial for the understanding of many aspects of the

physics of pnictides [8–11]. Correlation effects in  $\text{KFe}_2\text{As}_2$  were intensively studied: Terashima et al. [12] performed de Haas–van Alphen measurements of the Fermi surface in  $\text{KFe}_2\text{As}_2$ . They detected unusually large effective mass renormalizations and big differences in the masses of different bands, which is not found in other pnictides. The enhancement of the band mass was also measured by Yoshida et al. [13] in angular-resolved photoemission spectroscopy (ARPES) experiments. Hardy et al. [14] employed the Gutzwiller slave-boson mean-field method to study the strength of Coulomb correlations in  $\text{KFe}_2\text{As}_2$ . They confirmed the experimental conclusions of Terashima et al. [12] and Yoshida et al. [13], and proposed an orbital-selective scenario for its spectral properties.

A characteristic feature of the magnetic properties observed in the “1111” (compounds like  $\text{LaFeAsO}$ ) and “122” pnictide classes is the unusual linear-temperature increase in the paramagnetic susceptibility [15, 16]. There are two explanations of this phenomenon based either on the assumption of strong antiferromagnetic fluctuations in a two-dimensional Fermi liquid [17], or of peculiarities of the single-particle spectra [10, 11]. The temperature increase in the sus-

<sup>†</sup>The article is published in the original.

ceptibility was considered a universal property [18] of the pnictide superconductors and parent systems. By contrast, Cheng et al. [19] reported that in  $\text{KFe}_2\text{As}_2$  the magnetic susceptibility increases only at quite low temperatures, i.e., below 100 K, and then decreases slowly at least up to 300 K. The origin of that temperature dependence of the magnetic susceptibility of  $\text{KFe}_2\text{As}_2$  and its connection with the magnetic properties of the other end member of the “122” family,  $\text{BaFe}_2\text{As}_2$ , had not been explained yet. In particular, it was not studied by first-principle methods.

Today the most powerful technique that can account for correlation effects in real compounds and can describe the physics of the correlated paramagnetic phase, is the LDA+DMFT approach [20]. This method combines the advantage of density-functional theory (typically in the local density approximation, LDA) to describe the material-specific electronic structure of a weakly correlated system, with the ability of the dynamical mean-field theory [21] to treat the complete range of Coulomb correlations between the electrons in partially filled shells.

In this work, we investigate the temperature evolution of the paramagnetic susceptibility in  $\text{KFe}_2\text{As}_2$  in the framework of LDA+DMFT. We compare our results with experiments and our previously published LDA+DMFT data [11] obtained for the isostructural compound  $\text{BaFe}_2\text{As}_2$ . Thereby we demonstrate that the mechanism explaining the anomalous temperature behavior of the magnetic susceptibility in iron pnictides proposed in our previous investigations [10, 11] also allows one to understand the difference between the magnetic properties of these compounds and those of  $\text{KFe}_2\text{As}_2$ .

## TECHNICAL DETAILS

In the LDA+DMFT formalism employed here the material-specific band dispersion obtained within LDA is used as a starting point. Then matrix elements of the effective Hamiltonian  $H^{\text{LDA}}(\mathbf{k})$  are computed in the subspace of Wannier functions with the symmetry of  $p$  and  $d$  states using the projection procedure [22]. In the second step, the Coulomb interaction matrix  $U_{mm'}^{\sigma\sigma'}$ , parameterized by Slater integrals  $F_0$ ,  $F_2$ , and  $F_4$ , is calculated for each atom with partially filled shells. The values of  $F_0$ ,  $F_2$ ,  $F_4$  are computed using the on-site effective Coulomb parameter  $U$  and intra-atomic exchange parameter  $J$ . Finally, the following many-

electron Hamiltonian is iteratively solved by DMFT on the Matsubara contour:

$$\begin{aligned} & \hat{H}(\mathbf{k}) \\ &= \sum_{\mathbf{k}, im, jm', \sigma} [H_{im, jm'}^{\text{LDA}}(\mathbf{k}) - H_{im, jm'}^{\text{DC}}] \hat{a}_{\mathbf{k}, im\sigma}^\dagger \hat{a}_{\mathbf{k}, jm'\sigma} \\ & \quad + \frac{1}{2} \sum_{i, (m\sigma) \neq (m'\sigma')} U_{mm'}^{\sigma\sigma'} \hat{n}_{im\sigma}^d \hat{n}_{im'\sigma'}^d. \end{aligned} \quad (1)$$

Here,  $\hat{a}_{\mathbf{k}, im\sigma}^\dagger$  is the Fourier transform of  $\hat{a}_{im\sigma}^\dagger$  which creates an electron on the atom  $i$  in the state  $|m\sigma\rangle$ , where  $m$  labels the orbitals and  $\sigma = \uparrow, \downarrow$  corresponds to the spin projection. The particle number operator  $\hat{n}_{im\sigma}^d$  acts on the states localized at the atoms with partially filled shells (Fe- $d$  states in the present study). The term  $H^{\text{DC}}$  stands for a double-counting correction which corresponds to the Coulomb interaction energy already accounted for by LDA (see below).

In the present work the LDA band structure is calculated with the ELK full-potential code [23] with default parameters of the LAPW basis. By employing the constrained LDA method [24] we obtained the interaction parameters  $U = 3.5$  eV and  $J = 0.85$  eV. These values are typical for the pnictides and are in good agreement with previous estimations [9, 25]. The DMFT auxiliary impurity problem was solved by the hybridization function expansion quantum Monte-Carlo method [26]. The double-counting term is a diagonal matrix with only nonzero elements in the  $d$ - $d$  block expressed in the form  $E^{\text{DC}} = \bar{U}(n_d - 0.5)$ , where  $n_d$  is the number of Fe- $d$  electrons calculated within LDA+DMFT and  $\bar{U}$  is the average Coulomb parameter for the  $d$  states. This form of  $H^{\text{DC}}$  yields reliable results for magnetic and spectral properties of iron pnictides [8–11].

The orbitally-resolved spectral functions  $A_i(\omega)$  were computed as the diagonal elements of the real-energy Green function

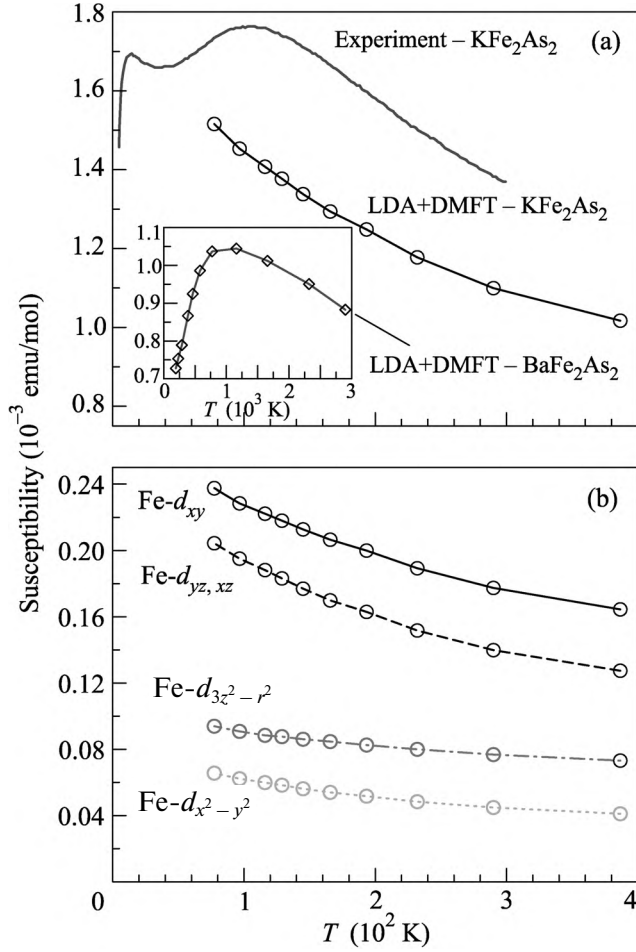
$$A_i(\omega) = \sum_{\mathbf{k}} \{ I(\omega + \mu) - [H^{\text{LDA}}(\mathbf{k}) - H^{\text{DC}}] - \Sigma(\omega) \}^{-1}_{ii}, \quad (2)$$

where  $\mu$  is the chemical potential calculated within DMFT,  $\Sigma(\omega)$  is the self-energy obtained with the use of Padé approximants [27], and  $I$  is the identity matrix.

The uniform magnetic susceptibility  $\chi(T)$  was calculated as the response to a small external magnetic field,

$$\chi(T) = \frac{\Delta M(T)}{\Delta E}, \quad (3)$$

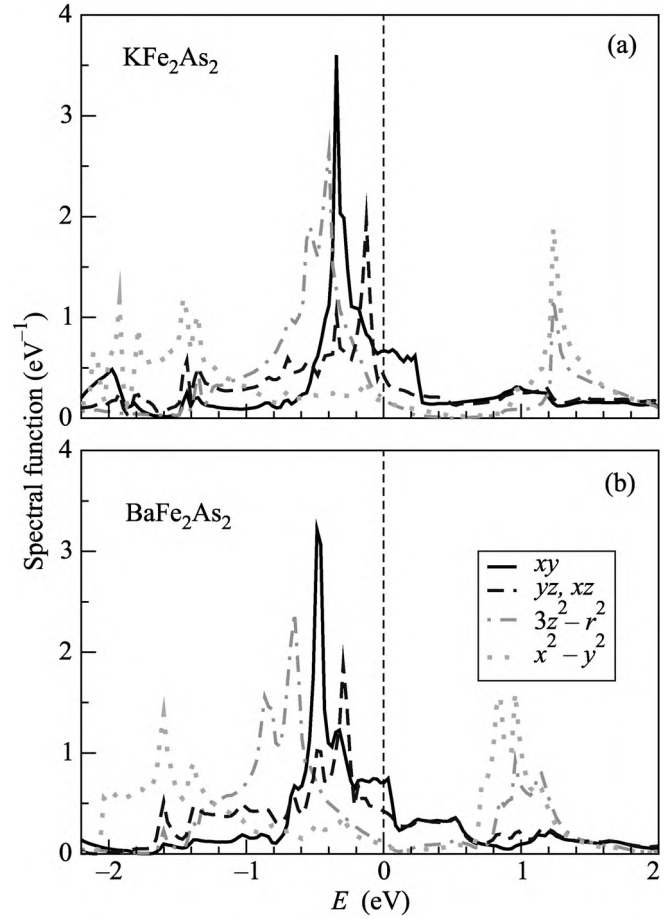
where  $\Delta E$  is the energy correction corresponding to the field and  $\Delta M = |N_\uparrow(T) - N_\downarrow(T)|$  is the occupation difference between the spin projections.



**Fig. 1.** Temperature dependence of the uniform susceptibility of  $\text{KFe}_2\text{As}_2$ . (a) Static susceptibility computed within LDA+DMFT (circles) is shown in comparison with experimental data [19] (solid curve). The inset shows the LDA+DMFT result for the susceptibility of  $\text{BaFe}_2\text{As}_2$  from [11]. (b) Temperature behavior of the orbitally-resolved contributions to the total susceptibility calculated by LDA+DMFT.

### TEMPERATURE DEPENDENCE OF THE UNIFORM MAGNETIC SUSCEPTIBILITY

In the upper panel of Fig. 1 the temperature behavior of the static magnetic susceptibility of  $\text{KFe}_2\text{As}_2$  as computed within LDA+DMFT is shown in comparison with the experimental result of Cheng et al. [19]. Both experimental and theoretical curves show a monotonic decrease in the temperature interval from 125 to 300 K. The slope of the calculated curve is in good agreement with experiment, while its absolute value is by about 20% smaller. The maximum in the experimental susceptibility observed at 100 K is not reproduced in the calculation. Temperatures lower than 77 K are not accessible in the present study. The temperature dependence of the LDA+DMFT calculated paramagnetic susceptibility in the other end



**Fig. 2.** Fe- $d$  orbitally-resolved densities of states of (a)  $\text{KFe}_2\text{As}_2$  and (b)  $\text{BaFe}_2\text{As}_2$  obtained within LDA (0 eV corresponds to the Fermi energy).

member of the “122” family is shown in the inset of Fig. 1. The similarities and differences of the curves are discussed in the Discussion section. The orbitally resolved Fe- $d$  contributions to the total susceptibility are presented in the lower panel of Fig. 1. The susceptibilities corresponding to the Fe- $d$  orbitals all show a decreasing behavior with temperature. The largest contributions come from the  $xy$  and  $yz(xz)$  orbitals.

### SPECTRAL PROPERTIES

The orbitally resolved densities of states of  $\text{KFe}_2\text{As}_2$  obtained within LDA are shown in the upper panel of Fig. 2 in comparison with the result obtained for  $\text{BaFe}_2\text{As}_2$ . In each case the Fe- $d$  states form a band with total width of  $W \approx 4$  eV located in the approximate interval  $(-2, +2)$  eV. Therefore the on-site Coulomb parameter  $U$  is comparable with the band width ( $W/U \sim 1$ ), implying that correlation effects are important. Both compounds have similar shape and relative positions of the spectral functions on the energy axis. However, in the case of  $\text{KFe}_2\text{As}_2$  the Fermi

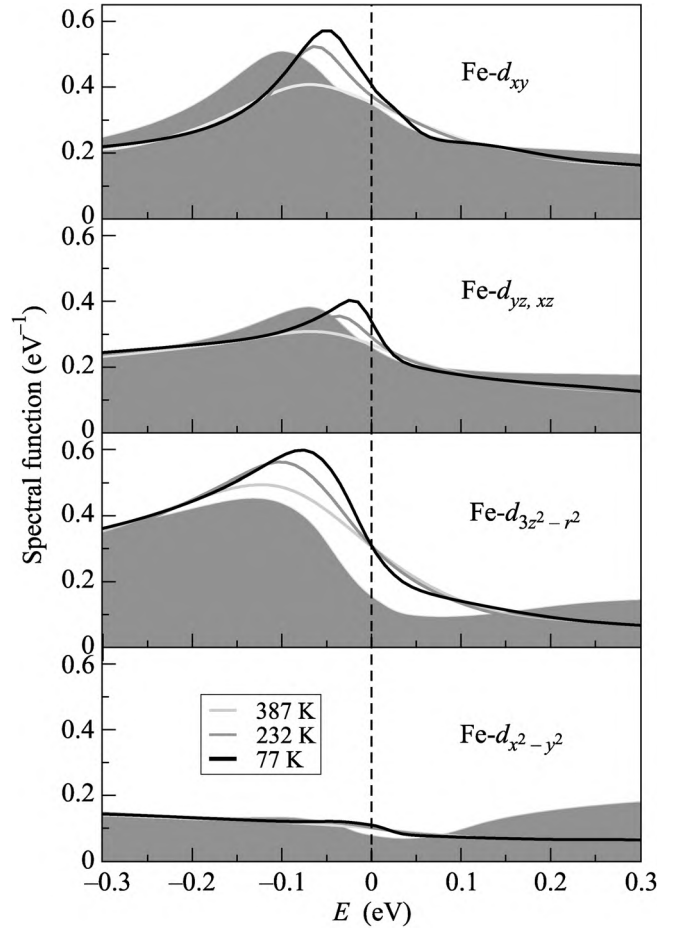
level is located approximately 150 meV lower than in  $\text{BaFe}_2\text{As}_2$  due to hole doping.

The Fe- $d$  spectral functions of  $\text{KFe}_2\text{As}_2$  computed within LDA+DMFT for the temperature window from 77 to 580 K are presented in Fig. 3 along with the result for  $\text{BaFe}_2\text{As}_2$  [11]. As in other pnictide superconductors the dynamical Coulomb correlations renormalize the spectrum in the vicinity of the Fermi energy and smear some fine details observed within the LDA, but the overall shape of the curves remains unchanged. This renormalization reduces the distance between the peaks in the Fe- $d$  spectral functions and the Fermi energy. In particular, the peak in the  $yz(xz)$  spectral function is now significantly closer to the Fermi level compared to that in  $\text{BaFe}_2\text{As}_2$ .

Quantitatively, the strength of the electronic correlations can be estimated by the increase in the effective masses in comparison with the LDA results. In the case of a single orbital the mass renormalization is expressed by the derivative of the self-energy  $\Sigma(\omega)$  as  $m^*/m_b = [1 - \partial \text{Re}\Sigma(\omega)/\partial \omega]$ , where  $m^*$  denotes the effective mass in LDA+DMFT and  $m_b$  is the band mass obtained in LDA. In our calculation the self-energy is a diagonal matrix which leads to an orbital dependence of the masses. The calculated values of  $m^*/m_b$  for every Fe- $d$  orbital are shown in table. The largest mass renormalization, 4.47, corresponds to the  $xy$  orbital. Electronic correlations in the other  $d$ -orbitals are weaker with  $m^*/m_b$  ranging from 2.22 to 4.02. The computed values of  $m^*/m_b$  are in good agreement with previous theoretical estimations [14] as well as with the ARPES data of Yoshida et al. [13]. The result that the electrons in the  $|xy\rangle$ -derived bands are the most correlated ones followed by the  $|yz\rangle$ ,  $|3z^2 - r^2\rangle$ , and  $|x^2 - y^2\rangle$  states, is in qualitative agreement with the conclusion on the proximity of  $\text{KFe}_2\text{As}_2$  to an orbital-selective Mott transition reported by Hardy et al. [14]. It should also be noted that the response of the electrons occupying states with larger  $m^*/m_b$  is more Curie–Weiss-like, while the temperature dependence of the susceptibilities corresponding to the other orbitals is less pronounced. A similar result was obtained in [28] for the local susceptibility of  $\text{LaFeAsO}$ .

## DISCUSSION

To explain why the magnetic susceptibility of  $\text{KFe}_2\text{As}_2$  behaves qualitatively different from that of the other iron pnictides it is instructive to compare the spectral properties of  $\text{KFe}_2\text{As}_2$  and the other end member of the “122” family,  $\text{BaFe}_2\text{As}_2$ . As was noted above, in  $\text{KFe}_2\text{As}_2$  the Fermi energy is lower than in  $\text{BaFe}_2\text{As}_2$  due to hole doping. Already on the level of LDA this results in a smaller distance between the peaks of the Fe- $d$  spectral functions and the Fermi energy. Since correlation effects in  $\text{KFe}_2\text{As}_2$  are stronger than in  $\text{BaFe}_2\text{As}_2$  the peaks obtained within



**Fig. 3.** Temperature evolution of Fe- $d$  spectral functions of  $\text{KFe}_2\text{As}_2$  computed by LDA+DMFT. The spectral functions of  $\text{BaFe}_2\text{As}_2$  corresponding to the temperature  $T = 232$  K taken from [11] are shown for comparison as shaded areas. The Fermi energy is set to 0 eV.

LDA+DMFT come to lie even closer to the Fermi energy. This is clearly seen in Fig. 3 where the orbitally resolved Fe- $d$  spectral functions of  $\text{BaFe}_2\text{As}_2$  are shown for comparison.

In our previous study [11] we investigated the temperature behavior of the magnetic susceptibility in a model where the spectral function has a sharp peak below the Fermi energy. It was shown that the behavior of the magnetic susceptibility is determined by the thermal excitations corresponding to the states forming the peak, and that the distance between the peak and the Fermi energy can be regarded as a parameter controlling the magnetic response of the system.

Effective mass enhancement  $m^*/m_b$  for different orbitals of the  $d$  shell

	$d_{xy}$	$d_{yz}$	$d_{3z^2 - r^2}$	$d_{x^2 - y^2}$
$m^*/m$	4.74	4.02	2.96	2.22

According to the present LDA+DMFT study, in  $\text{KFe}_2\text{As}_2$  the peaks of the Fe- $d$  spectral functions are significantly closer to the Fermi energy than in  $\text{BaFe}_2\text{As}_2$ . Physically this means that the excitation of the states forming the peaks in  $\text{KFe}_2\text{As}_2$  requires less energy than in  $\text{BaFe}_2\text{As}_2$ . An analysis of the model shows that the doping of 0.5 holes per iron atom is not sufficient to switch the system to the regime where the linear in  $T$  behavior of the susceptibility no longer exists. Therefore we expect the linear increase in  $\chi(T)$  of  $\text{KFe}_2\text{As}_2$  to start at a lower temperature than in  $\text{BaFe}_2\text{As}_2$ , while the overall shape of the susceptibility curves is similar. Indeed, the decreasing part of the experimentally measured susceptibility of  $\text{KFe}_2\text{As}_2$  is well described by our result.

We were not able to perform the susceptibility calculations for temperatures lower than 77 K because Monte-Carlo simulations become extremely time consuming. As a consequence the maximum of the susceptibility in  $\text{KFe}_2\text{As}_2$  is not captured by our calculations. In our previous investigation we showed that the increasing part of the curve below that maximum can be interpreted as a quasilinear region in the vicinity of a turning point. In  $\text{KFe}_2\text{As}_2$  a similar region is experimentally observed in the temperature window from 30 to 80 K. It remains to be seen whether this low-temperature behavior can be explicitly reproduced in future LDA+DMFT studies.

In conclusion, the temperature dependence of the uniform magnetic susceptibility of  $\text{KFe}_2\text{As}_2$  was investigated within the LDA+DMFT method. The temperature decrease in the computed susceptibility between 125 to 300 K agrees well with experiment. We found that, similar to other pnictides including the isostructural parent compound  $\text{BaFe}_2\text{As}_2$ , the Fe- $d$  spectral functions of  $\text{KFe}_2\text{As}_2$  show sharp peaks below the Fermi energy. However, these peaks lie significantly closer to the Fermi level than in  $\text{BaFe}_2\text{As}_2$ . Making use of the scenario developed in our previous study of the magnetic properties of iron pnictides, we conclude that the qualitative difference between the magnetic susceptibilities of the two isostructural end members of the “122” family is due to the smaller separation between the Fe- $d$  spectral functions and the Fermi energy in  $\text{KFe}_2\text{As}_2$ , which itself is a consequence of the effective hole doping and the stronger correlations in that compound.

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reported here were obtained using the “Uran” supercomputer, Institute of Metal Physics, Ural Branch, Russian Academy of Sciences.

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