


## Novel Fe-Based Superconductor $\text{LaFe}_2\text{As}_2$ in Comparison with Traditional Pnictides

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The recently discovered Fe-based superconductor (FeBS)  $\text{LaFe}_2\text{As}_2$  seems to break away from an established pattern that doping an FeBS beyond  $0.2e/\text{Fe}$  destroys superconductivity.  $\text{LaFe}_2\text{As}_2$  has an apparent doping of  $0.5e$ , yet superconducts at 12.1 K. Its Fermi surface bears no visual resemblance with the canonical FeBS fermiology. It also exhibits two phases, none magnetic and only one superconducting. We show that the difference between them nonetheless has a magnetic origin, the one featuring disordered moments, and the other locally nonmagnetic. We find that La there assumes an unusual valence of  $+2.6$  to  $+2.7$ , so that the effective doping is reduced to  $0.30 - 0.35e$ . A closer look reveals the same key elements: hole Fermi surfaces near  $\Gamma - Z$  and electron ones near the  $X - P$  lines, with the corresponding peak in susceptibility, and a strong tendency to stripe magnetism. The physics of  $\text{LaFe}_2\text{As}_2$  is thus more similar to the FeBS paradigm than hitherto appreciated.

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For more than a decade after the discovery of Fe-based superconducting pnictides [1] it seemed that superconductivity existed in a relatively narrow range of dopings away from the nominal  $\text{Fe}^{2+}$  valency, between  $-0.2e$  and  $0.15e$ , and disappeared or was rapidly suppressed after that [2]. It was rationalized in terms of the Cooper pair scattering between the hole pockets of the Fermi surface near the zone center and electron pockets near its corner [3]. One of the few examples of strongly overdoped (up to  $\text{Fe}^{1.5+}$  valency) pnictides was provided by Hosono and co-workers [4–6], namely the 1111 material  $\text{LaFeOAs}$ , with up to 50% of  $\text{O}^{2-}$  replaced by H. Intriguingly, they observed two superconducting domes, possibly with different pairing symmetries and/or mechanisms. Unfortunately, further study of this material, both theoretical and experimental, has been hindered by the volatility of hydrogen and natural disorder.

Recently, another compound with formally  $\text{Fe}^{1.5+}$  has been synthesized [7],  $\text{LaFe}_2\text{As}_2$  (La122), stoichiometric and isostructural with arguably the best studied iron pnictide,  $\text{BaFe}_2\text{As}_2$ . It was found experimentally that the material can exist in two distinctly different crystallographic phases: as-prepared samples exhibit a 6.5% shorter crystallographic  $c$  parameter and a 1.6% shorter  $a$  parameter than the same sample, annealed. In Ref. [7] they were named “collapsed-tetragonal” (CT) and “uncollapsed-tetragonal” (UT). The latter, but not the former, was exhibiting superconductivity at 12.1 K. A similar  $c$  parameter collapse had been observed in the  $\text{CaFe}_2\text{As}_2$  (Ca122) compound, where it is triggered by pressure and is accompanied by the formation of As-As dimers [8,9], and by the reduction of  $c$  and small increases of  $a$  and  $b$ . The formation of the As-As bond was initially

considered to be the driving force for the collapse [10], but a later investigation of  $\text{Ca}_{1-x}\text{Sr}_x\text{Fe}_2\text{As}_2$  suggested [11] that what drives the collapse is the loss of magnetism, while the As dimerization is a by-product. At first glance, neither idea is applicable to La122, because the As-As bond in the CT phase is considerably longer than in Ca122 ( $3.18 \text{ \AA}$  vs  $2.84 \text{ \AA}$ ), and the experiment does not show any ordered magnetism in the UT phase. Furthermore, the Fermi surface calculated in Ref. [7], at first glance, bears no resemblance with that of the traditional iron pnictides; the ubiquitous hole pockets near the zone center especially seem to be absent.

In this Letter, we will address structural, magnetic, and electronic properties of La122, and will show that the UT phase, as opposed to the CT one, carries a strong short-range magnetism of the stripe type driven by the next-nearest-neighbor exchange, with, however, different subdominant interactions. The structural changes are driven by the magnetic collapse, as in Ca122. The orbitals relevant for the low-energy physics are not the usual  $d_{xz}$  and  $d_{yz}$  (these are nearly completely filled) but  $d_{xy}$  and  $d_{z^2}$  instead. The former forms a quasi-2D cylinder at the zone center, which, contrary to the initial assertion, is quite similar to the hole pocket in traditional iron pnictides. This fact was overlooked because a very 3D  $d_{z^2}$  band forms a Fermi surface sheet that crosses the  $d_{xy}$  cylinder and hybridizes with it, hiding it from view if every sheet is plotted separately. Most importantly, La in this compound assumes a noninteger valence closer to  $2.7+$  than to  $3+$ , corresponding to the doping of  $\sim 0.35e$ , rather than  $0.5e$ ; it is thus overdoped, but not dramatically. The overextended electron pockets do not exclude the usual spin-fluctuation driven mechanism with

TABLE I. Structural parameters of  $\text{LaFe}_2\text{As}_2$  as determined experimentally (Ref. [7]) and obtained by full structural relaxation.

Structure	$a$ (Å)	$c$ (Å)	$z_{\text{As}}$
UT, exp.	3.9376	11.7317	0.3657
Stripe, theor.	3.9281	11.7960	0.3620
CT, exp.	4.0035	11.0144	0.3589
Nonmagnetic, theor.	3.9904	10.9535	0.3573

an overall  $s$  symmetry. However, in such a scenario the order parameter will nearly necessarily be nodal.

We use density functional theory (DFT) with a projector augmented wave basis as implemented in VASP [12] for structure prediction. All calculations employ a generalized gradient approximation (GGA) exchange correlation functional [13]. We use the all electron full potential local orbital (FPLO) basis [14] for electronic structure analysis [15] and energy mapping of magnetic states [16,17]. Based on a tight-binding model from projective Wannier functions [18], we determine a noninteracting susceptibility [19,20].

First, we address the structural properties, using density functional theory (DFT) as a tool. In a similar compound,  $\text{LaFe}_2\text{P}_2$ , DFT was shown to reproduce the experiment in much detail, arguably better than in  $\text{Fe}^{2+}$  pnictides [21,22]. We have performed the full optimization of the crystal structure, using two approaches: one spin unrestricted, and the other enforcing a nonmagnetic Fe state. In the former we have found the same stripe-order ground state as in  $\text{BaFe}_2\text{As}_2$ , with sizable magnetic moments of  $1.8 \mu_B$  inside the Fe PAW sphere, slightly smaller than in  $\text{BaFe}_2\text{As}_2$ . The structural parameters, listed in Table I, were extremely close to those experimentally determined for the UT phase. In contrast, the nonmagnetic calculations converged to a structure nearly identical with the experimental CT structure. It had been already well established (see, for instance, Ref. [23]) that in order to reproduce the crystal structure of paramagnetic iron pnictides one needs to account for the fluctuating local magnetic moments by allowing an appropriate magnetic order. Otherwise, the  $\text{Fe}^{2+}$  ionic radius is too small, the Fe-As bond too short, and  $c/a$  too small as

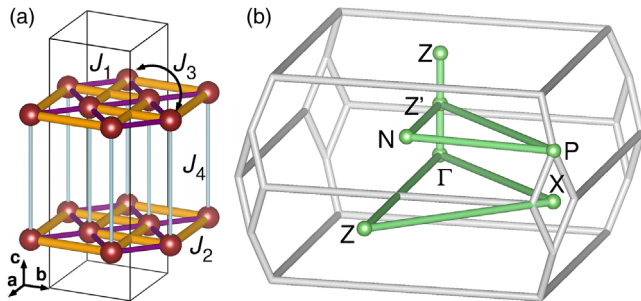

 FIG. 1. (a) Relevant exchange paths in  $\text{LaFe}_2\text{As}_2$ . (b) Brillouin zone of the  $14/mmm$  space group of  $\text{LaFe}_2\text{As}_2$ .

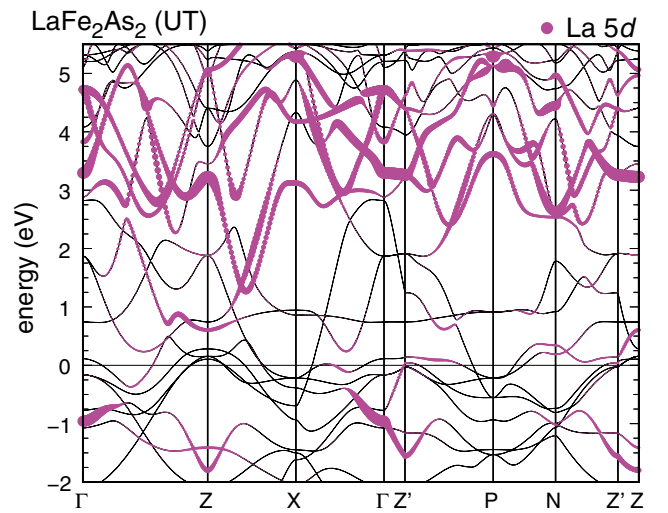
 TABLE II. Exchange couplings of  $\text{LaFe}_2\text{As}_2$  and  $\text{BaFe}_2\text{As}_2$  calculated by mapping GGA total energies of eleven spin configurations to a Heisenberg Hamiltonian. The exchange paths are visualized in Fig. 1(a).

Material	$J_1$ (K)	$J_2$ (K)	$J_3$ (K)	$J_4$ (K)
$\text{LaFe}_2\text{As}_2$	25 (13)	306 (7)	-108 (13)	63 (19)
$\text{BaFe}_2\text{As}_2$	75 (16)	400 (23)	-65 (40)	151 (8)

well. The only material where nonmagnetic calculations generate a correct structure is the CT phase of Ca122.

In pure Ca122 one cannot disentangle the effect of magnetism and the effect of As-As bonding; it had been generally believed that both contribute to the collapse, and one piece of evidence of the contrary [11] has not been universally accepted. Our result clearly shows magnetism in the driver seat. Experimentally and theoretically, As-As bonding is much weaker in CT La122 than in CT Ca122, yet their structural characteristics are amazingly similar.

Having established this fact, we have analyzed the magnetic interaction by fitting the calculated total energies in the UT phase onto the four nearest neighbor couplings of the Heisenberg Hamiltonian [the paths are shown in Fig. 1(a)]. The results are presented in Table II. Similar to other pnictides, the next-nearest-neighbor interaction  $J_2$  (the one supporting the  $s_{\pm}$  pairing [24]) dominates. Unlike those other materials,  $J_1$  is not only smaller than  $2J_2$ , assuring the stripe order, but is negligible. Furthermore, the third neighbor interaction, responsible for the double-stripe order in FeTe, is also quite sizable in La122, but is ferromagnetic rather than antiferromagnetic. It remains to be seen whether such an unusual behavior would follow from the standard low-energy itinerant model [25] and what particular effect it may have on the pairing symmetry, but it


 FIG. 2. Band structure of UT  $\text{LaFe}_2\text{As}_2$  along the path shown in Fig. 1(b) with total La 5d weights marked. The occupied La weight is mostly of  $5d_{xy}$  character.

is likely to modify the pairing interaction in a substantial and interesting way.

To this end, let us now present a detailed description of the electronic structure in the paramagnetic UT phase. As usual, the calculations are performed in the nonmagnetic case, deemed to be a good approximation to the paramagnetic state in pnictides (albeit not necessarily in more strongly correlated chalcogenides). It is worth noting that superconducting Fe pnictides are, in general, moderately correlated materials, which leads, for instance, to some

mass renormalization. Correlations become considerably stronger in strongly underdoped compounds, such as  $\text{KFe}_2\text{As}_2$ , which demonstrate qualitative changes due to strong correlations [26]. This is well understood as being due to the fact that  $\text{KFe}_2\text{As}_2$  is much closer to half-doping than  $\text{BaFe}_2\text{As}_2$ . The overdoped  $\text{LaFe}_2\text{As}_2$  is even farther from half-filling than doped  $\text{BaFe}_2\text{As}_2$  where DFT calculations reproduce the experimental Fermi surfaces rather accurately, so it is expected to be described by DFT as well as  $\text{BaFe}_2\text{As}_2$ . Since the main goal of this Letter is a

### LaFe<sub>2</sub>As<sub>2</sub> (UT)

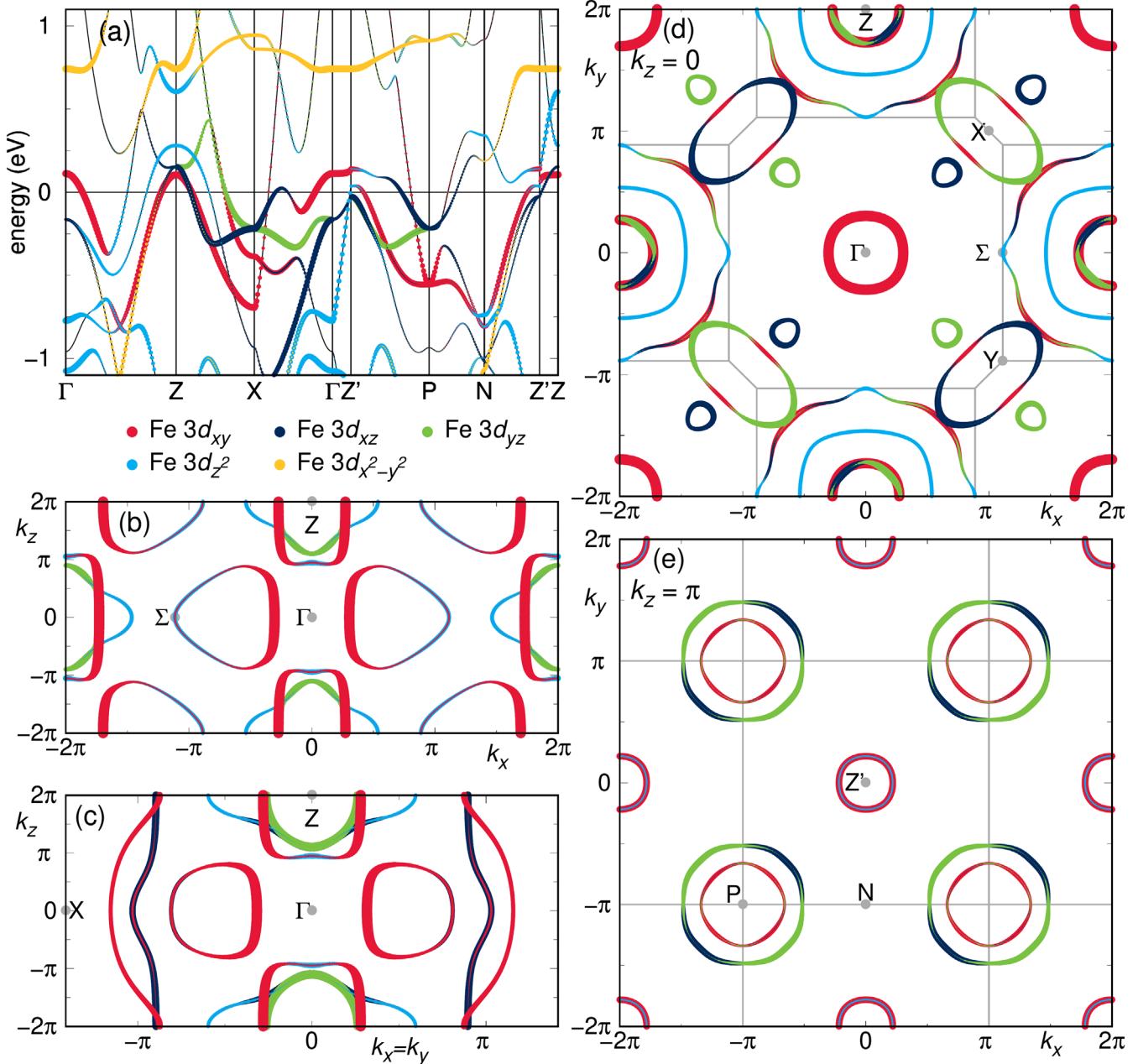


FIG. 3. Band structure and Fermi surfaces of UT  $\text{LaFe}_2\text{As}_2$  calculated within GGA. The high symmetry points are standard body-centered tetragonal points as listed in Ref. [27], except for  $Z'$  which is half way between  $\Gamma$  and Z [see the path marked in Fig. 1(b)].

comparison between the electronic structures and possible superconductivity mechanism between  $\text{LaFe}_2\text{As}_2$  and  $\text{BaFe}_2\text{As}_2$  the following analysis is conducted on a DFT basis.

Figure 2 shows the calculated band structure with the La  $5d$  character highlighted, and Fig. 3 shows the bands and Fermi surface cuts with Fe  $3d$  characters.

First and foremost, we see that one of the two La- $5d$   $e_g$  bands,  $5d_{xy}$ , which is strongly hybridized with As  $4p$ , has a huge dispersion, from its bottom at the  $\Gamma$  point at  $-1.5$  eV, to the top at  $X$  at  $+5$  eV (Fig. 2). Because of that, it becomes partially occupied, and, even though there are no pure La bands at the Fermi level, it absorbs some number of electrons, noticeably reducing the effective doping. Because of strong hybridization between this band and Fe orbitals, there is no rigorous way to assess this reduction. We have used two methods, one of which is supposed to give a lower bound, and the other the upper bound. In both cases we started from a tight-binding fit with all orbitals but Fe  $3d$  and La  $5d$  integrated out. The fit is not perfect around the  $X$  point, but pretty good closer to  $\Gamma$  and  $Z'$ . Then we set nondiagonal elements between La and Fe to zero and calculate the number of electrons in the (now pure) La  $5d$  band. This gives us  $0.22e$  per La. Next, we take the original fit, with Fe-La hybridization, and integrate the La  $5d_{xy}$  partial density of states. This gives  $0.47e$  per La. We consider these two numbers to be the lower and the upper bound, with  $0.3-0.4e$  the most likely number. Note that this corresponds to the actual Fe doping of  $0.30-0.35e/\text{Fe}$ , which is, of course, past optimal, but not nearly as heavy as  $0.5e$ . A more accurate estimate of the doping level is probably impossible without further experimental input, for instance, from photoemission spectroscopy.

Next, let us take a closer look at the Fe bands near the  $\Gamma$  point. We see that the  $d_{xz}/d_{yz}$  bands that play the leading role in the  $\text{Fe}^{2+}$  pnictides are now nearly entirely below the Fermi level in the vicinity of the  $\Gamma$  point (they do form a tiny 3D hole pocket around  $Z$ , which is basically irrelevant). This does not mean that the essential hole cylinder around  $\Gamma$ - $Z$  is gone; the  $d_{xy}$  band, which appears in many, albeit not all  $\text{Fe}^{2+}$  pnictides, is well visible near  $\Gamma$ , and the two cuts showing the vertical  $\Gamma$ - $Z$  direction [Figs. 3(b) and 3(c)] show it to be nearly 2D. This band is a perfect candidate for the standard  $s_{\pm}$  scenario. The reason that it was missed in Ref. [7] is that at  $k_z \sim (\Gamma$ - $Z)/2$  it is cut across by another, complicated Fermi surface, formed mostly by the  $d_{z^2}$  orbital, which gets gradually mixed with other orbitals as  $k_x, k_y$  increase. Note that this orbital extends along  $z$  and is thus more dispersive along  $k_z$  than in the  $k_x$ - $k_y$  plane. The corresponding Fermi surface is therefore very three dimensional. The  $d_{z^2}$  sheet hybridizes with the  $d_{xy}$  cylinder, creating a visually complicated topology, which, however, can be readily traced down to these two elements.

Having established the existence of a sizable quasi-2D hole pocket near the  $\Gamma$ - $Z$  line, let us see whether we can

reveal electron states sufficiently close to the  $X$  point to recover the standard pairing scenario [28] (note that because of the 3D character of the electronic structure we are using the standard notations for the body-centered tetragonal symmetry; point  $X$  in this notation corresponds to the  $M$  point in the often-used 2D nomenclature).

Again, let us begin with the  $d_{xz}/d_{yz}$  bands. At  $X$  they sit at a respectable 220 meV below the Fermi level, and disperse upward pretty much in the same way as they do in other iron pnictides. They strive to form a large Fermi surface cylinder ( $k_F \sim \pi/2a$ ), but this is interrupted by hybridization with other bands,  $d_{xy}$  and  $d_{z^2}$ . Right in the middle between  $\Gamma$  and  $Z$ , this hybridization is absent and the Fermi surface cut at this  $k_z$  looks amazingly similar to the Fermi surface topology in typical iron pnictide superconductors [Fig. 3(e)]. Given that the usual  $d_{xz}/d_{yz}$  hole pockets are absent, these states are unlikely to play a leading role in superconductivity.

Interestingly, the  $d_{xy}$  band also shows up near  $X$ . While at  $X$  it is located deep below the Fermi level ( $\sim 0.8$  eV), it disperses upward extremely rapidly, and along  $\Gamma$ - $X$ , where it cannot hybridize with the  $d_{xz}/d_{yz}$  bands by symmetry, it crosses the Fermi level already at 0.2 of the distance between  $\Gamma$  and  $X$ . Again, this simple fermiology is disrupted by hybridization with other states, except along  $\Gamma$ - $Z$ . However, it does not nullify the fact that there are plenty of  $d_{xy}$  states in the electronic pockets around the  $X$ - $P$ - $X$  vertical line, which share the character with zone-center hole states, and can lead to the same  $s_{\pm}$  superconductivity as in  $\text{Fe}^{2+}$  pnictides, despite a different doping level and visually extremely different Fermi surface.

This description is very reminiscent of the well-known scenario for superconductivity in optimally doped iron pnictides, except that instead of the  $d_{xz}/d_{yz}$  band showing up in both hole and electron pockets, we have  $d_{xy}$ . With this in mind, we have calculated the noninteracting susceptibility, including the orbital-defined matrix elements. It is displayed in Fig. 4. As expected, there is a large peak near

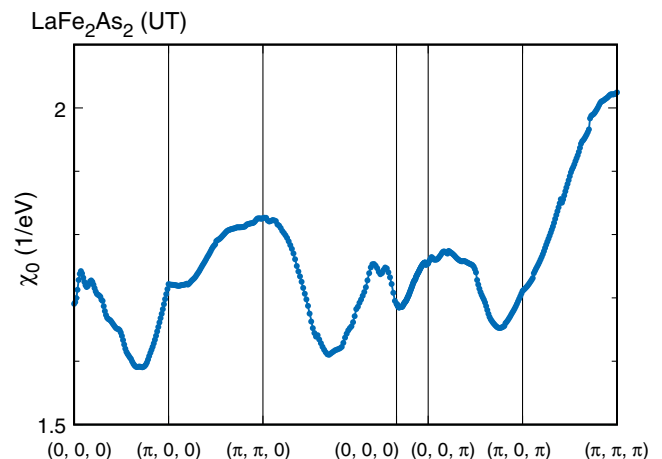


FIG. 4. Noninteracting susceptibility of UT  $\text{LaFe}_2\text{As}_2$ .

$\mathbf{Q} = (\pi/a, \pi/a, q_z)$ , both at  $q_z = 0$  and even stronger at  $q_z = \pi/c$ . Together with the fact that the calculated mean-field ground state is strongly stripe-type antiferromagnetic, it convincingly suggests that the dominant spin fluctuation has a  $(\pi/a, \pi/a)$  wave vector. Note that the calculations provide a sizable antiferromagnetic interlayer coupling, conforming to a global susceptibility maximum at  $\mathbf{Q} = (\pi/a, \pi/a, \pi/c)$ .

To summarize, we find that while  $\text{LaFe}_2\text{As}_2$  is unquestionably a unique, unusual, and highly interesting material, many of its apparent mysteries may have simple resolutions. First, the strange coexistence of two structurally different phases finds an explanation in different local magnetic states of Fe ions—despite the absence of a long-range order in either. Second, the real doping level of Fe bands is considerably smaller than the one derived from a purely ionic picture. Third, the Fermi surface of  $\text{LaFe}_2\text{As}_2$  is indeed very complex, but this complexity hides the same basic motif as in traditional iron-based superconductors: a hole pocket near  $\Gamma$  and electron pockets near  $X$ . Fourth, spin fluctuations are also peaked near  $\mathbf{Q} = (\pi/a, \pi/a, q_z)$ , potentially providing the necessary superconducting “glue.”

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*Note added.*—Recently, we became aware of independent work by Usui and Kuroki [29], who came to similar conclusions regarding the nature of superconductivity in UT  $\text{LaFe}_2\text{As}_2$ .

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