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NEWS AND VIEWS

Iron-based superconductors: A new family to find the origin of high T_c superconductivity

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Since the discovery of iron-based superconductors in 2008 [1], a new tide of study on high T_c superconductors spreads worldwide quickly. After a few years' intensive study, many new compounds of iron-based superconductors have been found and their properties have been disclosed. The great achievement is attributed to the modern experimental techniques, fast developing numerical methods and improved theories during the study of cuprate superconductors or more generally strongly correlated electron systems. For instance, the Fermi surface, band structure and superconducting gap for a new compound could be measured quickly by modern ARPES technique [2]. The improved LDA methods and powerful computers allow scientists to analyze the electronic structure of materials and predict the physical properties accurately [3, 4]. The theories help people understand the physics of superconductors and guide people in the search for new superconductors.

So far there have been many types of iron-based superconductors discovered. Basically, they can be divided into pnictides and chalcogenides. The iron pnictides include the 1111 compounds (e.g., LaFeAsO), 122 compounds (e.g., $SrFe_2As_2$), 111 compounds (e.g., LiFeAs), etc. The iron chalcogenides include the 11 compounds (FeTe or FeSe) and newly discovered 245-ferrochalcogenides (e.g., $K_xFe_{2-y}Se_2$). A typical phase diagram for the iron pnictides is shown in Fig. 1.

Soon after the discovery, people realize that magnetism plays an important role in iron-based superconductors, similar to cuprate superconductors (see Fig. 1). Short range spin fluctuation is believed to be a medium for Cooper pairing. Before doping, the parent compounds of most iron-based superconductors show long range antiferromagnetic (AF) orders. For iron pnictides, it is typically stripe like collinear AF phase with magnetic wave vector (π, 0), as shown in Fig. 2. From the local moment picture, the phase can be described by a J_1–J_2 Heisenberg model [5–8]. The corresponding spin wave calculations give consistent magnetic excitations with neutron scattering experiment. The effective exchange couplings are $J_{1a}\sim 50$ meV, $J_{1b}\sim -8$ meV, $J_2\sim 20$ meV for typical 122 compounds [9–11], where J_{1a} and J_{1b} are the nearest neighbor exchange couplings along a-axis and b-axis; J_2 is the next nearest neighbor exchange coupling shown

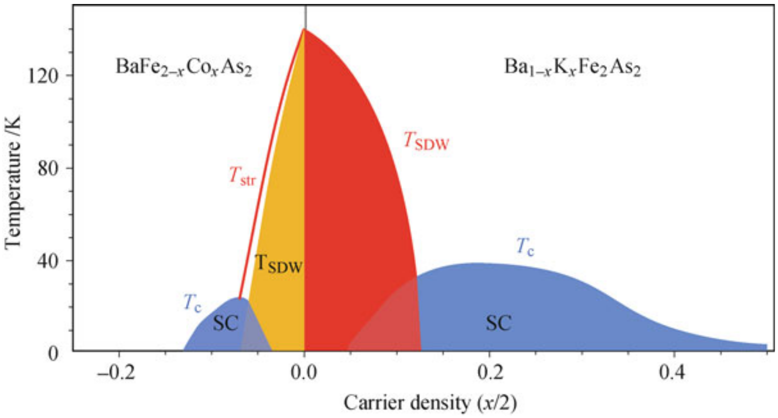

Fig. 1 Phase diagram of the Ba-122 compounds with both hole- and electron-doped cases. Reproduced from Ref. [37], Copyright © 2011 American Physical Society.

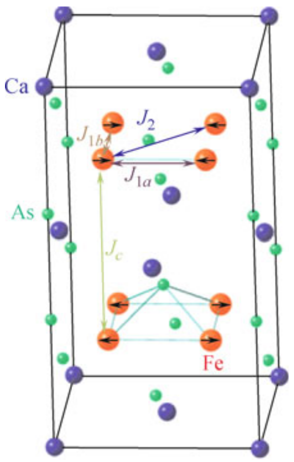

Fig. 2 Lattice and magnetic structure of $CaFe_2As_2$. Reproduced from Ref. [11], Copyright © 2009 Nature Publishing Group.

in Fig. 2. The couplings are smaller than the effective exchange coupling $J_1 \sim$120 meV in cuprates [12]. Moreover, the interlayer coupling for iron-based superconductors can be much larger than the cuprates, which means that $J_\perp/J_{//}$ can be 10^4 times bigger than the cuprates [9, 11]. The magnetism can also be understood by the itinerant electron picture because the parent compounds are poor metals. Within this picture, the long range magnetic order arises from the Fermi surface nesting. A better understanding may come from the combination of both local moments and itinerant electrons, like t–J model, Hubbard model, etc. For FeTe, the magnetic ground state is the bicollinear-antiferromagnetic state with a magnetic wave vector $(\pi/2, \pi/2)$ [13]. Within the local moment picture, this bi-collinear order can be described by a J_1–J_2–J_3 Heisenberg model with the nearest, next nearest, and next next nearest neighbor superexchange interactions. The long range J_3 can be understood by the itinerant 5p electrons at Fermi energy which mediate the exchange interactions [14]. The recently discovered alkaline iron selenide superconductors $A_xFe_{2-y}Se_2$ (A = K, Rb, Cs, Tl, etc.) have an AF block state with $\sqrt{5} \times \sqrt{5}$ Fe vacancy order, which is very different from iron pnictides [15]. It has generated great interest in the community because its pairing symmetry may be different from the sign reversed s-wave electron pairing proposed in other iron-based superconductors. The existence of long range magnetic order suggests that these compounds may be spin wave mediated superconductors [16]. However, a phase separation is found in the compounds recently [17, 18]. The inelastic neutron scattering experiment has shown that the magnetic order can be well described by an extended J_1–J_2–J_3 model [19]. Upon doping, the long range magnetic order tends not to survive in the superconducting state. However, neutron scattering experiments have shown that short range magnetic order still exists, like nematic phases. In particular, the neutron resonance peak has been associated with superconductivity, indicating a further connection with cuprate superconductors [20–22].

In most iron-based superconductors, on-site coulomb repulsion U is found in an intermediate range between strong correlation side (cuprate superconductors) and non-interacting side (BCS superconductors) from the fact that most parent compounds of the iron-based superconductors are AF metal with poor conductivity. In cuprates, the large U prohibits the double occupancy, and a Mott insulator can be formed. For BCS superconductors, the normal state is good metal without magnetic order. Numerical calculations indicate that U for Fe in iron-based superconductors is approximately half of the value for Cu in cuprates [23].

The Fe 3d electrons have multiorbital feature, which makes it a platform to study orbital physics. The polarization-dependent ARPES can identify the orbital character of electronic structures. It has been shown that d_{xz} and d_{yz} orbitals have the most important contribution although we need to include d_{xy}, $d_{x^2-y^2}$, $d_{3z^2-r^2}$ orbitals too in many cases. Theoretically, various multiorbital models have been proposed to describe the systems, like 2-, 3-, 4-, 5-orbital Hubbard models [24–26]. The Hund's coupling is found large ($\sim U/4$) in iron-based superconductors [26]. One can tempt to treat the iron-based superconductors as a multiband version of strongly correlated systems [27]. More simply, one may consider that partial d-electrons are itinerant (e.g., d_{xz}, d_{yz} electrons) and the rest of them are localized [28, 29]. The magnetic order can couple with the charge and orbital degrees to change the Fermi surface and band structure. The recent discovery of unidirectional electronic nanostructures or stripes in iron pnictides [30, 31] has shown new similarity between the Cu- and Fe-based superconductors. Looking for orbital order is a hot topic in the field of iron-based superconductors.

The superconducting gap for all iron-based superconductors is found to be singlet pairing from experiments like NMR [32]. The dominant pairing symmetry for most iron-based superconductors has been believed to be sign reversed s-wave pairing ($s^\pm$) with form factor $\cos k_x \cos k_y$ [33, 34]. The antiferromagnetic diagonal exchange coupling may play an important role in the pairing [35, 36]. Seen from the RPA study of multiorbital Hubbard models, several pairing symmetries are competing in the iron-based superconductors although the $s^\pm$ pairing dominates. This means that small tuning of parameters can change the dominant pairing symmetry dramatically. Then it is understandable that some bulk measurements have found the nodal superconductivity at certain doping levels of iron-based superconductors.

The origin of superconductivity in iron-based superconductors is still under debate. More and more evidences show that it may have similar superconducting mechanism as cuprate superconductors. Their phase diagrams are similar, and their parent compounds have long-range magnetic order. Superconductivity emerges when the long-range magnetic order is suppressed by carrier doping, and the short-range magnetic exchange interactions survive. The neutron resonance mode has been found in both families. The local AF exchange interactions in real space can help to mediate the electron pairing and drives the superconductivity. The matching of Fermi surface topology in reciprocal space and pairing form factor from the local AF interactions may be the key ingredients in the determination of high T_{c} [36]. Optimistically, we are in a good position to solve the high T_{c} problem after the 100 years' discovery of superconductivity.

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