

Chapter 2

Iron-Based Superconductors

Since Hideo Hosono discovered electron-doped iron-pnictide superconductor $\text{La}[\text{O}_{1-x}\text{F}_x]\text{FeAs}$ [1], scientists discovered various iron-pnictide superconductors containing FeAs layers and iron-selenide superconductors consisting of FeSe (and interstitial) layers. In the July of 2008, Johrendt group in the University of Munich suggested that BaFe_2As_2 in ThCr_2Si_2 structure could be a parent compound of iron-based superconductivity [2], and later discovered an optimal superconductivity with $T_c = 38$ K in potassium doped BaFe_2As_2 [3]. Meanwhile, Jin's group in the Institute of Physics in Beijing revealed $T_c = 18$ K superconductivity in LiFeAs [4]. Wu's group in Taiwan discovered the superconducting system based on FeSe [5]. Afterwards, superconductivity was achieved via carrier- or isovalent-doping in these systems [6–11]. According to the stoichiometric ratios of their chemical constituents, the main families of iron-based superconductors described above are denoted by '1111', '122', '111' and '11', respectively. Iron-based superconductors are the second class of high-temperature superconductors after cuprates. Their charge-carrier doping phase diagrams are similar to those for cuprates, while their parent compounds are poor metals instead of Mott insulators (Fig. 2.1). The comparison between iron-based and copper-oxide superconductors will provide new methods and insights for understanding high- T_c superconductivity [12]. In the studies of iron-based superconductors, many universal features among different families have been revealed. In this chapter, we will introduce some of these universal features that are associated with the studies of this thesis.

Figure 2.1 are schematic phase diagrams of copper-oxide and iron-based high-temperature superconductors [12]. Iron-based superconductivity is usually induced by doping charge carriers into its antiferromagnetic (AF) parent compound, which can be realized via element substitution in FeAs or its adjacent layer in various systems such as $\text{La}[\text{O}_{1-x}\text{F}_x]\text{FeAs}$ [1], $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ [3], $\text{BaFe}_{2-x}\text{T}_x\text{As}_2$ ($T = \text{Co}, \text{Ni}$) [6, 7], $\text{NaFe}_{1-x}\text{Co}_x\text{As}$ [8]. Superconductivity can also be induced by isovalent doping such as replacing Fe by Ru in $\text{BaFe}_{2-x}\text{Ru}_x\text{As}_2$ [9], As by P in $(\text{Eu}/\text{Ba})\text{Fe}_2(\text{As}_{1-x}\text{P}_x)_2$ [10, 11] and Se by Te in $\text{Fe}(\text{Se}, \text{Te})$ [5]. The doping gradually suppresses

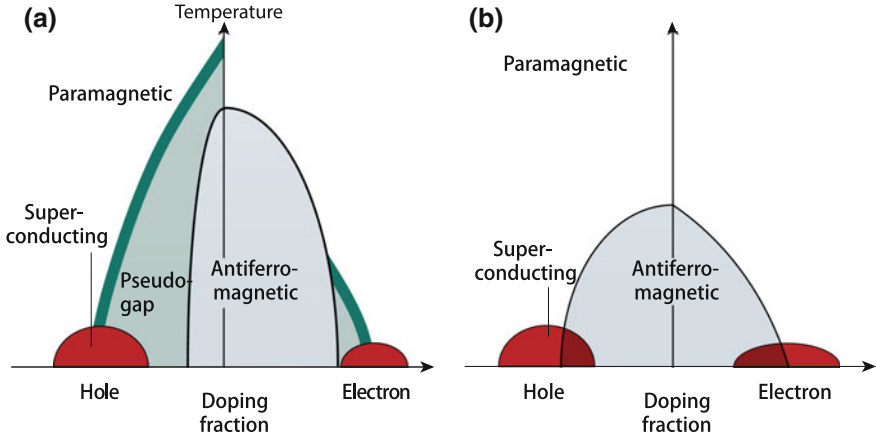


Fig. 2.1 Schematic phase diagrams of cuprate **a** and iron-based **b** high-temperature superconductors. Reprinted with permission from Macmillan Publishers Ltd: [12], Copyright 2010

the structural and magnetic phase transitions and induces optimal superconductivity at the border of structural and AF instability (Fig. 2.1). Besides doping, applying hydrostatic pressure is also efficient in inducing or enhancing superconductivity in some systems [13]. Thin films of some systems also exhibit superconductivity enhancement [14].

2.1 Basic Properties

2.1.1 Structure and Magnetic Structure

As shown in Fig. 2.2, iron-pnictide superconductors with layered structure consist of FeAs layers and interstitial layers, while iron-selenide superconductors are formed by stacked FeSe layers [15]. Within the FeX layer ($X = \text{As/P, Se/Te/S}$), four X ions surround one Fe^{2+} and form a tetrahedron (Fig. 2.2e). The geometry of the FeX_4 tetrahedron dominates various electronic properties of iron-based superconductors [16]. Parent compound of iron pnictides usually undergoes a tetragonal-to-orthorhombic structural transition (T_s), and a subsequent (or simultaneous) paramagnetic-to-AF transition (T_N). The tetragonal and orthorhombic unit cells of iron pnictides (122, 111, 1111 systems) are shown in Fig. 2.2f, where the orthorhombic unit cell are rotated by 45° and enlarged relative to the tetragonal unit cell ($a_o \approx b_o \approx \sqrt{2}a_T$). The magnetic ground state is a collinear stripe order (C-type) with magnetic wave vector $\mathbf{k} = (1, 0, 1)_{\text{ort}} = (1/2, 1/2, 1)_{\text{tet}}$ [17–22]. Compared with iron pnictides, iron selenides show different structural and magnetic transitions. Fe_{1+y}Te exhibit a simultaneous tetragonal-to-monoclinic structural and magnetic transition ($T_s = T_N \approx 70$

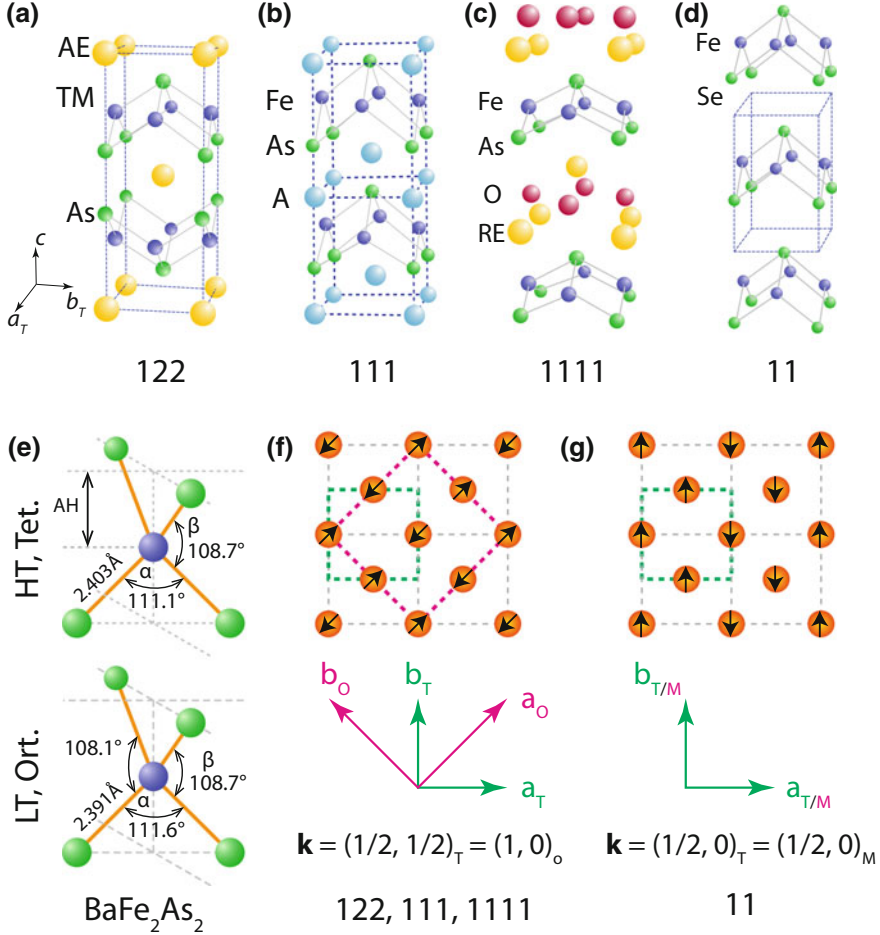


Fig. 2.2 Structures and magnetic structures of typical iron-based superconductors. **a–d** The tetragonal lattice structure for 122 (Space group: $I4/mmm$), 111, 1111 and 11 ($P4/nmm$) systems. Reprinted with permission from Macmillan Publishers Ltd: [15], copyright 2009. **e** Bond angle and bond length of FeAs tetrahedron in the tetragonal and orthorhombic state of BaFe₂As₂. α and β denote the two different types of bond angles [16]. AH (anion height) denotes the distance between the Fe²⁺ ion and the anion layer. **f** Spin arrangement of Fe²⁺ ions in FeAs layer for 122, 1111 and 111 system. The spins along c -axis are antiferromagnetically coupled. *Green square* and *pink diamond* mark the tetragonal and the orthorhombic/magnetic unit cells. **g** AF order for 11 system. The pattern itself is an AF unit cell. *Green square* denotes the tetragonal and the monoclinic unit cell

K). A bicollinear AF order (E -type, $\mathbf{k} = (1/2, 0, 1/2)_{\text{tet}} = (1/2, 0, 1/2)_{\text{mon}}$) emerges below T_N [23].

Since we focus on the studies of BaFe_{2- x} Ni _{x} As₂, we now turn to discuss the magnetic and structural properties of BaFe₂As₂ in detail. At high temperature,

BaFe_2As_2 shows tetragonal structure with space group $I4/mmm$ and lattice parameters $a = b = 3.963 \text{ \AA}$, $c = 13.02 \text{ \AA}$, as shown in Fig. 2.2. As cooling, BaFe_2As_2 undergoes a structural transition and a subsequent magnetic transition ($T_s \approx T_N + 0.2 \text{ K} \approx 138 \text{ K}$) [24]. The system enters an orthorhombic phase below T_s and then an AF state below T_N , with space group $Fmmm$ and lattice parameters $a = 5.615 \text{ \AA}$, $b = 5.574 \text{ \AA}$, $c = 12.95 \text{ \AA}$ at base temperature. The AF order of BaFe_2As_2 is a C-type collinear stripe order with magnetic vector $\mathbf{k} = (1, 0, 1)$ in the orthorhombic notation and $(1/2, 1/2, 1)$ in the tetragonal notation (Fig. 2.2). Relative to the tetragonal state, the orthorhombic unit cell are rotated by 45° with $a_o = \sqrt{2}a_T$. The other parent compounds of the 122 system such as CaFe_2As_2 , SrFe_2As_2 and EuFe_2As_2 have similar structural and magnetic properties [22, 25], though they show different lattice parameters, magnetic moments and structural and magnetic transition temperatures. The main difference among these 122 parent compounds is the order of the structural and the magnetic phase transitions [26]. BaFe_2As_2 exhibits second-order structural transition, as indicated by the gradual onset of the orthorhombic lattice distortion $\delta = (a_o - b_o)/(a_o + b_o)$ in Fig. 2.3a [24], and first-order magnetic transition that induces a hysteresis and a jump of δ via strong magnetoelastic coupling (Fig. 2.3a). With increasing electron doping, the temperature difference between T_s and T_N is enlarged and the magnetic transition becomes second order (Fig. 2.3b) [24]. The others, however, show simultaneous first-order structural and magnetic phase transitions in undoped and underdoped regime [21, 22, 25, 26]. The order of the structural and magnetic phase transitions, and whether they occur simultaneously, have significant influence on the electronic properties close to the transitions.

In the tetragonal state, electronic properties within ab plane of the doped BaFe_2As_2 systems show C_4 symmetry, as dictated by the structural symmetry and revealed by experimental studies. Similarly, samples in the orthorhombic phase

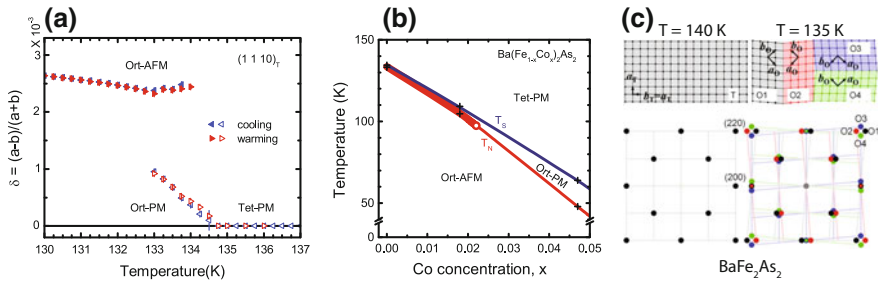


Fig. 2.3 **a** Temperature dependence of the orthorhombic lattice distortions (δ) in BaFe_2As_2 . The Ort, Tet, AFM and PM denote orthorhombic, tetragonal, AF and paramagnetic state, respectively. **b** Doping evolution of the structural transition and the magnetic transition in $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$. The thick red line marks the first-order magnetic transition. Reprinted with permission from [24]. Copyright 2011 by the American Physical Society. **c** Twinning caused by the tetragonal-to-orthorhombic structural phase transition in BaFe_2As_2 . Four kinds of domains form below T_s . **c** is reprinted with permission from [27]. Copyright 2009 by the American Physical Society

should exhibit two-fold (C_2) electronic properties. However, the tetragonal-to-orthorhombic structural transition results in twinning, as shown in Fig. 2.3c. Four kinds of domains formed with their a_o axis aligned along four different directions below T_s and hinder the measurements of the intrinsic electronic properties along a_o and b_o axes [27]. To measure the intrinsic electronic properties, the first step is to obtain a detwinned, single domain crystal. Tanatar et al. in Ames Lab [28] and Chu et al. in Stanford university [29] independently developed mechanical detwinning devices that can apply uniaxial stress for crystal detwinning. Their resistivity measurements on BaFe_2As_2 and $\text{BaFe}_{2-x}\text{T}_x\text{As}_2$ ($T=\text{Co, Ni}$) revealed strong resistivity anisotropy between ρ_a and ρ_b [29, 30]. ρ_a is smaller and shows metallic behavior below a characteristic temperature T^* , while ρ_b behaves like an insulator below T^* . T^* is much higher than T_s , indicating that this electronic anisotropy persists in the tetragonal state. The electronic anisotropy in the tetragonal state of uniaxial-pressure detwinned $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ is a solid evidence for the emergence of an electronic nematic in iron pnictides [29]. Similar electronic anisotropy in the tetragonal state has also been observed in uniaxial-strained $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$ but absent (or much weaker) in $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$, suggesting that it is easier to induce such anisotropy by doping FeAs layer [31, 32]. In addition, resistivity measurements on detwinned CaFe_2As_2 and SrFe_2As_2 reveal vanishingly small resistivity anisotropy above T_s and therefore suggested that the electronic nematic is sensitive to the order of the structural transition [28, 33]. To study the electronic nematic in iron pnictides, we use neutron scattering to study the magnetic order and spin excitations in uniaxial-strained $\text{BaFe}_{2-x}\text{Ni}_x\text{As}_2$. We shall discuss the details in Chap. 6.

The strong electronic anisotropy in the tetragonal state of uniaxial-strained $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ implies that the electronic properties of underdoped iron pnictides are susceptible to structural changes. Indeed, various studies have suggested that the electronic properties of iron pnictides are sensitive to the distortions of the FeAs_4 tetrahedron. To be specific, the anion height (AH) and the bond angle α of the FeAs_4 octahedron (Fig. 2.2) are correlated with the superconductivity in iron pnictides. As shown in Fig. 2.4a, Mizuguchi et al. summarized AH and T_c for many iron-based superconductors. As increasing AH, T_c firstly increases and then decreases, forming a peak at $\text{AH} = 1.38 \text{ \AA}$ [34]. Subsequently, Lee et al. plotted the relationship between T_c and α , as displayed in Fig. 2.4b. This plot suggests that a system containing undistorted FeAs_4 tetrahedron ($\alpha = 109.47^\circ$) exhibits higher T_c [35]. The structural effects above suggested that superconductivity can be induced by charge carrier doping as well as chemical pressure generated by element substitution. On the other hand, element substitution would induce impurity scattering, which is detrimental to superconductivity. Therefore, the emergence of superconductivity is driven and affected by various factors and cannot be simply explained by charge carrier doping.

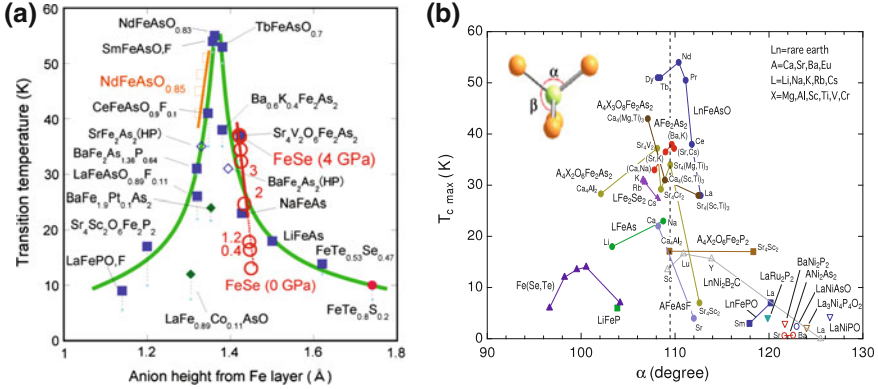


Fig. 2.4 **a** The relationship between AH and T_c . The maximum of T_c corresponds to 1.38 Å of AH [34]. © IOP Publishing. Reproduced with permission. All rights reserved. **b** As-Fe-As bond angle in FeAs_4 tetrahedron. The black dashed line marks $\alpha = 109.47^\circ$ for undistorted tetrahedron. Reprinted from [35]. Copyright 2012, with permission from Elsevier

2.1.2 Electronic Structure

Because of the common FeAs layer, iron pnictides exhibit similar Fermi surface topology. Compared with the single-band copper oxides, iron based superconductors are multi-band systems. Their Fermi surfaces usually consist of hole pockets around Γ point and electron pockets around $M(X)$ point.

Figure 2.5 shows the Fermi surface and band structure of LaOFeAs and LaOFeP calculated by LDA and measured by angle-resolved photoemission (ARPES), respectively [36–38]. The Fermi surface of LaOFeAs includes two hole pockets at the center of the Brillouin zone (Γ) and two electron pockets at zone corner (Fig. 2.5a). Some of the Fermi pockets show strong dispersion along k_z while the others are more two dimensional (Fig. 2.5b). Since the hole pockets at Γ show similar size to the electron pockets at M , Fermi surface nesting between them could occur with nesting vector $\mathbf{k} = (1/2, 1/2)_{\text{tet}} = (1, 0)_{\text{ort}}$ [36]. As suggested by theoretical calculation, the perfect Fermi surface nesting tends to induce an AF spin density wave ground state with wave vector $\mathbf{k} = (1/2, 1/2)_{\text{tet}}$ [36]. Subsequently, neutron diffraction measurements on LaOFeAs confirm the existence of the AF order in LaOFeAs [17]. Figure 2.5c depicts the contributions of different orbitals to the total electron density of states of LaOFeAs . The density of states close to Fermi surface are dominated by the orbitals of iron, while the p orbitals of As lie 3 eV below the Fermi surface. Therefore, the electronic properties of the system depends on the electron hopping between Fe ions. Figure 2.5d are band structures along high symmetry directions. The blue and green dashed curves are the band structures for 3.5 pm larger and smaller anion heights, respectively. Note the anion height for LaOFeAs is 130 pm. The change of the anion height induces similar band shift to that caused by charge carrier doping. As we have discussed in last section, the anion height has significant effects on the electronic

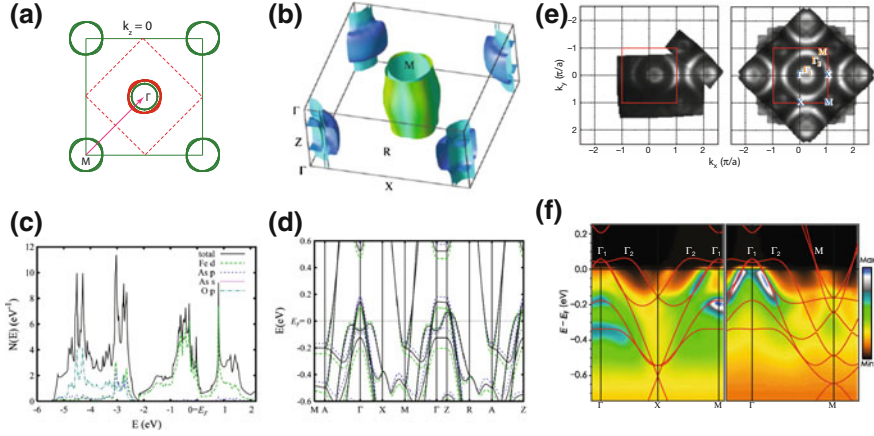


Fig. 2.5 **a** The Fermi surface of LaOFeAs at $k_z=0$. It consists of two hole pockets around Γ point and two electron pockets around M point [36]. **b** Three-dimensional Fermi surface of LaOFeAs calculated using LDA. **c** Electron density of states of LaOFeAs. **d** Electronic structure of LaOFeAs. The blue (green) dashed curves denote the electronic structure for 3.5 pm larger (smaller) anion height. **b–d** are reprinted with permission from [37]. Copyright 2008 by the American Physical Society. **e** Fermi surface and **f** band structure of LaOFeP measured by angle-resolved photoemission and their comparison with the results from LDA calculation. **e–f** are reprinted with permission from Macmillan Publishers Ltd: [38], copyright 2008

properties of iron pnictides. Figure 2.5e–f are Fermi surface and band structure of LaOFeP measured by ARPES, which is consistent with the results of LDA calculation [38]. The consistency between LDA results and the band structure measured by ARPES suggests that the system shows strong itinerancy and weak (or intermediate) electron correlations. However, as we shall discuss later, the real situation is more complicated.

As suggested by LDA calculation, 122 system exhibits similar Fermi surface topology and hosts two hole pockets at Γ point and two electron pockets at tetragonal zone corner (X point) [39]. As increasing charge carrier doping, the Fermi level shifts gradually, which changes the Fermi surface nesting condition. LDA calculation also suggests that the anion height decreases with hole doping. This can be ascribed to the enhanced attraction between Fe^{2+} and As^{3-} after the injection of holes into the Fe^{2+} sites and the decrease of the radius of Fe ions after hole injection.

2.2 Phase Diagrams

In this section, we will describe the phase diagrams of doped BaFe_2As_2 systems and discuss the emergence of the AF order, the orthorhombic lattice distortions and the superconductivity, and the interplay between these orders.

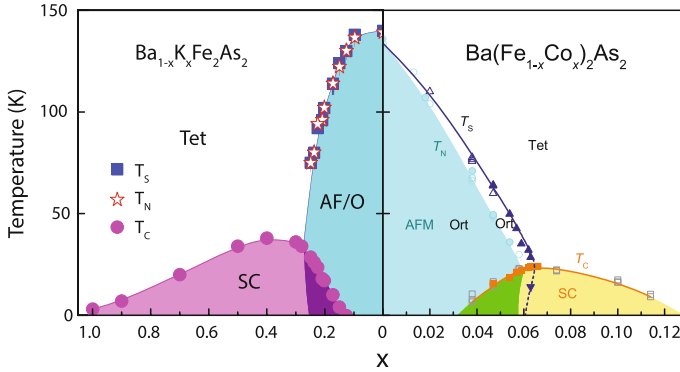


Fig. 2.6 **a** Hole- and **b** electron-doping phase diagrams of doped BaFe_2As_2 system [40, 41]. The AFM, Ort, Tet, SC are antiferromagnetic order, orthorhombic, tetragonal and superconductivity, respectively. The T_s , T_N and T_c are structural, antiferromagnetic and superconducting transition temperatures. The *left panel* is reprinted with permission from [40]. Copyright 2012 by the American Physical Society. The *right panel* is reprinted with permission from [41]. Copyright 2010 by the American Physical Society

Figure 2.6 shows the phase diagrams for hole- and electron-doped BaFe_2As_2 . In $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$, the substitution of Ba by potassium induces holes into the FeAs layers indirectly. The superconductivity emerges at $x = 0.1$ and persists to the end member $x = 1$, with optimal superconductivity ($T_c = 39$ K) achieved at $x = 0.4$ [40]. Compared with $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$, electron-doped $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ are distinct in various aspects [41]. The element substitution occurs at the Fe sites and induces electron doping in FeAs layers directly. Since the structure of FeAs layer dominates many electronic properties of iron pnictides, introducing charge carrier by element substitution in or out-of-FeAs layers are very different. As shown in Fig. 2.6, superconductivity in $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ appears from $x = 0.03$ and persists only before $x = 0.13$ with optimal $T_c = 26$ K occurred at $x = 0.062$, and the AF order is suppressed more quickly than that in $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$. This substantial electron-hole asymmetry reflects different electron correlation in these two sides. The microscopic origin, however, remains elusive.

In doped 122 systems, charge carrier doping in the interstitial layers adjacent to the FeAs layers are more effective in inducing superconductivity, for which optimal T_c is higher than 30 K in hole-doped $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ and $\text{Ba}_{1-x}\text{Na}_x\text{Fe}_2\text{As}_2$ and higher than 40 K in electron-doped $\text{Ca}_{1-x}\text{La}_x\text{Fe}_2\text{As}_2$. However, hole doping in FeAs layer fails to induce superconductivity because Cr and Mn that suppose to provide holes have strong magnetism and induce strong impurity scattering, which are detrimental to superconductivity. The electron- and isovalent-doping in FeAs layer, such as substituting Fe by Co, Ni, Ru and As by P, can induce superconductivity exhibiting optimal $T_c \sim 20\text{--}30$ K [6, 7, 9, 11]. With increasing doping, the AF order and orthorhombic state are gradually suppressed. The structural and the magnetic transitions are coupled first-order transition in $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ and BaFe_2As_2 .

$(\text{As}_{1-x}\text{P}_x)_2$, while T_s and T_N split with increasing doping in $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ and $\text{BaFe}_{2-x}\text{Ni}_x\text{As}_2$.

2.2.1 Spin Density Wave

Since the parent compounds of iron pnictides show poor metallic ground state, and their Fermi surface topology could allow Fermi surface nesting between the hole pockets at Γ point and the electron pockets at M point, Dong et al. proposed that a spin density wave (SDW) state could be formed in LaOFeAs , driven by the Fermi surface nesting (Fig. 2.5a) [36]. SDW is a symmetry-breaking state induced by the instability of Fermi surface in an itinerant magnetic system [42]. An AF order corresponding to the Fermi surface nesting was indeed discovered by neutron diffraction (Fig. 2.2) [17]. Because of the important role of Fermi surface nesting and itinerant magnetism in creating the AF groundstate and driving the magnetic dynamics of iron pnictides, it is necessary to introduce the basic ideas of Fermi-surface-nesting driven SDW.

As shown in Fig. 2.7a, the Fermi surface of one-dimensional electron gas are two points at $\pm k_F$. This special Fermi surface is susceptible to small perturbations, much different from its counterparts in higher dimensions. From linear response theory, electron density distribution caused by an external perturbation $\phi(\mathbf{q})$ can be expressed as:

$$\rho^{ind}(\mathbf{q}) = \chi(\mathbf{q})\phi(\mathbf{q}), \quad (2.1)$$

where $\chi(\mathbf{q})$ is the Lindhard Response Function of the system. The response function in d dimensions can be written as

$$\chi(\mathbf{q}) = \int \frac{d\mathbf{k}}{(2\pi)^d} \frac{f_k - f_{k+q}}{E_k - E_{k+q}}, \quad (2.2)$$

in which $f_k = f(\varepsilon_k)$ is Fermi distribution function. For the scattering between the occupied state and the unoccupied state in one dimension (Fig. 2.7a), $f_k - f_{k+q} \equiv 1$ while $E_k - E_{k+q}$ can be infinitesimal close to $q = 2k_F$, resulting in a divergence of the response function at $q = 2k_F$, as shown in Fig. 2.7b. This divergence corresponds to an unstable state, which is usually avoided by a periodic distribution of the electron (or spin) density with wave vector $q = 2k_F$, that is, density wave. The formation of the $q = 2k_F$ density wave folds the band structure and open a density-wave gap, leaving the system into a stable state [43]. Figure 2.7c shows the band folding and energy gap formation for a system with lattice parameter a . The period of the density wave is $2a$, corresponding to a smaller Brillouin zone $\frac{\pi}{a}$. Therefore, the periodicity of the density wave induces an energy gap at $\pm \frac{\pi}{2a}$ [43]. For higher dimensions $d = 2, 3$, only one q point on the Fermi surface meets the nesting condition, which cannot result in any divergence in the corresponding response function Eq. 2.2, as shown in Figs. 2.7b, d.

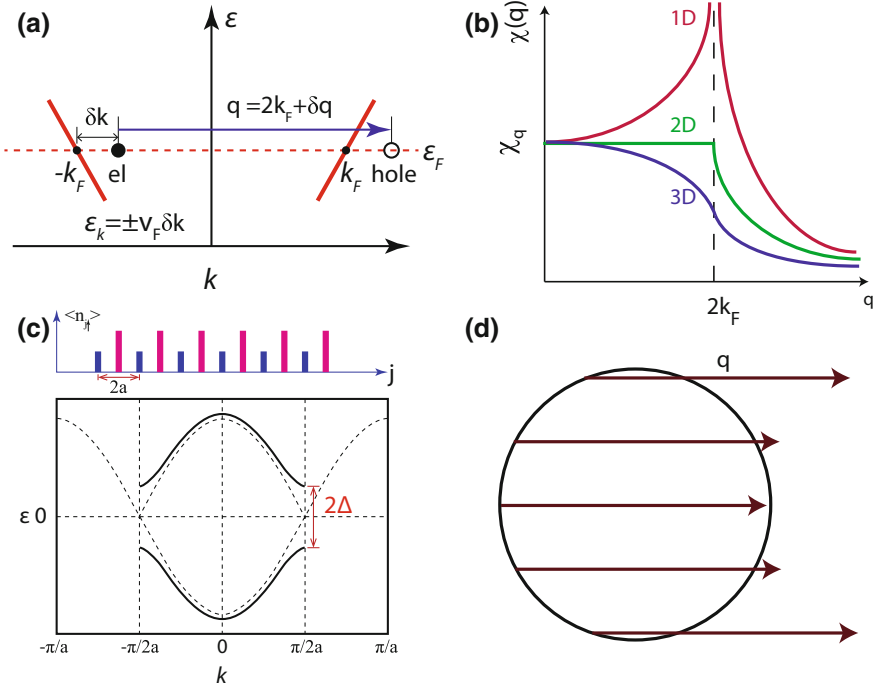


Fig. 2.7 **a** Schematic diagram of Fermi surface nesting in one-dimensional electron gas. **b** q dependence of the response function χ_q in dimensions $d = 1, 2, 3$. **c** Upper Spin density wave in real space. Lower Band structure of one-dimensional spin density wave. **d** Schematic of Fermi surface nesting in two-dimensional electron gas, in which only one q point meets the nesting condition. [42]

Free electron gas is a single-band system. Therefore, Fermi surface nesting cannot be realized in two and three dimensions. In the multiband iron pnictides, the interband scattering between the hole Fermi surface at Γ point and the electron Fermi surface at $M(X)$ point could induce Fermi surface instability and result in a SDW state with AF wave vector $(1/2, 1/2)\frac{2\pi}{a_T}$ (Fig. 2.2). Indeed, infrared optical measurements observed spectral weight transfer across the Néel temperature T_N in LaOFeAs, indicating an energy-gap opening below T_N , in agreement with the SDW picture [36, 44]. However, ARPES measurements revealed Fermi surface reconstruction instead of energy gap opening in iron pnictides [45, 46]. Therefore, whether the AF order is a SDW state remains an open question. Furthermore, the parent compound of 11 system (FeTe) has similar Fermi surface topology to iron pnictides but shows bicollinear AF order with wave vector $\mathbf{k} = (1/2, 0)(\frac{2\pi}{a_T})$ Fig. 2.2, suggesting that the AF order in iron-based superconductors cannot be fully described by the SDW picture [47]. In addition, the magnetic moment for FeTe, $\sim 2\mu_B/\text{Fe}$, is much larger than those in iron pnictides such as $0.35 \mu_B$ in LaOFeAs [17], $0.87 \mu_B$ in BaFe₂As₂ [18] and $\sim 0.1\mu_B$ in Na_{1- δ} FeAs [19], indicative of a local-moment picture. If the AF orders in these four families of

iron-based superconductors share the same origin, a comprehensive picture beyond SDW is required, for instance, theoretical attempts emphasizing correlation effects and Hund's coupling have been proposed [48, 49].

2.2.2 Superconductivity and Fermi Surface Nesting

In doped BaFe_2As_2 systems, it is well known that charge carrier doping gradually suppresses the long range AF order and induces optimal superconductivity at the boarder of the AF instability [40, 41]. In the view of band structure, charge carrier doping will change the chemical potential of the system and shift the Fermi surface. The band shift will change the sizes of the Fermi pockets and therefore vary the nesting condition [50–53]. In the theory of Fermi surface nesting, minor change of Fermi surface sizes can greatly change the nesting condition and suppress the AF order. Although the perfect nesting inducing the AF order will be broken, interband scattering between partial Fermi surface of the hole pockets and the electron pockets can persist in superconducting regime. Since this partial nesting could enhance AF spin fluctuations which could be a driving force for superconductivity, Fermi surface nesting has also been connected to the evolution of the superconductivity in these systems. As shown in Fig. 2.8a, b, in $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$, Fermi surface nesting between hole band α and electron bands ϵ and γ are enhanced in $x = 0.25$ and 0.4 sample, which was suggested to enhance the interband scattering (and spin fluctuations) and therefore improve superconductivity (T_c). As increasing hole doping to $x = 0.7$, nesting conditions become worse and T_c decreases to 22 K. The end member KFe_2As_2 ($x = 1$) shows only $T_c = 3$ K, where the γ pocket disappears and the ϵ band changes a lot in topology, both of which suppress the nesting condition. Similar doping evolution of Fermi surface nesting and superconductivity was also observed in electron-doped $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$. This consistency in the doping evolution between nesting and superconductivity in various systems indicates that Fermi surface nesting is intimately connected to the superconductivity in iron pnictides.

Since low energy spin fluctuations, including the spin resonance mode, have been suggested to arise from the interband scattering between the hole pockets at Γ and electron pockets at $M(X)$, better Fermi surface nesting condition means stronger spin fluctuations, which could enhance superconductivity if the superconductivity is indeed driven by spin fluctuations. The spin resonance mode was proposed to be an important evidence of the $s\pm$ -wave superconductivity in iron-based superconductors mediated by spin fluctuations [54]. Indeed, the spin resonance mode was subsequently discovered in various iron-based superconductors and strongly supports the $s\pm$ model. The $s\pm$ wave symmetry were also supported by the superconducting gaps in various pnictide superconductors measured by ARPES [55–58]. Scanning tunneling microscope measurements of the superconducting gap and the quasiparticle interference under magnetic field in $\text{Fe}(\text{Se},\text{Te})$ also favor the $s\pm$ wave symmetry [59].

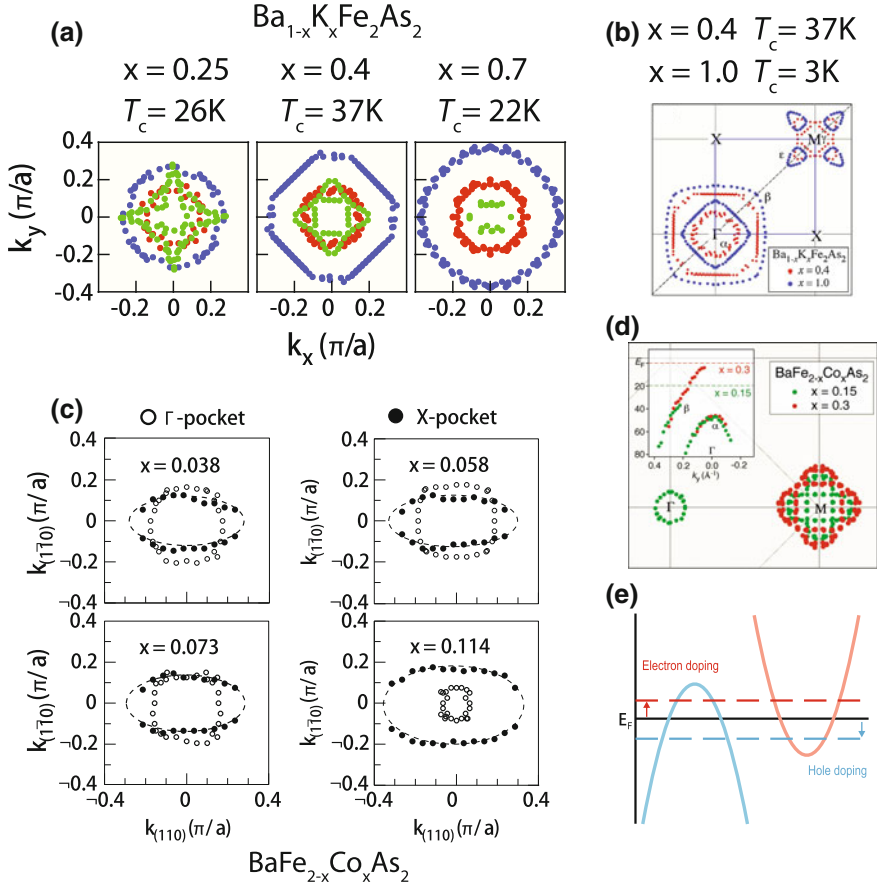


Fig. 2.8 **a–b** Doping evolution of the Fermi surfaces in hole-doped $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$. **a** is reprinted with permission from [50]. Copyright 2009 by the American Physical Society. **b** is reprinted with permission from [51]. Copyright 2011 by the American Physical Society. **c–d** Electron-doping evolution of the Fermi surfaces of $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ [52, 53]. **c** is reprinted with permission from Macmillan Publishers Ltd: [52], copyright 2010. **e** Fermi level shift induced by charge carrier doping in a rigid band picture

Although Fermi surface nesting was suggested to be essential for the spin fluctuations and the superconductivity in iron-based superconductors, experimental studies for their connections, and their doping evolution, are still lacking. One of our main goals is to explore the doping evolution of the Fermi surface, spin fluctuations and superconductivity, as well as their connections, in electron-doped $\text{BaFe}_{2-x}\text{Ni}_x\text{As}_2$, as we shall discuss in Chap. 7.

2.2.3 Coexisting and Competing Orders

The coexistence and competition between various orders such as AF order, orthorhombic state and superconductivity are crucial for understanding the microscopic mechanism of the superconductivity in iron-based superconductors. Studies of the interplay between these orders can reveal their connections and provide an experimental basis for developing a comprehensive theoretical model.

As we have discussed, underdoped BaFe_2As_2 samples undergo a structural phase transition ($T_s = 138$ K, $\delta = 0.36\%$ for BaFe_2As_2) and a magnetic phase transition ($T_N = 138$ K, $m = 0.87\mu_B$ for BaFe_2As_2). In the underdoped regime, with increasing doping, the structural transition and the magnetic transition are gradually suppressed. The transition temperatures (T_s and T_N), the orthorhombic lattice distortions (δ) and magnetic moment decrease monotonically with increasing doping. Meanwhile, superconductivity emerges and reach its maximum at the border of the structural and magnetic instability. The contrasting trends suggest a competition between superconductivity and orthorhombic AF state, and a coupling between the orthorhombic phase and the AF order. This interplay was an indirect speculation at early time, but became clear in the phase diagrams determined by transport, magnetic, neutron scattering and x-ray diffraction measurements in various systems. The underdoped region hosting orthorhombic state, AF order and superconductivity is of particular interest in the studies of the correlations between these orders. Figure 2.6 shows the research progress concerning this issue [40, 41].

When superconductivity emerges from the orthorhombic AF ground state, it has low T_c and small superconducting volume fraction. The interplay between these orders are not obvious. As increasing doping to weaken the orthorhombic AF state and enhance the superconductivity, a suppression of the orthorhombic lattice distortion (δ) and the AF order parameter occurs below T_c , as shown in Fig. 2.9a–c. In Fig. 2.9a–b, orthorhombic lattice distortions δ in $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ are heavily suppressed below T_c . In the optimal doping ($x = 0.063$), the system even re-enters the tetragonal state, as dictated by the merge of the two orthorhombic peaks at 8.3 K in Fig. 2.9a [41]. Figure 2.9c shows the split T_s and T_N and the suppression of the magnetic order parameter below T_c in $x = 0.047$ of $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ [60]. The suppression of the AF state becomes stronger at higher doping. In a doping close to optimal doping, the AF order parameter is almost completely suppressed at a temperature below T_c [41, 60, 62, 63].

The competition between superconductivity and AF order, and the strong magnetoelastic coupling have been discovered not only in many electron doped systems such as Co, Ni, Rh doped BaFe_2As_2 [64–67], but also in hole-doped $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ [40] and isovalent-doped $\text{Ba}(\text{Fe}_{1-x}\text{Ru}_x)_2\text{As}_2$ [68] and $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$ [69, 70]. These experimental facts indicate that the interplay is universal in iron pnictides. Thus far, we note that the systems showing weak impurity scattering, such as $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$ and $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$, exhibit strong suppression of the AF order, while some systems like $\text{BaFe}_{2-x}\text{Ni}_x\text{As}_2$ hosting stronger impurity scattering, show weaker suppression.

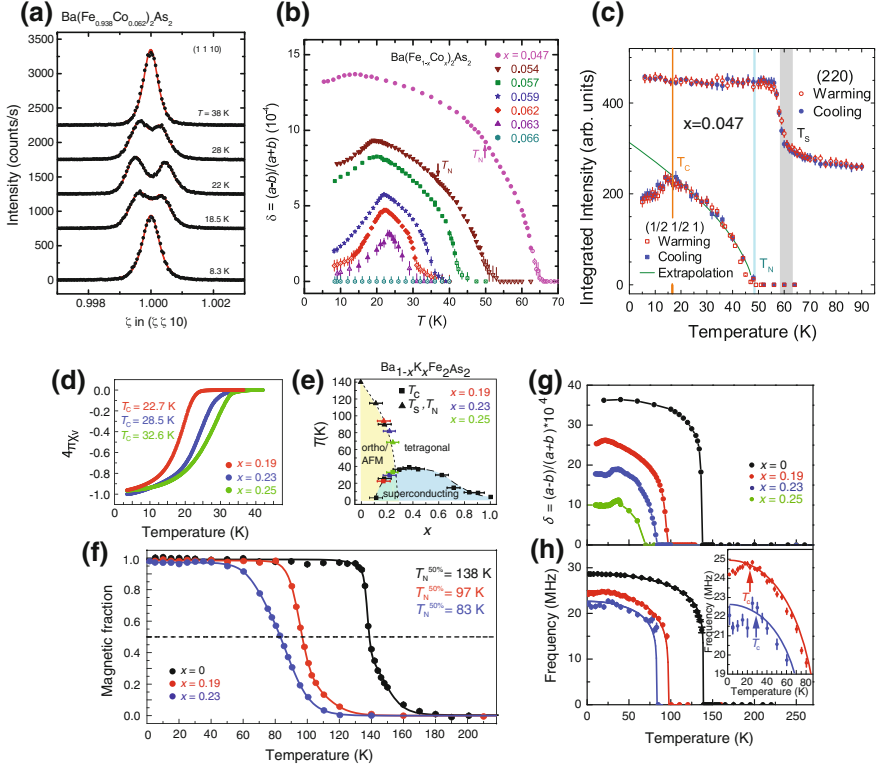


Fig. 2.9 **a** Temperature dependence of the tetragonal (1, 1, 10) Bragg peak in $\text{Ba}(\text{Fe}_{0.938}\text{Co}_{0.062})_2\text{As}_2$ [41]. **b** Orthorhombic lattice distortions (δ) as a function of temperature for $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ [41]. Reprinted with permission from [41]. Copyright 2010 by the American Physical Society. **c** Magnetic order parameter at $\mathbf{Q} = (1/2, 1/2, 1)$ and neutron extinction at $(2, 2, 0)$ nuclear Bragg peak of $\text{Ba}(\text{Fe}_{0.953}\text{Co}_{0.047})_2\text{As}_2$. Reprinted with permission from [60]. Copyright 2009 by the American Physical Society. **d–h** Microscopic coexistence of antiferromagnetism and superconductivity in $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ studied by μSR [61]. **d** Magnetic susceptibility for the three dopings used for the μSR study in Ref. [61]. **e** The phase diagram of $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$, where the three dopings shown in (e) are marked. **f** AF volume fraction measured by μSR . **g** Temperature dependence of the lattice distortions δ for $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$. **h** Magnetic order parameters of $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ measured by μSR . Reprinted with permission from [61]. Copyright 2011 by the American Physical Society

These unusual correlations have been interpreted by the competition between superconductivity and AF (SDW) state (since they share the same itinerant electrons) and the strong elastomagnetic coupling [63]. This also means that the superconductivity favors a paramagnetic tetragonal state, which is more isotropic (symmetric) than the orthorhombic AF state. This is an important point that must be taken into account in establishing a theoretical model for explaining the phase diagrams of iron pnictides.

Besides the competition, whether the AF order coexist with superconductivity in a microscopic scale is also an important question which is still controversial. Generally, it is difficult to judge the scale of this coexistence, since both microscopic and mesoscopic coexistence can describe the experimental observations from neutron scattering and x-ray diffraction. Some local probes such as muon spin rotation (μ SR) and nuclear magnetic resonance (NMR) support the microscopic coexistence of AF order and superconductivity. In a NMR study of $\text{Ba}(\text{Fe}_{1-x}\text{Ru}_x)_2\text{As}_2$ [71], Ma et al. found that magnetic volume fraction for underdoped samples is 100% below T_N and the magnetic signal falls sharply below T_c , providing a solid evidence for the microscopic coexistence of AF order and superconductivity. Similar conclusion was drawn in μ SR measurements of $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ [61]. In underdoped $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ hosting bulk superconductivity, the magnetic volume fraction below T_c is 100%, suggesting that AF order and the superconductivity coexist in a microscopic scale [61]. Complete understanding concerning this issue is still lacking and remains to be explored experimentally and theoretically. In this thesis, one important work is to clarify the correlations between the AF order, the lattice distortion and the superconductivity close to optimal doping of $\text{BaFe}_{2-x}\text{Ni}_x\text{As}_2$, as we shall discuss in Chaps. 4 and 5.

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