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## Charge redistribution and local lattice structure of (F, Zn)-codoped LaFeAsO superconductor

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**Abstract.** To understand the abnormal behavior of the superconducting transition temperature ( $T_c$ ) because of the presence of a non-magnetic Zn impurity in the (F, Zn)-codoped LaFeAsO system (Li *et al* 2010 *New J. Phys.* **12** 083008), we investigated its unique electronic and local structures via x-ray absorption spectroscopy and first-principles calculations. The data obtained showed that the presence of a Zn impurity induces an electron transfer from As to Fe atoms in both the F-underdoped and -overdoped regions. Moreover, due to the lattice mismatch, the local lattice structure is finely modulated by both F and Zn impurities. Actually, in the F-underdoped region doping by Zn is associated with regular FeAs<sub>4</sub> tetrahedra, while distorted FeAs<sub>4</sub> tetrahedra occur in the F-overdoped region where superconductivity is significantly suppressed.

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**1. Introduction**

The discovery of Fe-based superconductors [1, 2] opened up the possibility of understanding better the mechanism of high-temperature (high- $T_c$ ) superconductivity [3, 4] and renewed interest in it, thus triggering new studies in the condensed matter community [5]. Similar to the  $\text{CuO}_2$  layer in cuprates, the FeAs layer of pnictide systems is considered to be the corresponding superconducting layer. Parent compounds of iron pnictides are antiferromagnetic systems and poor metals. In these materials either chemical doping or pressure may suppress the long-range magnetic order, favoring the emergence of superconductivity. However, the main—and probably the most challenging—issue regarding iron pnictides is pairing symmetry. Many experiments and theoretical calculations have pointed out that the electronic structure of Fe-based superconductors is characterized by a multi-band nature [6]. In this scenario, the superconductivity should be associated with the inter-pocket nesting among electron-like pockets and hole-like ones [7]. However, in the so-called  $s^\pm$ -pairing framework, the pockets are characterized by an opposite sign of the superconducting order parameters [8]. Recent detailed angle-resolved photoemission spectroscopy experiments on  $A_x\text{Fe}_2\text{Se}_2$  ( $A = \text{K}, \text{Cs}$ ) showed that the Fermi surface nesting does not necessarily exist as previously suggested, and a conventional  $s$ -wave pairing could better describe these systems [9]. At the same time, evidence of  $d$ -wave type in iron pnictides has also been reported [10, 11]. The scenario is then contradictory, and to clarify this fundamental issue accurate investigation is required.

According to Anderson's theorem [12], a conventional  $s$ -wave superconductor is less sensitive to non-magnetic impurities (NMI), whereas for a  $d$ -wave superconductor or in the case of  $s^\pm$ -pairing, NMI may lead to severe pair breaking. Then this type of substitution is believed to play an important role in identifying the pairing symmetry. A few cases of Zn-doped Fe-based superconductors have been described. Guo *et al* [13] observed a large decrease of  $T_c$  by minimal Zn doping in an oxygen-deficient  $\text{LaFeAsO}_{0.85}$  compound. They also found a linear decrease of  $T_c$  with increasing doping in Zn-doped  $\text{BaFe}_{1.89}\text{Co}_{0.11}\text{As}_2$  [14]. In contrast, Li *et al* [15] found no effects with Zn doping and possibly an enhancement of  $T_c$  in the  $\text{LaFeAsO}_{0.9}\text{F}_{0.1}$ . The presence of Zn impurities also hardly affects superconductivity in the case of optimally hole-doped  $\text{Ba}_{0.5}\text{K}_{0.5}\text{Fe}_2\text{As}_2$  [16]. The contradictory experimental results point out the complex dependence of  $T_c$  on the presence of Zn impurities in different Fe-based superconductor systems. A systematic study by Li *et al* [17] in the  $\text{LaFeAsO}_{1-x}\text{F}_x$  system demonstrates the strong F-doping dependence of  $T_c$  on Zn impurities. They showed that  $T_c$  increases in the underdoped regime ( $x = 0.05$ ), while it remains constant at optimal doping ( $x = 0.10$ ) [17]. In addition, superconductivity is severely suppressed in the F-overdoped region ( $x = 0.15$ ) [17]. This influence of Zn impurity on Fe-based superconductors is complex and

different to that of cuprates with d-wave pairing, in which the Zn impurity can severely suppress the superconductivity [18].

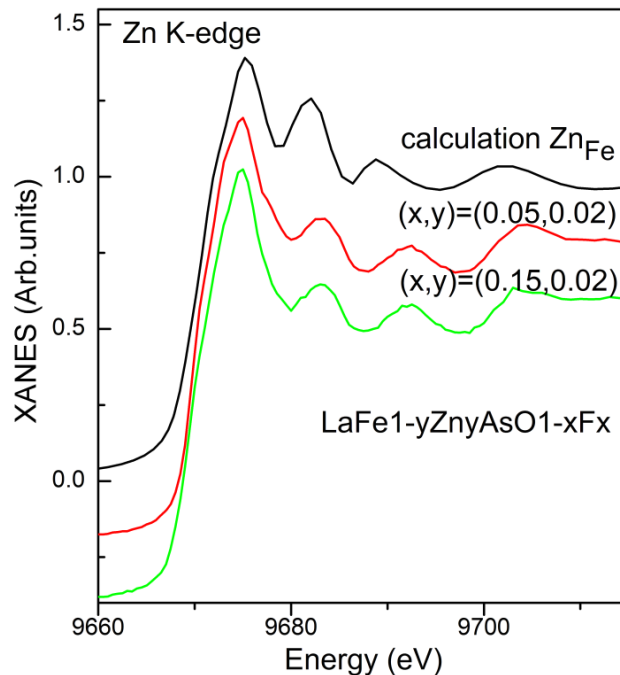
A few studies have focused on the effect of NMI on the microscopic lattice structure and electronic structure of complex codoped compounds. Recently, nuclear magnetic resonance and nuclear quadrupole resonance investigations in the Zn-substituted LaFeAsO<sub>0.85</sub> system showed that Zn impurities do not affect the crystal structure and electronic states [19]. Because the FeAs layer in Fe-based superconductors is considered to be a superconducting layer, detailed investigation of the characteristic properties of this layer may provide valuable information on the microscopic superconducting mechanism, and is fundamental for a better understanding of these systems [20, 21]. In this paper, we present a combined study using x-ray absorption spectroscopy and first-principles electronic structure calculations of NMI substitutions in iron pnictides. In the proposed scenario of a charge redistribution and possible local lattice distortions, the goal of this research is to identify cooperative mechanisms among F and Zn ions in the (F, Zn)-codoped LaFeAsO system.

## 2. Experiments and calculations

Polycrystalline compounds of LaFe<sub>1-y</sub>Zn<sub>y</sub>AsO<sub>1-x</sub>F<sub>x</sub> ( $x = 0.05, y = 0, 0.02; x = 0.15, y = 0, 0.02$ ) were synthesized by conventional solid-state reaction methods [17]. Samples were ground into fine powder and then brushed onto tapes. We collected both Fe and As K-edge extended x-ray absorption fine structure (EXAFS) spectra in the transmission mode at the U7C beamline of the National Synchrotron Radiation Laboratory (NSRL) in Hefei, China. The storage ring worked at the electron energy of 800 MeV with a maximum stored current of about 250 mA. Also, Zn K-edge x-ray absorption near edge spectroscopy (XANES) of LaFe<sub>1-y</sub>Zn<sub>y</sub>AsO<sub>1-x</sub>F<sub>x</sub> ( $x = 0.05, y = 0.02; x = 0.15, y = 0.02$ ) compounds was measured in the fluorescence mode using a four-element Si drift detector at the 14W1 station of the Shanghai Synchrotron Radiation Facility, running at an electron energy of 3.5 GeV with a maximum stored current of about 250 mA.

Zn K-edge XANES simulations were carried out in the framework of the multiple scattering (MS) theory [22, 23] using the FEFF code [24]. For the calculations, we used the tetragonal lattice parameters of the parent compound LaFeAsO in which the Fe atom is replaced by a Zn atom as the photoabsorber, and the Hedin–Lundqvist exchange-correlation potential [23, 25]. A cluster size of up to 59 atoms was considered for obtaining an accurate self-consistent field calculation, while a large cluster (127 atoms) was used for full MS calculations.

Electronic structure calculations were performed by using the density functional theory, as implemented in the Vienna *Ab Initio* Simulation Package (VASP) [26, 27]. The projector augmented wave was used to describe the electron–ion interaction and the exchange-correlation potential was described by the generalized gradient approximation in the form of the Perdew–Burke–Ernzerhof [28]. To model the doping condition in the LaFeAsO, we considered a  $2 \times 2 \times 2$  supercell in the tetragonal  $P4/nmm$  symmetry where we replaced one O in the cell with an F atom, while one Fe atom was replaced by Zn at random. These simulations correspond in the LaFe<sub>1-y</sub>Zn<sub>y</sub>AsO<sub>1-x</sub>F<sub>x</sub> system to the doping sets ( $x = 0.0625, y = 0$ ) and ( $x = y = 0.0625$ ). For the calculations we choose structural parameters obtained from x-ray diffraction (XRD) experimental data [17] of the doped samples: ( $x = 0.05, y = 0$ ) and ( $x = 0.05, y = 0.06$ ). To achieve convergence, an energy cutoff of 600 eV was chosen while the irreducible Brillouin zone was performed considering a  $6 \times 6 \times 4$  Monkhost–Pack  $k$ -points grid [29].



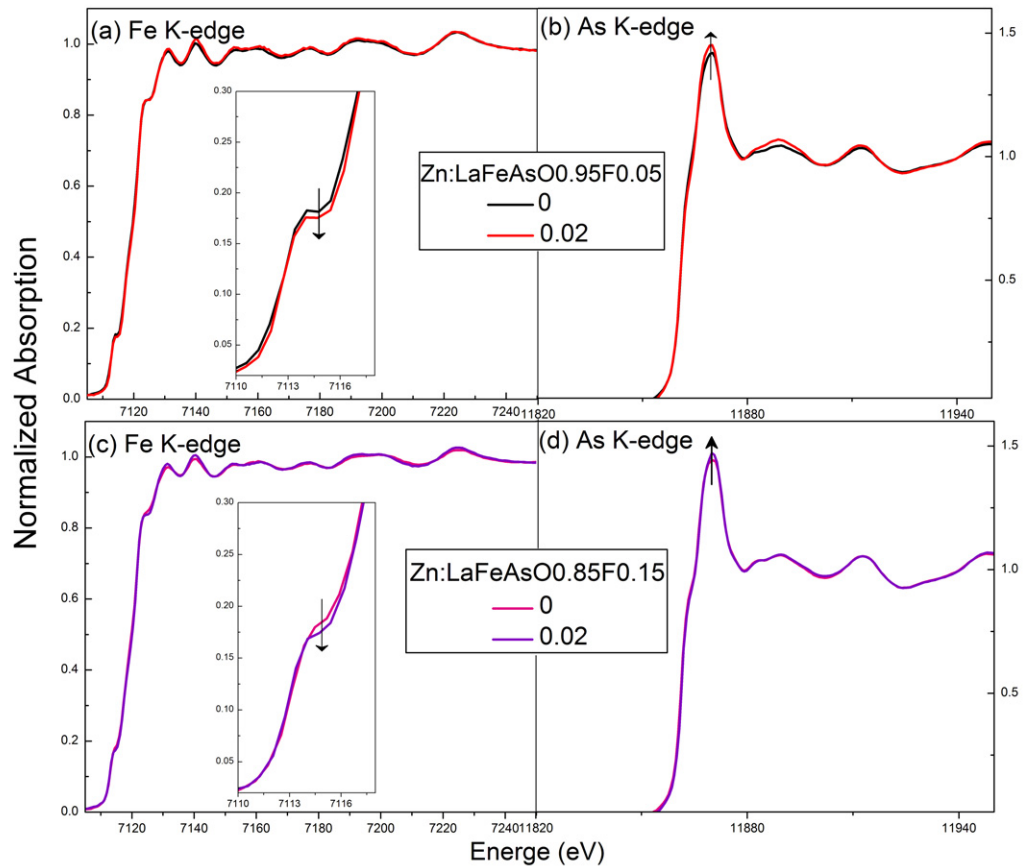
**Figure 1.** Comparison of the experimental Zn K-edge XANES spectra with a theoretical MS calculation where a Zn photoabsorber has replaced a Fe atom.

### 3. Results and discussions

Although it is well known that F atoms select an O site in  $\text{LaFeAsO}_{1-x}\text{F}_x$  [1], for doped compounds, in particular in the codoped system, the first issue is to identify the occupation site of the dopant. Here, we present XANES calculations at the Zn K-edge in  $\text{LaFe}_{1-y}\text{Zn}_y\text{AsO}_{1-x}\text{F}_x$  ( $x = 0.05, y = 0.02$ ;  $x = 0.15, y = 0.02$ ). A comparison of experimental Zn K-edge XANES spectra with theoretical simulations is shown in figure 1. Data support a scenario in which Zn ions are embedded in the  $\text{LaFeAsO}_{1-x}\text{F}_x$  matrix and Zn K-edge calculations with a Fe atom replaced by Zn successfully reproduce all XANES features, i.e. Zn occupies the Fe site.

Typical Fe and As K-edge XANES spectra of (F, Zn)-codoped  $\text{LaFeAsO}$  compounds are shown in figure 2. With respect to singly F-doped samples, XANES spectra of (F, Zn)-codoped compounds have the same energy position, a result compatible with the same chemical valence of Fe and As ions. With increasing Zn doping, the intensity of the pre-edge feature at the Fe-edge that probes the amount of the local and partial empty density of states decreases. The result points out an increase of occupation on Fe-d/As-p hybridized states just above the Fermi energy ( $E_F$ ). Effects on the electronic structure of this system induced by Zn doping are also evident at the main peak at the As K-edge. This transition involves 1s core-level electrons excited to 4p-like unoccupied orbital. In (F, Zn)-codoped samples, the main peak at the As K-edge is higher than that in F-doped compounds. Therefore, we observe a redistribution of the electron density between Fe and As atoms, i.e. a transfer of electrons from As-p orbital to Fe-d states.

To better understand Zn-doping effects on the electronic structure, we performed first-principles calculations using VASP. Figure 3 shows the  $2 \times 2 \times 2$  supercell of the  $\text{LaFeAsO}$  system where one O atom has been replaced by F, and the four possible sites occupied by a



**Figure 2.** Normalized Fe and As K-edge XANES spectra of  $\text{LaFe}_{1-y}\text{Zn}_y\text{AsO}_{1-x}\text{F}_x$  ( $x = 0.05, y = 0, 0.02$ ;  $x = 0.15, y = 0, 0.02$ ) samples. The arrows in (a) and (c) show the excitation of  $1s$  core-level electrons to the Fe-d/As-p hybridized orbital in tetrahedral symmetry (see the magnified view in the inset); the arrows in (b) and (d) indicate the increasing intensity of the main peak at the As K-edge XANES.

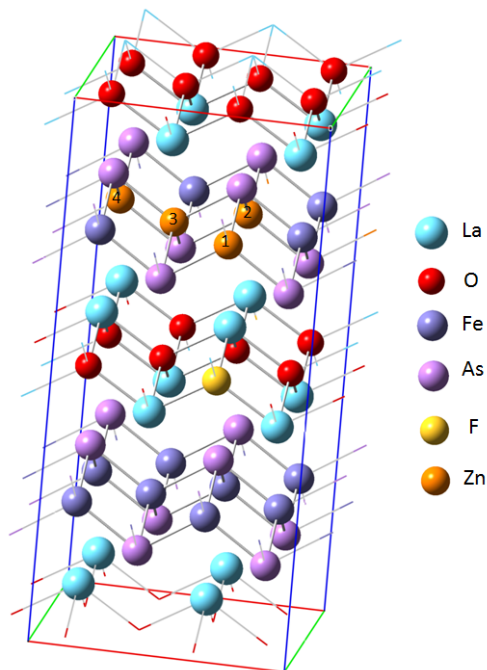
Zn impurity correspond to those of the F-underdoped system. Two or more O atoms have to be replaced and many more possible sites have to be considered for Zn doping in the case of the F-overdoped system. This much more complex geometry will not be discussed here.

In order to evaluate the relative stability of the different Zn sites, we compare their total energies in table 1. Differences between the four sites are negligible, indicating a unique, almost stable structure. However, in (F, Zn)-codoped compounds, four extra electrons injected by the Zn ion are present in the system. In comparison with a singly F-doped sample, extra electrons are localized around Zn impurity sites [30]. To clarify the effective charge transfer between Fe and As atoms observed in the XANES spectra, we present here a charge analysis based on the Bader scheme [31]. Table 1 summarizes both the total number of electrons and the charges of both Fe and As atomic species for F-doped and (F, Zn)-codoped compounds. We find that  $\sim 0.02$  electron is transferred from As to Fe via Zn doping, a value consistent with experimental XANES data.

As revealed by the XANES analysis and by electronic structure calculations, a non-negligible charge transfer occurs both in F-underdoped and -overdoped regimes. However, the

**Table 1.** Total energies calculated for different Zn locations and charges belonging to Fe and As atomic species, as obtained by Bader analysis.

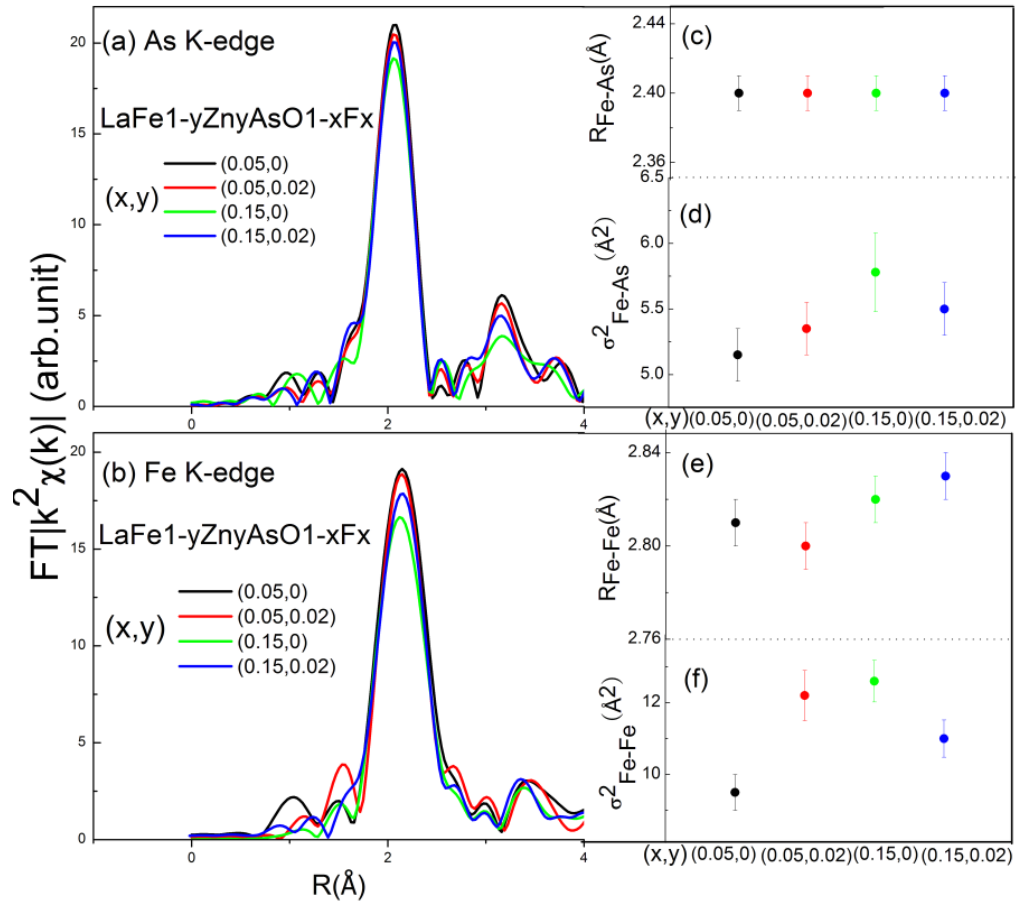
	F-doped	F, Zn1-codoped	F, Zn2-codoped	F, Zn3-codoped	F, Zn4-codoped
Total energy (eV)	−481.195	−472.366	−472.371	−472.370	−472.373
Total electrons	481	485	485	485	485
<i>Charge</i>					
Fe	7.8182	7.8399	7.8401	7.8400	7.8396
As	5.8402	5.8195	5.8196	5.8195	5.8198

**Figure 3.** The  $2 \times 2 \times 2$  supercell used in VASP calculations for the (F, Zn)-codoped LaFeAsO system. Adding one F atom to the supercell, we have four possible locations for the Zn ion marked from 1 to 4.

$T_c$  response to Zn doping is significantly different in the two regimes [17]. To understand fully the underlying mechanism, we look at the local lattice structure, which is much more sensitive to impurities.

Figure 4 shows Fe and As K-edge Fourier transforms (FT) of EXAFS signals of  $\text{LaFe}_{1-y}\text{Zn}_y\text{AsO}_{1-x}\text{F}_x$  samples as well as their fits. In the EXAFS analysis, we isolated the first peak of the FT using a rectangular window at the As K-edge and at the Fe K-edge in the ranges 1.4–2.5 and 1.6–3.0 Å, respectively. For the As K-edge, we considered the nearest Fe–As pair, while at the Fe K-edge we fit experimental data including both the nearest Fe–As and the next-nearest Fe–Fe correlations. Due to the low doping level of Zn, contributions of Zn–As and Zn–Fe shells have been neglected in the fit. The results shown in figure 4 indicate that the Fe–As pair is unaffected or rigid by F and Zn doping, while the bond distance of the Fe–Fe pair changes. Moreover, doping also affects the behavior of the Debye–Waller factor  $\sigma^2$



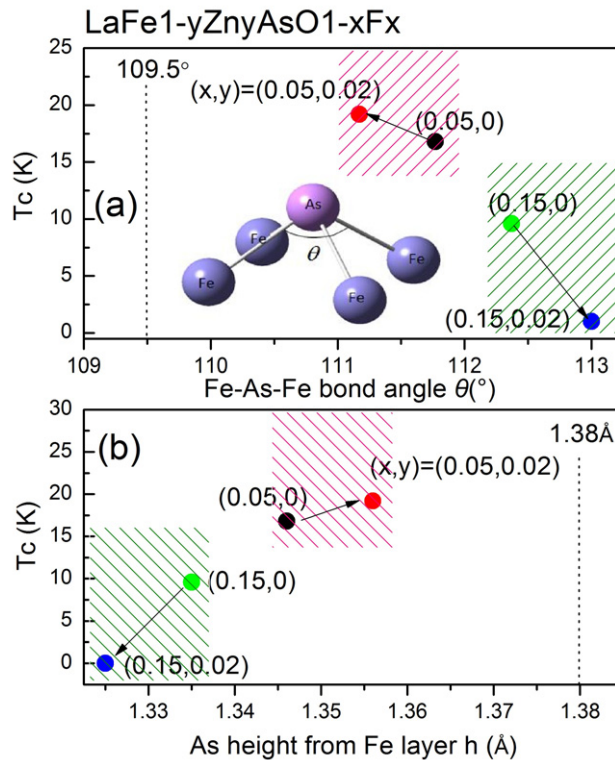


**Figure 4.** FTs of the  $k^2\chi(k)$  EXAFS signals of  $\text{LaFe}_{1-y}\text{Zn}_y\text{AsO}_{1-x}\text{F}_x$  ( $x = 0.05$ ,  $y = 0, 0.02$ ;  $x = 0.15$ ,  $y = 0, 0.02$ ) compounds at the As (a) and Fe K-edge (b). Results of the fit of the Fe–As/Fe–Fe bond distances and mean-square relative displacements are shown in panels (c)–(f). Error bars correlating with the uncertainty value associated with the EXAFS analysis are given.

that probes the mean-square relative displacement of the photoabsorber–backscatterer pairs. In the F-underdoped region, i.e.  $x = 0.05$ , both  $\sigma_{\text{Fe–As}}^2$  and  $\sigma_{\text{Fe–Fe}}^2$  increase versus Zn doping, while with Zn doping they decrease for  $x = 0.15$ . In a previous report on the K-doped  $\text{BaFe}_2\text{As}_2$  system, it was shown that an increased disorder in the iron layer due to the softening of the Fe–Fe bond partly or fully suppressed the structural phase transition and the spin-density-wave (SDW) observed in the parent  $\text{BaFe}_2\text{As}_2$  compound inducing a superconducting behavior [21]. In a similar way, the increase of the  $\sigma_{\text{Fe–Fe}}^2$  by Zn doping in the F-underdoped  $\text{LaFeAsO}$  system may be partly associated with suppression of the structural transition or of the SDW, so that better superconductivity may occur. In these Fe-based and codoped superconductors data are consistent with a model in which dopants control the disorder of the system playing a role in the increase of  $T_c$ .

Several investigations have already established a correlation between the superconducting behavior of Fe-based superconductors and the geometry of  $\text{FeAs}_4$  tetrahedra and anion distance from the Fe layer [32–34]. Data showed that  $T_c$  increases as the  $\text{FeAs}_4$  coordination approaches





**Figure 5.** The Fe–As–Fe bond angle (a) and the height of the As from the Fe layer (b) in the  $\text{LaFe}_{1-y}\text{Zn}_y\text{AsO}_{1-x}\text{F}_x$  as a function of both F and Zn concentrations.

a regular tetrahedron [32], a condition that can be monitored looking at the Fe–As–Fe bond angle. Moreover, for a typical Fe-based superconductor,  $1.38 \text{ \AA}$  is the optimal anion height to achieve the highest  $T_c$  [33]. Starting from these two assumptions we may evaluate in the  $\text{LaFe}_{1-y}\text{Zn}_y\text{AsO}_{1-x}\text{F}_x$  system the relationship between the (F, Zn)-doping level and the layer structure versus the superconducting properties. In this paper, using the bond lengths obtained by EXAFS analysis, we plot the Fe–As–Fe bond angle and the height between the As and the Fe layer as a function of both F and Zn concentrations. As shown in figure 5(a) in the F-underdoped region ( $x = 0.05$ ), the Zn doping induces structural changes driving the Fe–As–Fe bond angle towards the value of a perfect tetrahedron ( $109.5^\circ$ ). In contrast, in the F-overdoped regime ( $x = 0.15$ ), 2% of Zn impurity is sufficient to induce a deviation of the Fe–As–Fe bond angle from the value of a perfect tetrahedron and superconductivity is dramatically suppressed. Therefore, the opposite behavior of the Fe–As–Fe bond angle going from the F-underdoped to the overdoped regions in the presence of a Zn impurity can be correlated to the observed changes of  $T_c$  versus Zn doping. The behavior of the distance between the As ion and the Fe layer shown in figure 5(b) presents the same trend. At  $x = 0.05$  the Zn doping can be associated with an As height near the optimal value of  $1.38 \text{ \AA}$ , while in the F-overdoped ( $x = 0.15$ ) region, the Zn doping gradually reduces the distance of the As from the Fe layer.

Summarizing, in the (F, Zn)-codoped  $\text{LaFeAsO}$  system the cooperative contribution of F and Zn impurities fine-tune the local structure, e.g. modify both the Fe–As–Fe bond angles and the height of As from the Fe layer. In the F-underdoped region, Zn doping leads to a more symmetric  $\text{FeAs}_4$  coordination, while  $T_c$  increases accordingly. In contrast, the  $\text{FeAs}_4$

tetrahedron is distorted by Zn doping and a severe suppression of the superconductivity in the F-overdoped regime is observed. Similarly, the Zn doping in the cuprate compound  $\text{GdBa}_2\text{Cu}_3\text{O}_{7-\delta}$  could markedly influence the crystal structure distortion and therefore suppress the superconductivity [18].

#### 4. Summary

We have studied Zn-doping effects on the electronic structure and local lattice structure of the  $\text{LaFe}_{1-y}\text{Zn}_y\text{AsO}_{1-x}\text{F}_x$  system. Due to the presence of a Zn impurity, a charge redistribution, i.e. a charge transfer from As to Fe atoms, is evident from both Fe and As K-edge XANES spectra, and is clearly supported by first-principle calculations. As shown by the EXAFS analysis, the concurrent contribution of F and Zn dopants in the local lattice deformations should be responsible for the opposite behavior of  $T_c$  versus Zn impurity between F-underdoped and F-overdoped regions. The Zn doping leads to more symmetric  $\text{FeAs}_4$  tetrahedra in the F-underdoped region ( $x = 0.05$ ), different from the behavior of the F-overdoped region, in which the increasingly distorted  $\text{FeAs}_4$  tetrahedra induce the superconductivity to disappear. Therefore the crystal structure, especially the regularity of  $\text{FeAs}_4$  tetrahedra, is the most essential factor for determining the superconductivity of Fe-based superconductors, similar to the cuprate compound of Zn-doped  $\text{GdBa}_2\text{Cu}_3\text{O}_{7-\delta}$ . This structural deformation can determine the band filling and Fermi-surface nesting, and the spin fluctuation driven by the nesting plays an important role in Fe-based superconductors; therefore our new findings on the local structural deformation may provide interesting insights into the role of impurities in Fe-based superconductors.

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