



DFT study of electronic structure properties of SrAFe₄As₄ (A = Rb and Cs) superconductors

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ABSTRACT

Using the full-potential linearised augmented plane wave method and the PBE generalized gradient approximation, the electronic structure properties of SrAFe₄As₄ (A = Rb and Cs) superconductors were determined and compared with those of their parents SrFe₂As₂ (*Fmmm*), SrFe₂As₂ (*I4/mmm*), RbFe₂As₂ and CsFe₂As₂. It is found that associated with the Van Hove singularities, densities of states of SrAFe₄As₄ around Fermi energy level, mostly caused by Fe-3d orbitals, are relatively high but not enough to account for enhancement of T_c in these materials. We suggest rather a relationship between T_c values and interband scattering strength, which depends on the number of electronic bands crossing E_F and forming hole-like pockets around the Γ point and electron-like pockets at the corners of Brillouin zone. It is established that Fermi surfaces of SrAFe₄As₄ are described by 2D and manifest the behaviour of $\pm s$ -wave gap in Cs- and nodal gap in Rb-based. Electron Localization Function demonstrates the presence of both valence and metallic bondings. However, there is a stronger covalent bonding in AFe₂As₂ than in SrAFe₄As₄, suggesting that the weakness of covalency accompanies higher T_c values.

1. Introduction

One of the most significant breakthroughs in the fields of superconductivity took place in 1986 when Bednorz and Müller discovered superconductivity at $T_c = 30$ K in the La-Ba-Cu-O system [1]. This event has triggered a widespread and intensive research work aimed at searching for higher values of T_c and physical mechanism underlying the superconductivity. As a tremendous result, many high- T_c superconductors both stranded on Cu-oxides with T_c up to 164 K [2] and other e.g., MgB₂ [3] or Fe-based [4] were reported. At the same time, various rival theories for high- T_c superconductivity have been postulated and of course they need experimental endorsement for their validity [5]. In general, there are three representative models for high- T_c unconventional superconductivity. In the first model, the explanation is based on the BCS theory [6,7], which deals with the pairing of fermion quasi-particles at the same temperature as onset of superconductivity. Accordingly, the critical temperature T_c in the layered structure BCS-type superconductors can be enhanced by the interlayer coupling [8] or by the inter-band interactions between nested Fermi-surface sheets [9]. The second one is leaned on an assumption that the superconductivity has an origin of interactions from high-temperature regime, e.g., the condensation of boson pairs sets in already at T^* above T_c [10–12] or incoherent electronic correlations in the normal state enhance a

conventional pairing [13]. Finally, several scenarios which could belong to the third model are these ascribing an intimate relationship of superconductivity to exotic phenomena; There are, i.a., resonating valence bonding [14], spin-fluctuation [15] spin and/or charge (SDW/CDW) instabilities [16–19], and so on. Clearly, a unified model of the superconducting mechanism for different high- T_c -materials was still lacking. Therefore, understanding of electronic properties of new superconductors is essential and highly desired for investigating the fundamental superconductivity.

The discovery of superconductivity in the Fe-based materials, especially, in so-called “122” FeAs-based superconductors, was surprising and exciting, not because of exhibiting many similarities (also differences) to high- T_c cuprate superconductors of tetragonal structure, but also owing to tunable superconducting properties by doping [20–23], applying pressure [24–26] or magnetic field [27,28]. Basically, all FeAs-based superconductors possess a common layered structure consisting of a planar layer of iron atoms joined by tetrahedrally coordinated As anions arranged in a stacked sequence separated by blocking layers of alkali, alkaline earth or rare earth. In such arrangement of atoms, quasi-2D transport properties are anticipated, although the superconductivity may depend on the blocking layers, giving a rise to the electron-phonon interaction.

The presence of magnetism in FeAs-based materials is an important

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Table 1

Crystallographic parameters of studied compounds from literature: SrRbFe₄As₄ [39], SrCsFe₄As₄ [39], SrFe₂As₂ [20] SrFe₂As₂ [42], RbFe₂As₂ [43] and CsFe₂As₂ [42].

Compound	SrRbFe ₄ As ₄	SrCsFe ₄ As ₄	SrFe ₂ As ₂	SrFe ₂ As ₂	RbFe ₂ As ₂	CsFe ₂ As ₂
Space group	<i>P4/mmm</i>	<i>P4/mmm</i>	<i>Fmmm</i>	<i>I4/mmm</i>	<i>I4/mmm</i>	<i>I4/mmm</i>
a (nm)	0.38971	0.39101	0.5783	0.39259	0.37818	0.38894
b (nm)	0.38971	0.39101	0.55175	0.39259	0.37818	0.38894
c (nm)	1.34175	1.37293	1.22965	1.23750	1.45254	1.50665
At. positions	$z_{Fe} = 0.2246$, $z_{As1} = 0.3336$, $z_{As2} = 0.1193$	$z_{Fe} = 0.2246$, $z_{As1} = 0.3336$, $z_{As2} = 0.1193$	$z_{As} = 0.3612$	$z_{As} = 0.36$	$z_{As} = 0.3401$	$z_{As} = 0.342$

Table 2

Crystallographic data of the studied compounds after the optimization of geometrical parameters.

Compound	SrRbFe ₄ As ₄	SrCsFe ₄ As ₄	SrFe ₂ As ₂	SrFe ₂ As ₂	RbFe ₂ As ₂	CsFe ₂ As ₂
Space group	<i>P4/mmm</i>	<i>P4/mmm</i>	<i>Fmmm</i>	<i>I4/mmm</i>	<i>I4/mmm</i>	<i>I4/mmm</i>
a (nm)	0.36869	0.38717	0.55750	0.38336	0.36277	0.38894
b (nm)	0.36869	0.38717	0.55149	0.38336	0.36277	0.38894
c (nm)	1.31889	1.37157	1.22947	1.16480	1.45247	1.50108
At. positions	$z_{Fe} = 0.2307$, $z_{As1} = 0.3316$, $z_{As2} = 0.1328$	$z_{Fe} = 0.24251$, $z_{As1} = 0.344897$, $z_{As2} = 0.13293$	$z_{As} = 0.3491$	$z_{As} = 0.3551$	$z_{As} = 0.3403$	$z_{As} = 0.3430$

Table 3

Muffin-tin radii values of atoms in the 122 and 1144 compounds.

	R_{Sr} (a.u.)	R_{Rb} (a.u.)	R_{Cs} (a.u.)	R_{Fe} (a.u.)	R_{As} (a.u.)
SrRbFe ₄ As ₄	2.600	2.600		2.10175	2.10175
SrCsFe ₄ As ₄	2.600		2.800	2.2347	2.2347
SrFe ₂ As ₂ (<i>Fmmm</i>)	2.600			2.234	2.234
SrFe ₂ As ₂ (<i>I4/mmm</i>)	2.600			2.124	2.124
RbFe ₂ As ₂		2.600		2.231	2.231
CsFe ₂ As ₂			2.800	2.231	2.231

issue, because over a long-time period, it was commonly assumed that magnetism cannot coexist with conventional superconductivity. Nowadays the magnetism from 3d electrons is believed to be the integral element of superconductivity in FeAs-based materials [29]. It is remarkable that the magnetic phase transition is always associated with the tetragonal-orthorhombic distortion [30–32], and furthermore this structural transition has been ascribed due to an orbital ordering [33] or antiferromagnetic fluctuation [34].

Among the “122” FeAs-based superconductors, RbFe₂As₂ and CsFe₂As₂ are superconductors with a low T_c value ~ 2 K [35–38]. On the other hand, non-superconducting orthorhombic SrFe₂As₂ at ambient pressure becomes superconducting under hydrostatic pressures, with maximum $T_c \sim 27$ K around 3 GPa [26]. It is worthwhile to recall that a high pressure recovers the tetragonal ThCr₂Si₂ type structure for SrFe₂As₂. Based on what has been considered, it is very tempting to conclude that both the layer-type structure and Fe-magnetism are essential factors to high- T_c superconductivity.

Recently, Iyo et al. discovered superconductivity in tetragonal SrAFe₄As₄ (A = Rb, Cs) (hereafter denoted as 1144) materials with relatively high T_c (~ 35 K in SrRbFe₄As₄ and ~ 37 K in SrCsFe₄As₄) [39]. The compounds crystallize also in layer-type structure with the characteristic Fe₂As₂ building layers. The Sr and A atoms are alternately inserted between these layers, so the space group has been changed from *I4/mmm* to *P4/mmm*, as compared to that of the parent 122 compounds. From this perspective of electron-hole count, stoichiometric SrRbFe₄As₄ and SrCsFe₄As₄ may be viewed as hole-doped SrFe₂As₂, but without tetragonal-orthorhombic distortion. In contrast to SrFe₂As₂, the high- T_c superconductivity realizing in the 1144 materials does not require hydrostatic pressure.

In this work, we further characterize the superconductivity in SrAFe₄As₄ reporting the DFT calculations using the Full-Potential

Linearized Augmented Plane Wave (FP-LAPW) method implemented in ELK code [40]. The aim of the present work was not only investigate the ground state electronic structure (GSES) properties, including densities of states (DOS), electronic band structures (EBS), Fermi surfaces (FS), Electron Localization Function (ELF) of SrAFe₄As₄ (A = Rb, Cs) superconductors, but also compare the obtained data with those of their parents SrFe₂As₂, RbFe₂As₂ and CsFe₂As₂. Eventual differences in GSES properties between the 112 and 1144 compounds would give rise to a better understanding why the T_c in the 1144 materials can attain high values. To the best of our knowledge, this work is the first *ab initio* calculation of the GSES properties accomplished on this newly discovered superconductors. Nonetheless, a similar research has been carried out by Suetin and Shein on closely-related CaFe₄As₂ (A = K, Rb and Cs) superconductors [41].

2. Computational details

We started DFT calculations with the crystal structure parameters available in the literature [20,39,42]. The lattice parameters and atomic positions of the studied compounds before and after structure optimization are listed respectively in Tables 1 and 2. A comparison of two sets of crystallographic data reveals a volume reduction after structural optimization less than 2%, suggesting that the change in electronic band structures due to this volume decrease is insignificant. For this reason, we performed GSES properties based on experimental crystallographic parameters.

The GSES properties of the 122 and 1144 materials were performed using the Full-Potential Linearized Augmented Plane Wave (FP-LAPW) method implemented in ELK code [40]. In our calculations, spin-orbit coupling and the Generalised Gradient Approximation (GGA-PBE) functional [44] for the exchange-correlation energy were applied. Currently, exchange-correlation functionals based on GGA-PBE or Local Density Approximation (LDA) [45] are the most popular used ones in condensed matter physics. Though, the LDA has long been the standard choice of the exchange-correlation functional [46], but some time this leads to an overestimating the electron correlation energies [47]. On the other hand, the GGA depending on both the local density and spatial variation of the density, generally provides improved bond angles, lengths, and valence-valence exchange energies [48,49]. Therefore, GGA allows to perform DFT calculations better than LSD for bulk solids, and the usage of GGA in our calculations was preferred.

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