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Electronic structure of novel multiple-band superconductor $SrPt_2As_2$

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We present LDA calculated electronic structure of recently discovered superconductor $SrPt_2As_2$ with T_c=5.2K. Despite its chemical composition and crystal structure are somehow similar to FeAs-based high-temperature superconductors, the electronic structure of $SrPt_2As_2$ is very much different. Crystal structure is orthorhombic (or tetragonal if idealized) and has layered nature with alternating $PtAs_4$ and $AsPt_4$ tetrahedra slabs sandwiched with Sr ions. The Fermi level is crossed by Pt-5d states with rather strong admixture of As-4p states. Fermi surface of $SrPt_2As_2$ is essentially three dimensional, with complicated sheets corresponding to multiple bands. We compare $SrPt_2As_2$ with 1111 and 122 representatives of FeAs-class of superconductors, as well as with isovalent $(Ba,Sr)Ni_2As_2$ superconductors. Brief discussion of superconductivity in $SrPt_2As_2$ is also presented.

In 2008 new class of FeAs based high-temperature superconductors was discovered [1]. Reviews of most of pioneering papers were presented in Refs. [2, 3]. Lots of experimental and theoretical investigations were published since then and the search for new promising compounds is continuing. Recent report on coexistence of superconductivity ($T_c = 5.2\,\mathrm{K}$) and CDW by Kudo et al. [4] in the new arsenide compound $SrPt_2As_2$ motivated us to compare its electronic structure with that of different representatives of FeAs class of superconductors investigated by us earlier [5 – 9]. We shall see that despite expectations expressed in Ref. [4] this system cannot be considered an analogue of Fe pnictides, though by itself presents an interesting case of a new multiple band superconductor with very complicated electronic structure close to the Fermi level.

As reported in Ref. [10] $SrPt_2As_2$ has orthorhombic structure with the space group *Pmmn*. To some extent it reminds $CaBe_2Ge_2$ type tetragonal crystal structure with the space group $P4/nmm$. The later one is presented in Fig.1. There are two layers of $PtAs_4$ and $AsPt_4$ tetrahedra in the elementary cell (shown in Fig.1). In one layer square lattice of Pt ions is coordinated with As tetrahedra and vice versa in the next layer. Corresponding tetrahedra are connected with lines in Fig.1. The most similar 122 polymorhic form to $SrPt_2As_2$ is $BaFe_2As_2$ pnictide [11] where two mirrored $FeAs_4$ tetrahedra layers are contained in the elementary cell [6]. Other pnictide systems belong mainly to the space group $P4/nmm$ [9].

In present work we neglect for simplicity of comparison to other pnictides small atomic position modulations in the $PtAs_4$ layer of $SrPt_2As_2$ leading to the *Pmmn* structure detected in Ref. [10]. Thus we transform the real *Pmmn* structure to an idealized $P4/nmm$ as described below. To obtain the tetrahedral a lattice parameter we have taken the average of a=4.482Å and b=4.525Å parameters of orthorhombic structure, while c=9.869Å parameter was taken the same as in the experimentally observed structure. Wyckoff Positions of ions were changed from *Pmmn* to $P4/nmm$ like this: Sr 2a(1/4,1/4,0.7469)→2c(1/4,1/4,0.7469); for $PtAs_4$ layer Pt1 4e(1/4,0.8163,0.9989)→2a(1/4,3/4,0) and As2 4e(1/4,0.294,0.1263)→2c(1/4,1/4,0.1263); for $AsPt_4$ layer Pt2 2a(1/4,1/4,0.3817)→2c(1/4,1/4,0.3817) and As1 2b(1/4,3/4,0.4997)→2b(1/4,3/4,1/2). Thus we do not account for alternating half filled 4e positions of Pt1 and As2 and slightly change appropriate coordinates for the atoms.

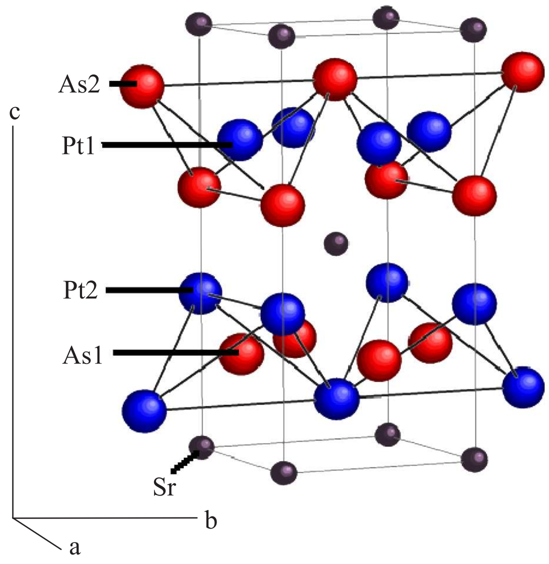

Fig.1. Idealized tetragonal crystal structure of $SrPt_2As_2$

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Using this idealized $SrPt_2As_2$ tetragonal crystal structure we performed electronic structure calculations within the linearized muffin-tin orbitals method (LMTO) [12] with default settings.

In Fig.2 we present band dispersions obtained within LDA calculations for $SrPt_2As_2$ plotted along high-symmetry Brillouin zone directions. Upper panel shows total overview of bands on a large energy scale. Lower panel highlights those bands crossing the Fermi level within the k_z=0 plane and in a narrow energy interval relevant to superconductivity. Letters marking bands on lower panel of Fig.2 correspond to LDA Fermi surface (FS) sheets plotted in Fig.3 and described below.

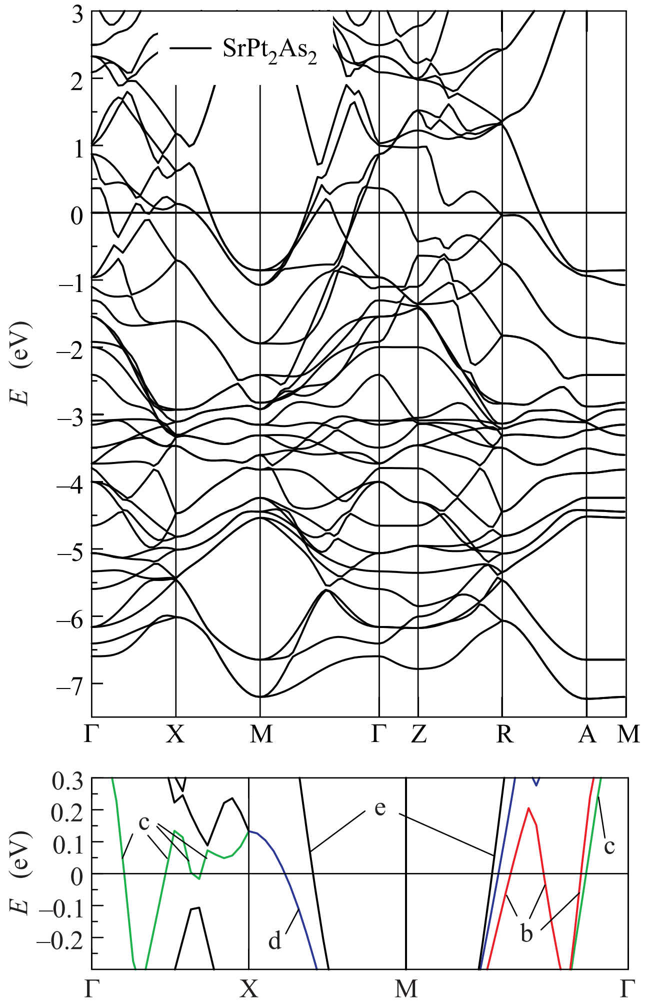

Fig.2. LDA calculated band dispersions of $SrPt_2As_2$: upper panel – total overview; lower panel – bands in the k_z=0 plane in a narrow energy interval around the Fermi level. On lower panel letters correspond to Fermi surface sheets shown in Fig.3. The Fermi level is at zero energy

One should note that $SrPt_2As_2$ bands in general share some common features with e.g 1111 FeAs systems [5, 8], for example around M-point. But basically in the vicinity of the Fermi level bands are completely different from 1111 and 122 systems. However, the multiple band nature of electronic spectrum close to the Fermi level is obvious. There are four band crossings of the Fermi level between Γ and M-points and up to six bands at the Fermi level in M-Γ direction.

Fig.4 displays LDA densities of states (DOS) of $SrPt_2As_2$. Upper panel shows total DOS (solid line). Since there are two layers of tetrahedra as discussed above we present DOSes for $PtAs_4$ layer as solid lines (Pt1 – triangles, As2 – crosses) and for $AsPt_4$ layer as dashed ones (Pt2 – squares, As1 – pluses). Contribution of Pt1-5d states forming square lattice on the Fermi level is almost twice larger than of the other states. However, Pt2 and both As1,As2 also give considerable contribution to the DOS on E_F. This distinguishes $SrPt_2As_2$ system from Fe pnictides where As states almost do not appear at the Fermi level [5, 8]. Most of Pt-5d states are situated much further down from the Fermi level in contrast to the pnictides. This can be attributed to the fact that Pt has more d-electrons than Fe. Also Pt-5d states are obviously more extended with larger bandwidth than that of Fe-4d.

Lower panel of Fig.4 shows orbital resolved DOSes for Pt1 and Pt2 5d states. Pt1 belongs to $PtAs_4$ tetrahedron layer and Pt2 to $AsPt_4$ one. Because of tetragonal symmetry we still can use cubic notations for the 5d orbitals. For both Pt ions largest contribution on the Fermi level comes from $x^2 - y^2$ orbital (solid line), while other orbitals give smaller contribution. Situation here differs from that in pnictides [6, 7], where all of t_{2g} orbitals contribute to DOS at the Fermi level. Here as mentioned above most of Pt-5d states lie below the Fermi level.

Finally in Fig.3 we present LDA Fermi surfaces. In Fig.3a we show all FS sheets in the first Brillouin zone. In Figs.3b–3e we present different FS sheets separately. Letters (b, c, d, e) denoting Fermi sheets correspond to bands marked with the same letters as on lower panel of Fig.2. One can see that in total there are six FS sheets. Most of them except Fig.3e are essentially three dimensional. This fact also makes $SrPt_2As_2$ different from 1111 or 122 pnictides. Crossection of the FS at k_z=0 is shown in Fig.3f with the same letters coding. Here we also see much more complicated multiple FS sheets picture in contrast to Fe pnictides.

Thus we have in $SrPt_2As_2$ the multiple band structure with rather complicated multiple sheet FS topology, which is quite different from that of Fe pnictides. In general, the multiple band system may be also very complicated from the point of view of possible types of Cooper pairing, with different energy gaps on differ-

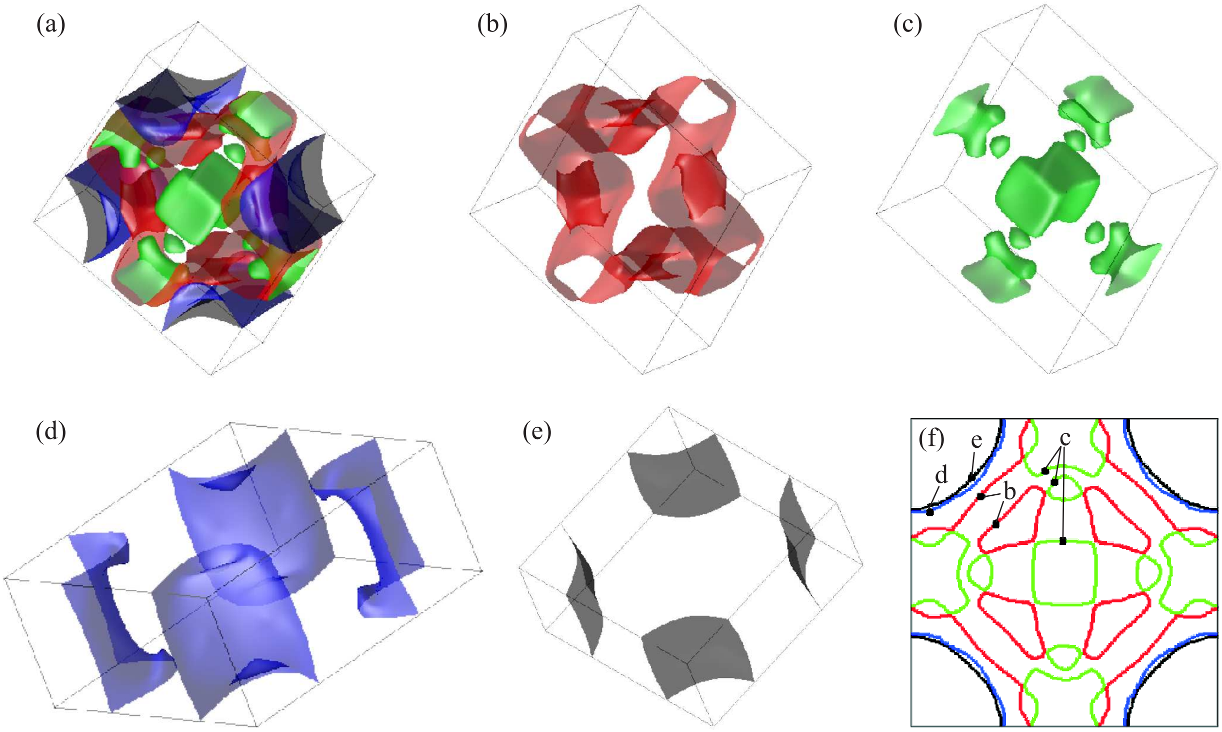

Fig.3. LDA calculated FS for $SrPt_2As_2$. (a) – all FS sheets together; (b), (c), (d), (e) – separate view of each of four FS sheets. Among these (b) is electron-like, (c) is hole-like and (d) and (e) are electron-like. (f) – crossection of FS at k_z=0 with color coding corresponding to Fermi sheets (b), (c), (d) and (e)

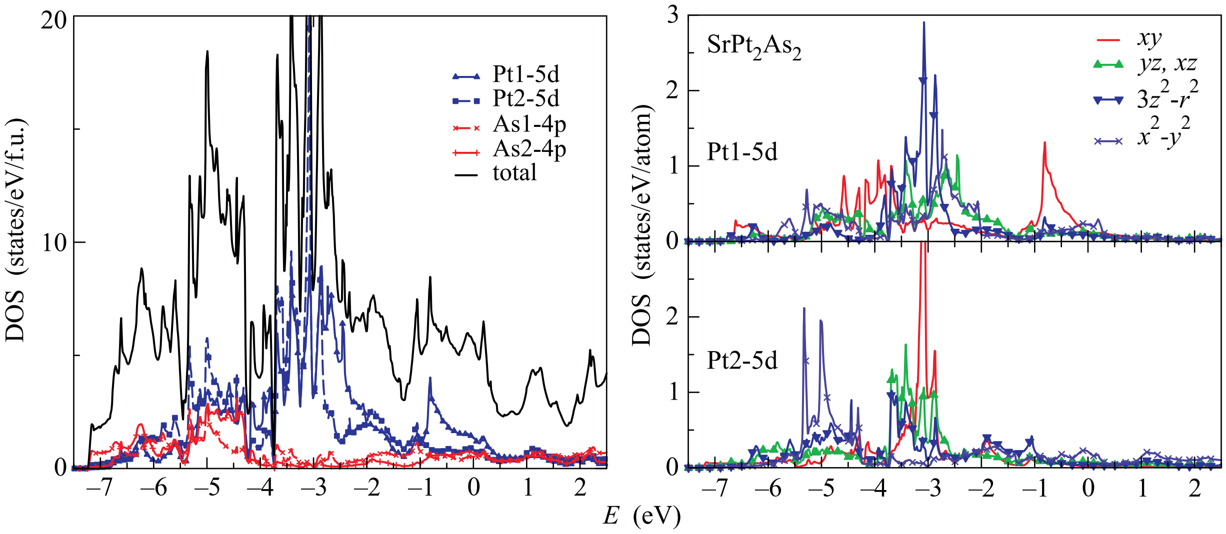

Fig.4. Upper panel: Densities of states from LDA calculations for $SrPt_2As_2$. Solid line – total DOS; solid line with triangles – Pt1-5*d* DOS; dashed line with squares – Pt2-5*d* DOS; solid line with crosses – As1-4*p* DOS; dashed line with pluses As2-4*p* DOS. Lower panel: DOSes for different orbitals of Pt1 and Pt2 5*d* shells. The Fermi level energy is zero

ent FS sheets, like in FeAs systems [13, 14]. From the general symmetry analysis [15, 16] it is known that in case of tetragonal symmetry and in spin – singlet case we can in principle observe either the usual isotropic or anisotropic *s* – wave pairing or several types of *d* – wave pairing. Nothing can be concluded from symmetry considerations alone on the possibility of $s^{\pm}$ pairing, with e.g. isotropic gap on different FS sheets changing sign between different sheets, as it is most probably is in the case of Fe pnictides [2, 14].

As to the value of T_c and gap ratios on different FS sheets in the multiple band system these are actually defined by rather complicated interplay of intraband and interband couplings in Cooper channel, partly determined by relations between partial DOS'es at these FS sheets [13, 14]. However, we can make some simple estimates based on elementary BCS approach. Consider the value of total DOS at the Fermi level $N(E_F)$ which is 5.6 states/eV/cell in our calculations. If we calculate corresponding T-linear coefficient of the specific heat we obtain γ=13.1 mJ/mol/K^2, which agrees rather well with experimental value of 9.7 mJ/mol/K^2 [4]. Then one can immediately estimate the dimensionless pairing coupling constant λ value using the BCS expression $T_c = 1.14\omega_D e^{-1/\lambda}$, with Debye frequency ω_D, corresponding to the experiment. If we chose ω_D=200K and T_c=5.2 K in agreement with Ref. [4] for $SrPt_2As_2$ we get λ=0.26. Now we can can estimate T_c values for isovalent systems $BaNi_2As_2$[17] and $SrNi_2As_2$[18] which are also found to be superconductors, but with much lower experimental superconducting temperatures of 0.7K[17] and 0.62K[18]. To do so we performed LDA calculations for BaNi and SrNi systems to get appropriate values of N(E_F) for these systems. Actually, our results agree well with the previous LDA calculations of Refs. [19, 20]. We got N(E_F)=3.86 states/eV/cell for BaNi and N(E_F)=2.81 states/eV/cell for SrNi system. As BCS coupling is always proportional to N(E_F) and assuming the same value of dimensional coupling in all these systems, we directly obtain $\lambda_{\rm BaNi}$=0.18, $\lambda_{\rm SrNi}$=0.13 with corresponding T_c values of 0.97 K and 0.13 K in rather good agreement with experiment. Thus, similar to our work on pnictides [9] we see that the values of T_c are well correlated with the total DOS value at the Fermi level $N(E_F)$.

In conclusion, our results show that the novel superconductor $SrPt_2As_2$ is essentially a multiple-band system. Despite its crystal structure similarity to that of 122 pnictides, its electronic structure is quite different – more bands cross the Fermi level, Pt-5d states lie at lower energies than Fe-3d bands and mostly Pt1-5d x^2-y^2 orbital comes to the Fermi level instead of all t_{2g} orbitals, contribution of As-4p states at the Fermi level is much stronger. Fermi surface has much more complicated multiple sheet topology and is definitely three dimensional, which can lead to rather complicated picture of Cooper pairing. Finally we note that rather non monotonous behaviof the DOS near the Fermi level (cf. Fig.4) suggest the possibility of significant changes of T_c due to doping.

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