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Electronic structure of new multiple band Pt-pnictide superconductors APt_3P

I. A. Nekrasov[+1)], *M. V. Sadovskii*[+*1)]

[+] *Institute for Electrophysics UB RAS, 620016 Ekaterinburg, Russia*

[*] *Institute for Metal Physics UB RAS, 620990 Ekaterinburg, Russia*

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We report LDA calculated band structure, densities of states and Fermi surfaces for recently discovered Pt-pnictide superconductors APt_3P (A = Ca, Sr, La), confirming their multiple band nature. Electronic structure is essentially three dimensional, in contrast to Fe pnictides and chalcogenides. LDA calculated Sommerfeld coefficient agrees rather well with experimental data, leaving little space for very strong coupling superconductivity, suggested by experimental data on specific heat of $SrPt_3P$. Elementary estimates show, that the values of critical temperature can be explained by rather weak or moderately strong coupling, while the decrease of superconducting transition temperature T_c from Sr to La compound can be explained by corresponding decrease of total density of states at the Fermi level $N(E_F)$. The shape of the density of states near the Fermi level suggests that in $SrPt_3P$ electron doping (such as replacement Sr by La) decreases $N(E_F)$ and T_c, while hole doping (e.g. partial replacement of Sr with K, Rb or Cs, if possible) would increase $N(E_F)$ and possibly T_c.

1. Introduction. After the discovery of first iron-pnictide high-temperature superconductors [1] (see reviews in Refs. [2, 3]) several other iron-pnictide and iron-chalcogenide families of superconductors were intensively studied in recent years (see reviews in Refs. [2, 3] and pnictide-chalcogenide comparison in Ref. [4]). The search for new systems produced several new superconductors, which are chemical analogues of iron-pnictides and chalcogenides, such as $BaNi_2As_2$ [5], $SrNi_2As_2$ [6], $SrPt_2As_2$ [7], SrPtAs [8], but with pretty low superconducting T_c. Recently, another family of Pt-based superconductors with chemical composition APt_3P (A = Sr, Ca, La) [9] was discovered with experimental values of T_c equal to 8.4, 6.6, and 1.5 K correspondingly. Based on the observation of nonlinear temperature behavior of Hall resistivity, the authors of Ref. [9] supposed the multiple band nature of superconductivity in these new systems, while specific heat data on $SrPt_3P$ has lead them to a conclusion on very strong coupling nature of superconductivity [9].

Below we present the results on LDA calculated electronic structure for $SrPt_3P$ and $LaPt_3P$, as well as some comparison with previously studied Pt-based superconductor $SrPt_2As_2$ [10]. We also present some elementary estimates concerning superconductivity in APt_3P system.

2. Crystal structure. Crystals of $SrPt_3P$ system have tetragonal space group $P\frac{4}{n}mm$ with $a = 5.8094$ Å and $c = 5.3833$ Å [9]. Between Sr layers there are antiperovskite Pt_6P octahedra where basal Pt1 atoms occupy $4e$ (1/4, 1/4, 1/2) positions and apical Pt2 occupy $2c$ (0, 1/2, 0.1409). Phosphorus inside octahedra also occupies $2c$ position, but with $z = 0.7226$. These octahedra are not ideal – distance from basal plane to apical Pt2 atoms is different, while basal Pt1 atoms form perfect squares. From Fig. 1 it is clear that because of alternating edge sharing Pt_6P octahedra, basal Pt1 atoms form two dimensional square lattice. For $LaPt_3P$ we assume the same crystal structure as for $SrPt_3P$.

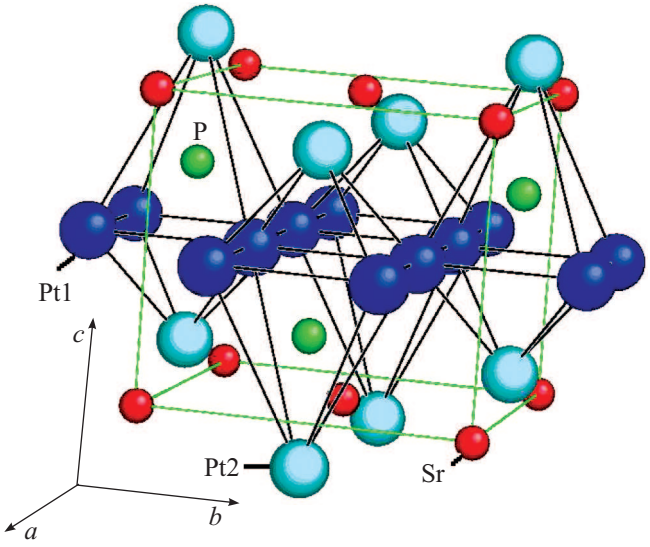

Fig. 1. Crystal structure of $SrPt_3P$. Pt_6P octahedra are shown by Pt–Pt bonds

[1)] e-mail: nekrasov@iep.uran.ru; sadovski@iep.uran.ru

3. Electronic structure. Using the experimentally established crystal structure [9] we performed LDA band structure calculations within the linearized muffin-tin orbitals method (LMTO) [11] with default settings.

In Fig. 2 we present LDA calculated densities of states (DOS) of $SrPt_3P$ (upper panel) and $LaPt_3P$

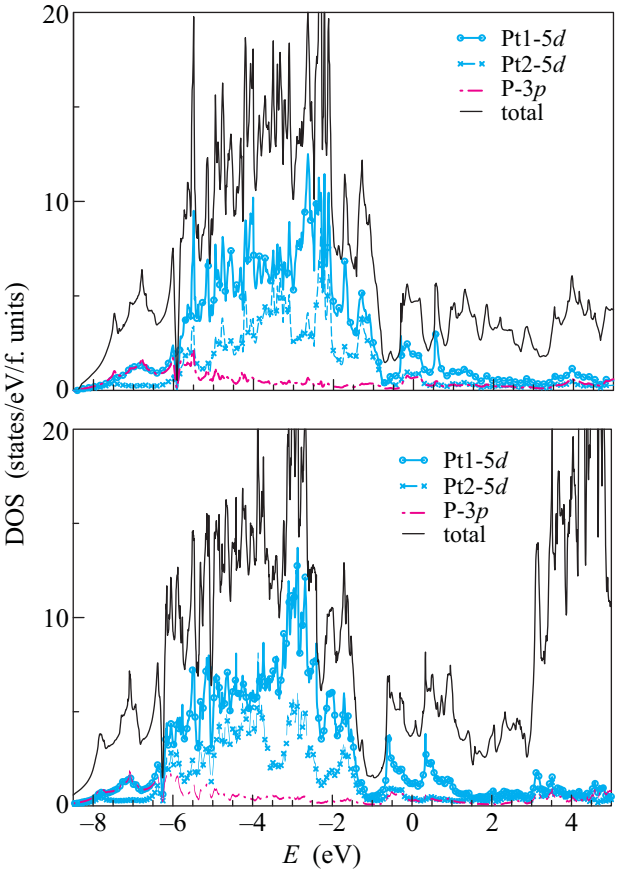

Fig. 2. LDA calculated densities of states (DOS) of $SrPt_3P$ (upper panel) and $LaPt_3P$ (lower panel). Solid black line – total DOS, line with circles – Pt1-5d DOS, line with × – Pt2-5d DOS and dot-dashed line – P-3p DOS. The Fermi level E_F is at zero energy

(lower panel). Most of spectral weight from −8 up to 2 eV belongs to Pt1 (line with circles) and Pt2 5d states (line with ×). Phosphorus 3p states give rather small contribution to the DOS (dot-dashed line). DOS at the Fermi level is formed mainly by Pt1-5d states (Pt1 atoms make 2d-square lattice, see Fig. 1) with a bit of admixture of Pt2-5d and P-3p states.

The values of the DOS at the Fermi level $N(E_F)$ for Sr and La compounds are correspondingly 4.69 and 3.77 states/eV/cell. These values are comparable with those for pnictides with moderate T_c values [12]. Calculating Sommerfeld coefficient $\gamma_b = \frac{\pi^2}{3} N(E_F)$ we obtain 11 and 8.9 mJ/mol/K^2 for $SrPt_3P$ and $LaPt_3P$, respectively. For Sr compound the experimental value of Sommerfeld coefficient is $\gamma^{exp} = 12.7$ mJ/mol/K [9] and agrees rather well with our band structure estimates. In fact γ^{exp} should be larger than calculated (free electron) γ_b, because of DOS renormalization due to electron-phonon interaction (or interaction with other collective modes): $\gamma = (1 + \lambda)\gamma_b$, where λ is corresponding dimensionless coupling constant. Comparing experimental data and calculated results we get an estimate of λ of the order of 0.15 only, which corresponds to rather weak coupling and is too small to obtain the experimental values of T_c (see below). Note also that experimental estimates [9] of Wilson ratio produced the values of $R_W \sim 1$, which signifies the absence of strong correlations in $SrPt_3P$.

Our results for DOS show that in $SrPt_3P$ the Fermi level is located just in the middle of the slope of a peak in the DOS, so that electron doping decreases $N(E_F)$, while hole doping the other way around increases it. This may be important for superconductivity (see discussion below).

In Fig. 2 we show band dispersions of $SrPt_3P$ (black lines) and $LaPt_3P$ (gray lines) in the vicinity of the Fermi level. These are quite different from band dispersions reported for chemically similar material $SrPt_2As_2$ [10] and also from iron pnictides and chalcogenides [4]. First of all, both APt_3P compounds are essentially three dimensional as one can see from dispersions in Γ-Z direction. From chemical composition point of view (neglecting lattice relaxation effects) $LaPt_3P$ is "electron doped" $SrPt_3P$ system (one extra electron in La). This results in almost rigid shift of the La compound bands down in energy for about 0.3 eV with respect to the bands of Sr compound (see Fig. 3). Close to the Fermi level for $LaPt_3P$ there are several band crossings and Van-Hove singularities. Thus Fermi surface topology can be changed rather easy upon doping.

In Figs. 4 and 5 we present LDA calculated Fermi surfaces (FS) of $SrPt_3P$ and $LaPt_3P$ correspondingly and also separately drawn different FS sheets. Overall shape of the APt_3P FS is very different from those in typical iron pnictides or chalcogenides [13, 14]. First of all it looks pretty three-dimensional and does not have any well developed cylinders.

The overall conclusion on electronic structure of APt_3P family is that it really the new class of multiple band superconductors, as was expected from Hall measurements in Ref. [9]. $SrPt_3P$ system is essentially two-band superconductor, while $LaPt_3$ band structure in the vicinity of the Fermi level is even more complicated. Fermi surfaces of both systems are characterized by multiple sheets and pockets in the Brillouin zone,

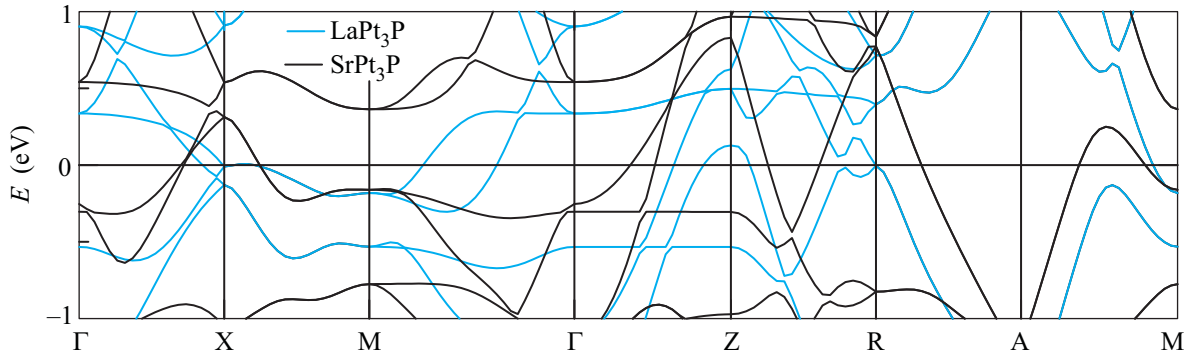

Fig. 3. LDA calculated band dispersions in the vicinity of the Fermi level for $SrPt_3P$ (black line) and $LaPt_3P$ (gray line). The Fermi level is at zero energy

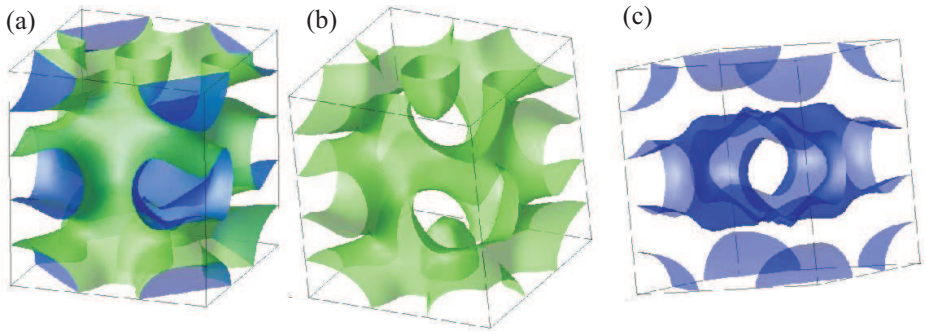

Fig. 4. LDA calculated Fermi surface for $SrPt_3P$ (a) and its separate sheets (b, c)

which produce very complicated topology and variability under doping.

4. Remarks on superconductivity. 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 Cooper pairing or several types of d-wave pairing. Most probable is, of course, the case of s-wave superconductivity, as proposed in Ref. [9]. Additional complications arise from multiple band nature of the APt_3P compounds. The three-dimensional multiple sheet FS topology may lead to complicated superconducting gap structure, with different energy gaps on different FS sheets. The T_c value and gap ratios in the multiple band systems are actually determined by rather complicated interplay of intraband and interband couplings in Cooper channel, as well as by partial DOS ratios at different FS sheets [17, 18].

Nevertheless simple BCS approach allows us to make simple estimates of dimensionless coupling constant λ value from experimental values of T_c. Using the simple BCS expression $T_c = 1.14\omega_D e^{-1/\lambda}$ with experimental value of Debye frequency $\omega_D = 190\,K$ [9] we obtain weak coupling value of $\lambda = 0.31$ for $T_c = 8.4\,K$. Reducing this value of λ proportionally to the decrease of DOS at the Fermi level (from 4.69 states/eV/cell in Sr compound to 3.77 states/eV/cell in La system) we obtain $T_c = 4\,K$ for $LaPt_3P$ in a reasonable agreement with experimental value of 1.5 K.

As simple BCS expression for T_c is probably too crude, we also used the McMillan expression [19]:

$$T_c = \frac{\omega_D}{1.45} \exp\left[-\frac{1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\lambda)}\right], \qquad (1)$$

where μ^* is the Coulomb pseudopotential. Quite similar results were also obtained with Allen-Dynes formula [20], considered to be the best interpolation expression for T_c in strongly coupled superconductors. Taking the "optimistic" value of Coulomb pseudopotential $\mu^* = 0$, we repeat our previous analysis. Now Eq. (1) gives $\lambda = 0.61$ for $SrPt_3P$ and corresponding $T_c = 5.6\,K$ for $LaPt_3P$. Once we assume more typical value of $\mu^* = 0.1$, we get $\lambda = 0.85$ for $SrPt_3P$ and then $T_c = 5.4\,K$ for La compound is obtained.

To sum up we see that the values of T_c for Sr and La systems reasonably correlated with DOS behavior at Fermi level, which is similar to our estimates for iron pnictides and chalcogenides [4, 12]. At the same time, these estimates correspond to weak or intermediate coupling superconductivity in APt_3P supercon-

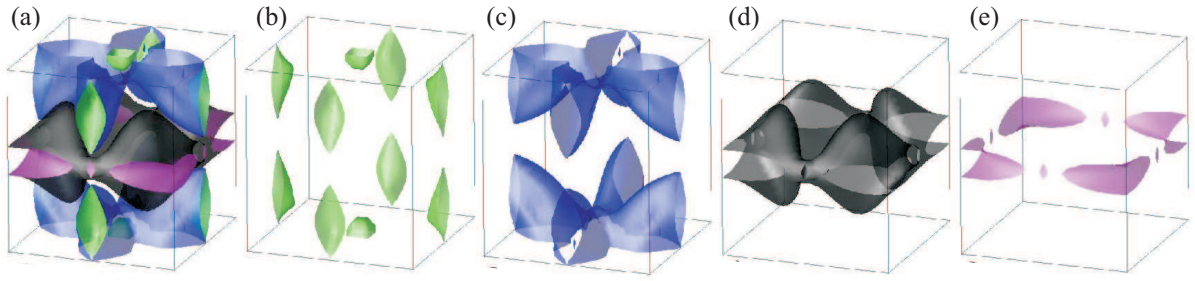

Fig. 5. LDA calculated Fermi surface for $LaPt_3P$ (a) and its separate sheets (b–e)

ductors, which cannot explain (compare [20]) unusually high $2\Delta/T_c$ ratios obtained from specific heat data in Ref. [9]. This stresses the need for independent experimental estimates of $2\Delta/T_c$ ratios in these systems.

5. Conclusion. In this work we presented LDA results for band dispersions, densities of states and Fermi surfaces for recently discovered Pt-pnictogen superconductors APt_3P (A = Sr, La) [9]. We confirm experimental predictions concerning the multiple band superconductivity in these systems, with complicated multiple sheet FS topology. In contrast to typical iron pnictides and chalcogenides we find Pt systems to be essentially three dimensional. Our LDA data and simple estimates of superconducting T_c leave little space for strong coupling superconductivity in new Pt-compounds. The observed correlation of T_c values with DOS behavior close to Fermi level stresses the importance of doping. It seems probable, that hole doping of $SrPt_3P$, if possible, can lead to higher values of T_c.

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