Electronic Structure of Novel Multiple-Band Superconductor SrPt$_2$As$_2$<sup>II</sup>

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The electronic structure of the recently discovered superconductor SrPt$_2$As$_2$ with $T_c = 5.2$ K has been calculated in the local-density approximation. Despite its chemical composition and crystal structure are somehow similar to FeAs-based high-temperature superconductors, the electronic structure of SrPt$_2$As$_2$ is very much different. The 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$_2$As$_2$ is essentially three-dimensional, with complicated sheets corresponding to multiple bands. We compare SrPt$_2$As$_2$ with 1111 and 122 representatives of FeAs-class of superconductors, as well as with isovalent (Ba,Sr)Ni$_2$As$_2$ superconductors. Brief discussion of superconductivity in SrPt$_2$As$_2$ is also presented.

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described below. To obtain the tetrahedral lattice parameter we have taken the average of \(a = 4.482\,\text{Å}\) and \(b = 4.525\,\text{Å}\) parameters of orthorhombic structure, while \(c = 9.869\,\text{Å}\) parameter was taken the same as in the experimentally observed structure. Wyckoff Positions of ions were changed from \textit{Pmmn} to \textit{P4/nnmm} like this: \text{Sr} 2a(1/4, 1/4, 0.7469) \rightarrow 2c(1/4, 1/4, 0.7469); for PtAs\textsubscript{4} layer Pt1 4e(1/4, 0.8163, 0.9989) \rightarrow 2a(1/4, 3/4, 0) and As2 4e(1/4, 0.294, 0.1263) \rightarrow 2c(1/4, 1/4, 0.1263); for AsPt\textsubscript{4} layer Pt2 2a(1/4, 1/4, 0.3817) \rightarrow 2c(1/4, 1/4, 0.3817) and As1 2b(1/4, 3/4, 0.4997) \rightarrow 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.

Using this idealized SrPt\textsubscript{2}As\textsubscript{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 calculated in the local-density approximation (LDA) for SrPt\textsubscript{2}As\textsubscript{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.

One should note that SrPt\textsubscript{2}As\textsubscript{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 \(\Gamma\) and M-points and up to six bands at the Fermi level in M–\(\Gamma\) direction.

Figure 4 displays LDA densities of states (DOSs) of SrPt\textsubscript{2}As\textsubscript{2}. Upper panel shows total DOS (solid line). Since there are two layers of tetrahedra as discussed above we present DOSs for PtAs\textsubscript{4} layer as solid lines (Pt1 with triangles, As2 with crosses) and for AsPt\textsubscript{4} layer as dashed ones (Pt2 with squares, As1 with pluses). Contribution of Pt-5\(d\) 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\textsubscript{2}As\textsubscript{2} system from Fe pnictides where As states almost do not appear at the Fermi level [5, 8]. Most of Pt-5\(d\) 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-5\(d\) states are obviously more extended with larger bandwidth than that of Fe-4\(d\).

Lower panel of Fig. 4 shows orbital resolved DOSs for Pt1 and Pt2 5\(d\) states. Pt1 belongs to PtAs\textsubscript{4} tetrahedron layer and Pt2 to AsPt\textsubscript{4} one. Because of tetragonal symmetry we still can use cubic notations for the 5\(d\) 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 5\(t_2\) orbitals contribute to DOS at the Fermi level. Here as mentioned above most of Pt-5\(d\) 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 FS sheets correspond to bands marked with the same letters as on