Electronic Structure of New LiFeAs High-T<sub>c</sub> Superconductor<sup>¶</sup>

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We present results of ab initio LDA calculations of electronic structure of “next generation” layered iron-pnictide high-T<sub>c</sub> superconductor LiFeAs (T<sub>c</sub> = 18 K). Obtained electronic structure of LiFeAs very similar to recently studied ReOFeAs (Re = La, Ce, Pr, Nd, Sm) and AFe<sub>2</sub>As<sub>2</sub> (A = Ba, Sr) compounds. Namely close to the Fermi level its electronic properties are also determined mainly by Fe 3d-orbitals of FeAs<sub>4</sub> two-dimensional layers. Band dispersions of LiFeAs are very similar to the LaOFeAs and BaFe<sub>2</sub>As<sub>2</sub> systems as well as the shape of the Fe-3d density of states and Fermi surface.

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Recently several series of new layered iron-pnictide superconductors with T<sub>c</sub> about 40–55 K has attracted a lot of scientific interest. At present there are two types of such systems (i) Re111 (Re = La, Ce, Pr, Nd, Sm) with parent compound LaO<sub>1–x</sub>F<sub>x</sub>FeAs [1–8] and (ii) A122 (A = Ba, Sr) with parent system BaFe<sub>2</sub>As<sub>2</sub> [9–11]. The A122 systems are found to form large enough single crystals [12]. A new type of FeAs based superconductor, LiFeAs, was just obtained experimentally [13]. With Li ion deficiency for the composition Li<sub>0.6</sub>FeAs T<sub>c</sub> = 18 K was observed.

Electronic structure of La111 series obtained by means of LDA were reported by several groups [14–16] and qualitatively agreed with the first one calculated for LaOFeP [17]. It was also shown for Re111 that band structure is rather irrelevant to the Re type [18]. For the Ba122 first LDA density of states (DOS) were published in [19, 20]. Detailed comparison of prototype systems La111 and Ba122 was performed in [21].

In this short note we present LDA and structure analysis for newly discovered iron-pnictide system LiFeAs. The obtained LDA band dispersions, DOS and Fermi surface for LiFeAs comparison with the one previously reported for La111 and Ba122 [18, 21] are discussed.

1. CRYSTAL STRUCTURE

The crystal structure of LiFeAs was recently refined [22]. LiFeAs crystallized in tetragonal structure with the space group P4/nmm and lattice parameters a = 3.7914(7) Å, c = 6.364(2) Å. The experimentally obtained crystallographic positions for Fe (2b) (0.75, 0.25, 0.5), Li (2c) (0.25, 0.25, z<sub>Li</sub>), As (2c) (0.25, 0.25, z<sub>As</sub>), z<sub>As</sub> = 0.26351, z<sub>Li</sub> = 0.845915 [22].

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As-Fe-As angles in the case of LiFeAs have values ~103.1° and ~112.7°. Thus one pronounced layered structure presuming quasi two-dimensional electronic properties. To some extent, it resembles the crystal structure of La111 [1] and Ba122 [23].

Most relevant interatomic distanced Fe-Fe and Fe-As are 2.68 and 2.42 Å correspondingly. At the moment it is spatially most compact crystal structure (see for comparison [21]). As-Fe-As angles in the case of LiFeAs have values ~103.1° and ~112.7°. Thus one
should expect some fine distinctions for LiFeAs with respect to La111 and Ba122 [21].

2. ELECTRONIC STRUCTURE

The electronic structure of LiFeAs compound was calculated within the local density approximation (LDA) by using linearized muffin-tin orbital basis (LMTO) [24]. In upper part of Fig. 2 LDA calculated total, Fe-3d and As-4p DOS (left panel) matched with the band dispersions (right panel) are presented. Analyzing Fig. 2 one can see that around the Fermi level from −2.5 eV to +2.5 eV there are Fe-3d states while As-4p states are lower in energy from −2.5 eV down to −6.0 eV. In the ($k_x$, $k_y$) plane band dispersions around the Fermi level have similar shape as reported before for La111 and Ba122 [21] (see Fig. 2, lower panel).

To compare directly LiFeAs with La111 and Ba122 materials in Fig. 3 we show Fe-3d DOS (upper panel) together with the total DOS in the vicinity of the Fermi level (lower panel) for all of them. A bit larger bandwidth of Fe-3d states in LiFeAs is connected with tighter As tetrahedron coordination. For the same reason As-4p states are lower in energy for LiFeAs as to La111 and Ba122. The value of total DOS on the Fermi level is 3.86 state/eV/cell (see Fig. 3, lower panel) which is slightly less than those for La111 (4.01) and Ba122 (4.22) [21]. In principle, this fact alone may lead to lower values of superconducting $T_c$ in this compound, as compares with other iron-pnictide supercon-