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Electronic Structure of New LiFeAs High-T_c Superconductor

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We present results of *ab initio* LDA calculations of electronic structure of "next generation" layered ironpnictide High-T_c superconductor LiFeAs (T_c=18K). Obtained electronic structure of LiFeAs is very similar to recently studied ReOFeAs (Re=La,Ce,Pr,Nd,Sm) and AFe_2As_2 (A=Ba,Sr) compounds. Namely close to the Fermi level its electronic properties are also determined mainly by Fe 3*d*-orbitals of $FeAs_4$ two-dimensional layers. Band dispersions of LiFeAs are very similar to the LaOFeAs and $BaFe_2As_2$ systems as well as the shape of the Fe-3*d* density of states and Fermi surface.

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Recently several series of new layered ironpnictide superconductors with T_c about 40–55K 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 $LaO_{1-x}F_xFeAs$ [1, 2, 3, 4, 5, 6, 7, 8] and (ii) A122 (A=Ba,Sr) with parent system $BaFe_2As_2$ [9, 10, 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 – LiFeAs [13]. With Li ion deficiency for the composition $Li_{0.6}FeAs$ T_c=18K was observed.

Electronic structure of La111 series obtained by means of LDA were reported by several groups [14, 15, 16] and qualitatively agreed with the first one calculated for LaOFeP [17]. Also it was 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 Refs. [19, 20]. Detailed comparison of prototype systems La111 and Ba122 was performed in Ref. [21].

In this short note we present LDA band structure analysis for newly discovered ironpnictide system LiFeAs [13]. Also we propose complete set of crystallographic data for LiFeAs obtained within LDA optimization of crystal structure since no atomic positions were presented in Ref. [13]. Then our LDA band dispersions, DOS and Fermi surface for LiFeAs in comparison with one previously reported for La111 and Ba122 (Refs. [18, 21]) are discussed.

1. CRYSTAL STRUCTURE

LiFeAs crystal structure to some extend resembles one for La111 [1] and Ba122 [22]. LiFeAs crystallize in tetragonal structure with the space group $P4/nmm$ with lattice parameters a = 3.76 Åand c = 6.28 Å. The crystal structure of LiFeAs is displayed in Fig. 1. Corresponding Wyckoff positions of the space group for different atoms are Fe(2a) (0,0,0), Li(2b) (0,0,0.5), and As(2c) (0,0.5,z_{As}). The crystal structure of LiFeAs displayed in Fig. 1 has pronounced layered structure presuming quasi two-dimensional electronic properties.

Arbitrary parameter z_{As}=0.21696 was obtained from crystal structure optimization using the linearized augmented planewave (LAPW) method within WIEN2k code [23, 24] and the generalized gradient approximation (GGA) of Perdew, Bruke and Ernzerhof (PBE) [25]. One should mention that in our "first shot" optimization calculations no magnetic order on Fe ions or correlation effects were assumed (which are not reported by experimentalists so far). However as it is shown in Ref. [26] account of these details might affect optimized crystal structure for these particular compounds rather strong.

Most relevant interatomic distances Fe-Fe and Fe-As are 2.66 and 2.32 Å correspondingly. At the moment it is spatially most compact crystal structure (see for comparison Ref. [21]). As-Fe-As angles in the case of LiFeAs have values $\sim 108.5^\circ$ and $\sim 110.0^\circ$. 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 orbitals basis (LMTO) [27]. In upper part of Fig. 2 LDA calculated total, Fe-3*d* and As-4*p* DOS (left panel) matched with the band dispersions (right panel) are presented. Analyzing Fig. 2 one can see that around the Fermi

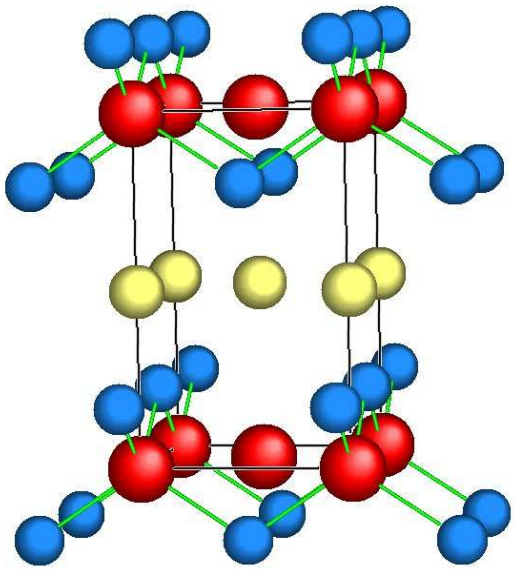

Fig. 1. Crystal structure of LiFeAs. Fe ions (red) within the As (blue) tetrahedra form two-dimensional layers separated by Li ion (yellow) stratum.

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 Ba112 [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 more tight As tetrahedron coordination. For the same reason As-4p states are lower in energy for LiFeAs as to La111 and Ba112. The value of total DOS on the Fermi level is 3.24 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 compared with other ironpnictide superconductors. The orbitally resolved Fe-3d DOS for LiFeAs is shown in Fig. 4. One can see three Fe-3d orbitals of t_{2g} symmetry – xz, yz, xy mainly contributing to the bands crossing the Fermi level.

In Fig. 5 we show LDA calculated Fermi surface of LiFeAs. If compared with Fermi surfaces for Ba122 (and to a lesser extend La111) systems one can see that two hole cylinders around Γ point are significantly closer to each other. This fact can be viewed also in the band dispersions (see Fig. 2, lower panel).

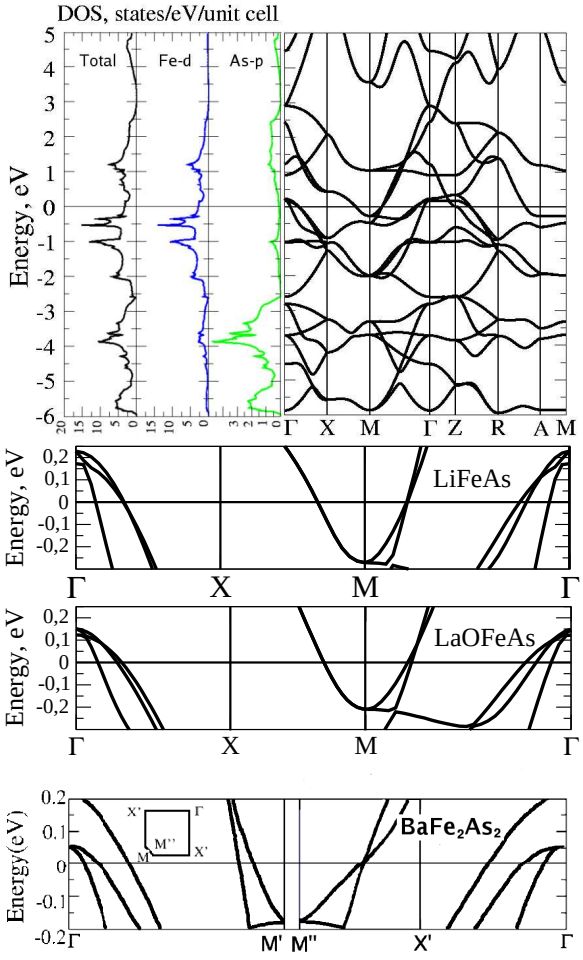

Fig. 2. Upper panels LDA densities of states (left) vs. band dispersions (right) for LiFeAs. Low panel – magnified band dispersions around the Fermi level for (k_x, k_y) plane for LiFeAs, La111 and Ba112. The Fermi level corresponds to zero.

3. CONCLUSION

To summarize, we have presented the LDA calculation results of "next generation" prototype ironpnictide high-temperature superconductor LiFeAs. To complete crystallographic data necessary for band structure computations we perform optimization of the crystal structure with respect to unknown z_{As} coordinate. Further comparison of our LDA data with previously reported Re111 and A122 series shows resembling electronic properties for all of them. However for LiFeAs hole cylinders around Γ-point are found to be remarkably closer to each other than in La111 and Ba122 compounds. Despite that in ironpnictides including LiFeAs two-dimensional $FeAs_4$ layer provides electronic states in the vicinity of the Fermi level which are important to superconductivity investigation in those compounds.

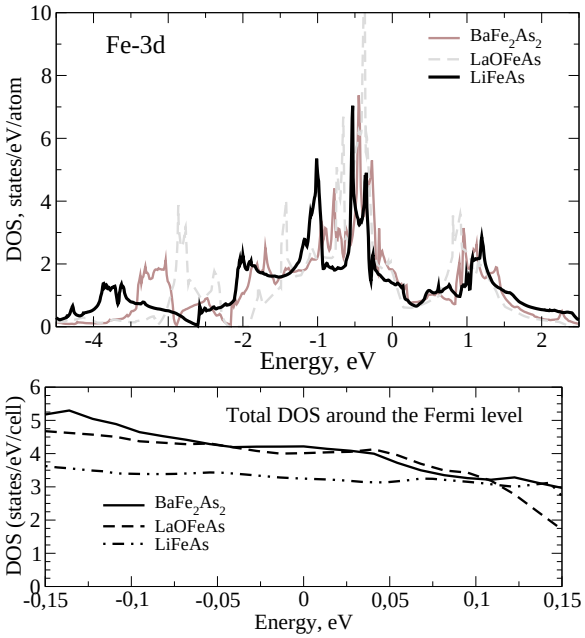

Fig. 3. Comparison of LDA Fe-3*d* DOS (upper panel) for LiFeAs (black solid line), La111 (gray dashed line) and Ba122 (brown solid line). Lower panel – total DOS of LiFeAs, La111 and Ba122 in the vicinity of the Fermi level. The Fermi level corresponds to zero.

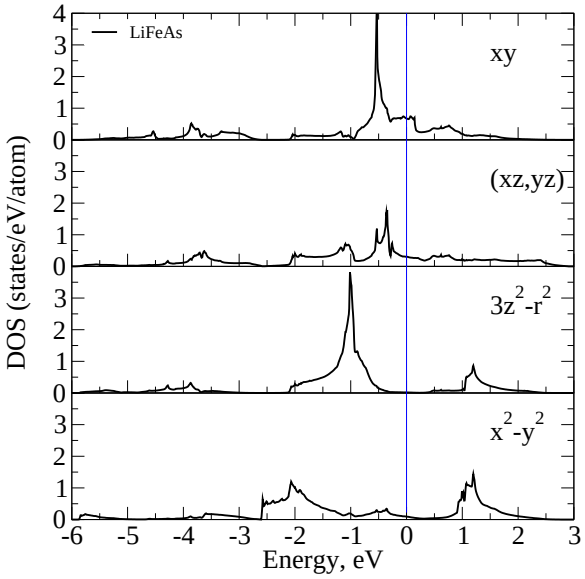

Fig. 4. Orbitally resolved LDA calculated Fe-3*d* DOS for LiFeAs. The Fermi level corresponds to zero.

4. ACKNOWLEDGEMENTS

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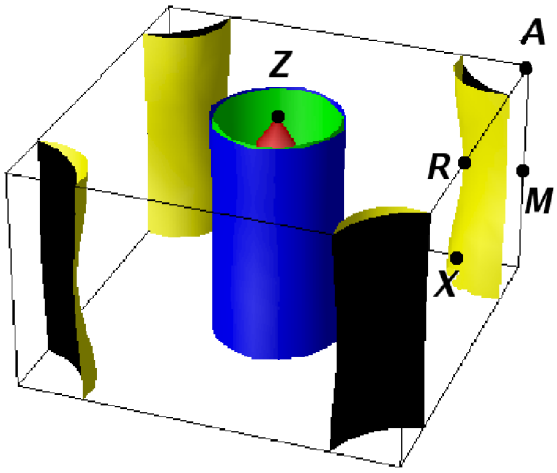

Fig. 5. LDA Fermi surface of LiFeAs shown in the first Brillouin zone centered at Γ point.

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