Electronic Properties of Iron Pnictide Superconductor LiFeP

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Abstract. A Density Functional Theory (DFT) based computation was conducted to study the electronic band structure, electron density of states (DOS), integrated DOS and partial DOS of LiFeP, a new iron pnictide superconductor, using Generalized Gradient Approximation (GGA) with ultrasoft pseudopotentials. The dominance of 3s state of 'P' in the region far below the Fermi level and thereof 3d state of 'Fe' near the Fermi level and also of 'Li' above the Fermi level are seen. The overlapping of bands near the Fermi level shows the metallic nature of LiFeP.

INTRODUCTION

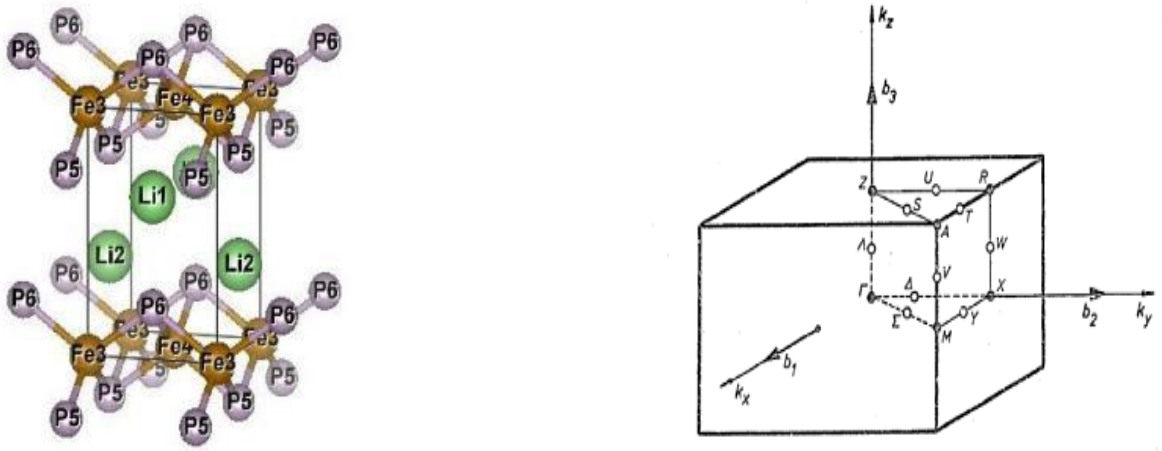
After the discovery of superconductivity at Tc ~ 26K in LaFeAsO1-xFx[1], the researchers in the field have developed a broad range of FeAs based layered superconductors [2-4]. The use of such, FeAs family materials found to be more effective than cuprates due to the brittleness of cuprates [5]. Also, designing the cuprates in preferred structure requires complex processes. The study on NaFeAs and LiFeAs are also reviewed by Dai et al. [6]. Generally, iron pnictide layers are contained in pnictide compounds, which are the reason for the superconducting current connected with charge reservoir, which can be alkali metal (e.g. potassium) [7] or alkaline earth metal (e.g. magnesium) [8]. It is also stated that the itinerant behavior of this superconductor at normal state can be useful to comprehend the phenomena of high temperature superconductivity occurring in pnictide superconductors [9]. The recent detection of an iron pnictide superconductor, LiFeP, which consists of FeP layer has a similar structure like as LiFeAs [9]. It is the first analogue of the family of "111" iron pnictides, which is free of arsenic. As the transition temperature Tc ~ 6K, it is a low temperature superconductor [9]. The present work reports the electronic properties viz; electronic band structure, electron density of states (DOS), partial DOS and integrated DOS of LiFeP, pnictide superconductor.

METHOD OF COMPUTATION

The Density Functional Theory (DFT) based calculations were carried out to study the ground state electronic structure of LiFeP, pnictide superconductor. The calculations were done using Quantum Espresso [10] in theWinmostar environment [11]. The Generalized Gradient Approximation (GGA) [12] with the functional suggested by Perdew-Burke-Einzerhof indulged the exchange correlation effects. Plane waves were taken with kinetic energy cutoff 20 Ry and charge density cutoff 80 Ry have been considered. A k-points mesh of 4×4×4 was taken to carry out integration over Brillouin zone. The ultrasoft pseudopotentials [13] of three different elements i.e. Li, Fe and P are used for the present computation.

Equilibrium geometry was obtained by optimizing the atomic positions of the structure. The structure was considered to be converged when the accuracy in energy of 10^{-6} Ry was achieved. LiFeP has a tetragonal structure with space group P4/nmm. It consists of alternating [Fe_2P_2] blocks which surrounds the Li atoms. The crystal

structure and first Brillouin zone for LiFeP is shown in fig. 1. The experimental values for the lattice parameters are a = 3.692 Aº and c = 6.031 Aº[9]. The obtained optimized values for the lattice parameters are a = 3.707 Aº and c = 6.167 Aº, which are in excellent agreement with the experimental values. The band structure was generated for major symmetry points along the path Γ → Z → R → X → M → A.



(a) (b)

Figure 1. (a) Crystal structure of LiFeP and (b) First Brillouin zone for tetragonal structure.

RESULTS AND DISCUSSION

Figure 2 shows the electronic band structure of LiFeP. While, fig. 3 shows the total electron density of states (DOS) of LiFeP. The partial DOS of Li, Fe, P and the integrated DOS are shown in fig. 4.

Here, from fig. 2, it can be seen that the two lowest bands below the Fermi level near -11 eV are mainly due to 3s state of element 'P' (fig. 4c). The area around Fermi level is formed by the states of [Fe_2P_2], hence near the Fermi level all bands are dominated by the states of elements 'Fe' and 'P'. While, in the region above the Fermi level, the contribution of 'Li' element is dominant. The quasi-core pnictogen bands are shown at -2.5 eV below the Fermi level. The gap between the Fermi level and the beginning edge of the pnictogen band is found of the order of 5.8 eV.

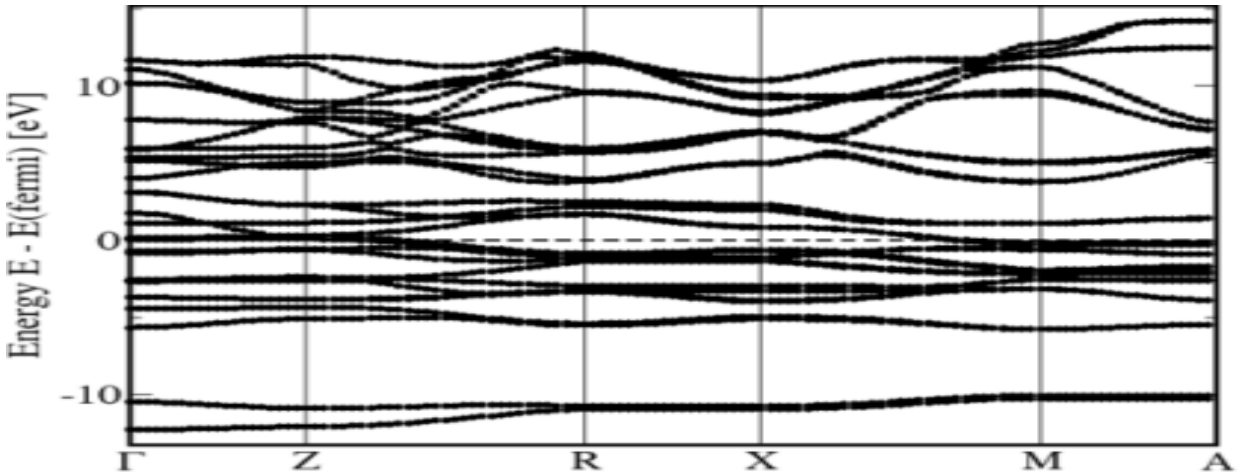


Figure 2. Electronic band structure of LiFeP.

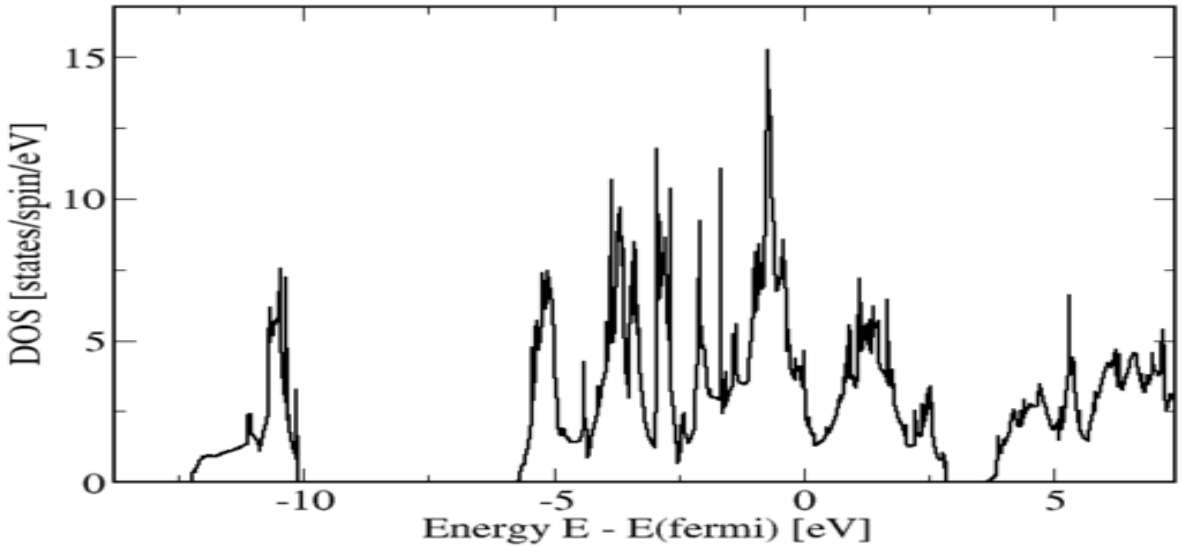


Figure 3. Total electron density of states of LiFeP.

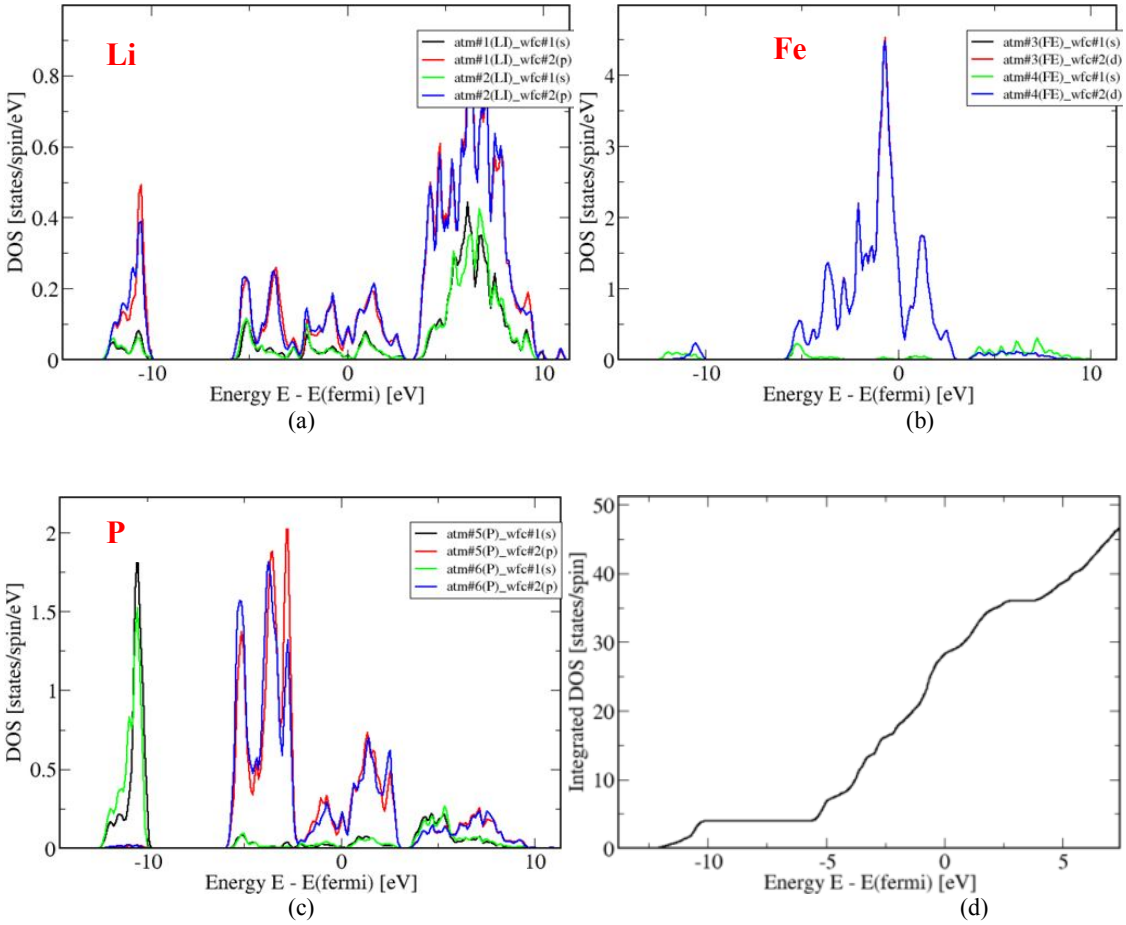


Figure 4. Partial DOS of (a) Li, (b) Fe and (c) P and (d) integrated DOS of LiFeP.

CONCLUSION

In conclusion, we studied the electronic band structure, DOS, partial DOS and integrated DOS of the first arsenic free analogue of the family of said "111" FeAs superconductors, LiFeP using the GGA approach, with ultrasoft pseudopotentials under DFT. The dominance of 3d state of 'Fe' is observed near the Fermi level in LiFeP. From the overlapping of bands in the band structure near the E_F, the metallic character of LiFeP is confirmed.

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