



The study on the effect of Ruthenium(Ru) in LaFeAsO

M. A. Afrassa¹, P. Singh²

Adama Science and Technology University, Adama, Ethiopia

mesfingn171@gmail.com

Addis Ababa University, Department of Physics, Addis Ababa, Ethiopia

ABSTRACT

We study the effect of Ru substitution at Fe site on $\text{LaFe}_{1-x}\text{Ru}_x\text{AsO}$ compounds for $x = 0, 0.25, 0.50, 0.75$ and 1 . We produce density of state (DOS), Fermi surface (FS) and a band structure based on Density Functional Theory(DFT). The result on the band structures show that Ru substitution changes the hole bands and not the electron bands. One of the possible reason is perhaps that Ru substitution does not induce additional electrons, which is in agreement with NMR and resistivity measurement report. We conclude that the change in the whole bands is the reason for suppressing effect of Ru. The DOS is much affected for over doped region($x > 0.50$) around the Fermi level. For Ru = 0.50, the Fermi surfaces is close to nesting, and we calculated the value of T_c applying McMillan equation. The result indicates that the alloy can be a superconductor only for strong pairing potential($x > 0.7$).

Indexing terms/Keywords

Superconductivity, Band structure, Density of state(DOS), Fermi surface.

Academic Discipline And Sub-Disciplines

Condensed matter Physics, Superconductivity

SUBJECT CLASSIFICATION

Physics

TYPE (METHOD/APPROACH)

Electronic structural calculation with Density Functional Theory(DFT)

1. INTRODUCTION

The study on the mechanism of Superconductivity has attracted lots of attention on iron based superconductors following the report on $\text{LaFeAsO}_{1-x}\text{F}_x$ [1]. In many studies, much effort has been made theoretically and experimentally to identify the main cause of their novel properties. A deeper understanding on the doping effect of the electronic structure of this compound can provide insight into the properties of superconductivity and the mechanism of superconducting critical temperature- T_c .

Ln1111 family of iron pnictides (with Ln a lanthanide ion) shows the highest critical temperature- T_c . Different experimental work on Ln1111 families of pnictides result in various phase diagrams[2]. Superconductivity achieved on the parent compound LaFeAsO with different techniques including applying pressure and doping. Experimental report shows that Superconductivity is induced by hole doping for instance on $\text{La}_{1-x}\text{Sr}_x\text{FeAsO}$ ($T_c=25\text{K}$) [3] and electron doping in $\text{Gd}_{0.8}\text{Th}_{0.2}\text{FeAsO}$ compound [4]. The pairing mechanism in such compounds is not well understood.

On the contrary the suppression of Superconductivity was reported by Mn substitution on Fe site [5]. The pair breaking effect due to the doping is not well explained but there is a report from NMR and resistivity measurement indicating that no charge doping rather localized magnetic impurities play the role[6]. It is also reported that a quantum critical point is observed in La based compound[7].

Electronic structural calculation on Ln1111 shows a significant progress in understanding the system. Ru substitution on Fe site shows different properties. In $\text{PrFe}_{1-x}\text{Ru}_x\text{AsO}$, Ru substitution reduce SDW[8]. Similarly in 122 family, $\text{Ba}(\text{Fe}_{1-x}\text{Ru}_x)_2\text{As}_2$ it was reported that Ru substitution suppresses spin density wave[9].

In most of the experimental result Superconductivity appears when magnetism is reduced or disappears. The electronic structure calculation[10] shows that Ru substitution does not induce magnetic property. In Ru doped experiment Fig (2) of Ref.[11], $\text{LaFe}_{1-x}\text{Ru}_x\text{AsO}_{1-y}\text{F}_y$, μSR measurement shows that there is a short range of magnetic ordering compare to Sm based compound.

In this work we tried to see the effect of Ru substitution on the band structure, DOS, and FS for different concentration of Ru($x=0, 0.25, 0.50, 0.75$, and 1).

COMPUTATIONAL DETAILS

We apply first principle calculation in Density Functional Theory(DFT) approach with Quantum Espresso(QE)[12]. We use the value of the tetragonal lattice parameter(a and c) together with internal coordinates of La and As, from Ref. [10]. The bands are plotted along the high symmetry direction (Γ -X-M- Γ -Z-R-A-Z) in the Conventional Tetragonal-TET Brillouin zone[13]. The DOS calculation were performed using tetrahedron method. For 0.25 and 0.75 Ru substitution, we doubled

the cell in the c-axis and we did a band folding to compare band structure in the first Brillouin zone. In general we did non magnetic calculations.

3. RESULT AND DISCUSSION

3.1 Electronic Band structure calculation

We calculate the band structure for a tetragonal lattice following the path Γ -X-M- Γ -Z-R-A-Z. We checked the effect of Ru substitution on the number, shape and size of bands. In all our calculations we found at least four bands at E_F , indicating the multi band nature. Our results are shown in Fig 1, Fig 2, and Fig 3.

We first calculated the electronic structure of the parent compound with out Ru to compare with literature. We found our result is in a good agreement with previous calculations except a small change in the Fermi level due to the difference parameters in different codes. In the remaining calculation we replace for example, 50 % Ru concentration was achieved by the substitution of two Ru out of four Fe, etc. Since Ru has a larger atomic size than Fe, it is expected a wider band and a larger FS.

In Fig. 1, it is found that, the shapes of the electron bands and hole bands are similar for all substitutions. The number and size of electrons band is not changed (at M) with Ru substitution but the size of hole band is changed for all substitutions at the Γ - and Z points. This may show that Ru substitution does not introduce additional electrons.

We compared the energy of each band at Γ and Z points for the hole bands and at M and X point for electron bands. The electrons band at M and X point have the same energy value for each substitution. But the energy change ΔE with respect to the Fermi level is higher for whole band than electrons band for different Ru substitutions. We also noticed that Ru changes the Fermi level E_F linearly.

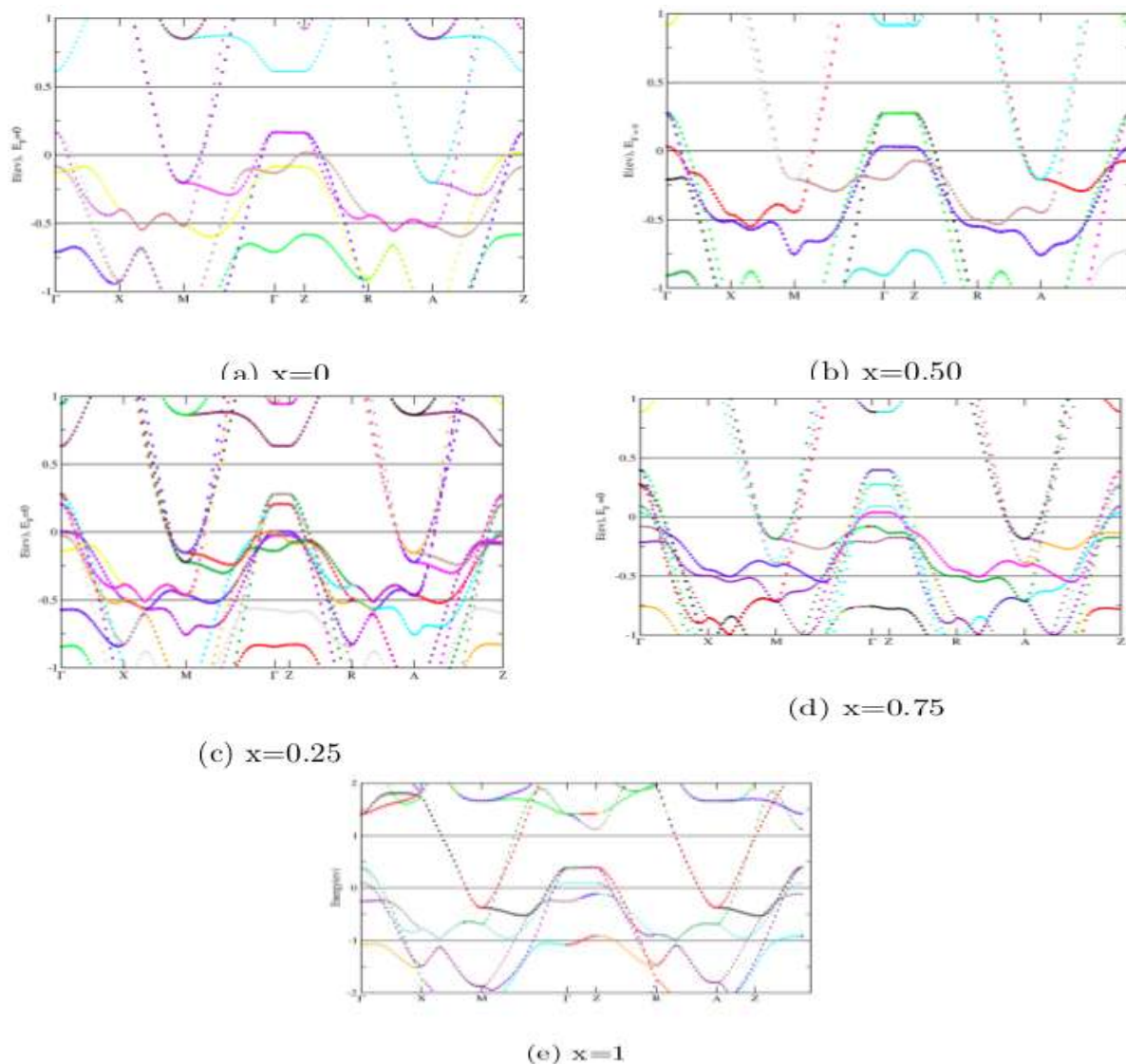


Figure 1: Band structure for $\text{LaFe}_{1-x}\text{Ru}_x\text{AsO}$

Fig. 2 shows that the shape of DOS is similar for all substitutions but the total value is changing. The DOS around E_F is changed quickly in the over doped region after 0.50Ru. The highest peak is between -1 and 0 Ru = 0.50 may be where the higher T_c can be achieved.

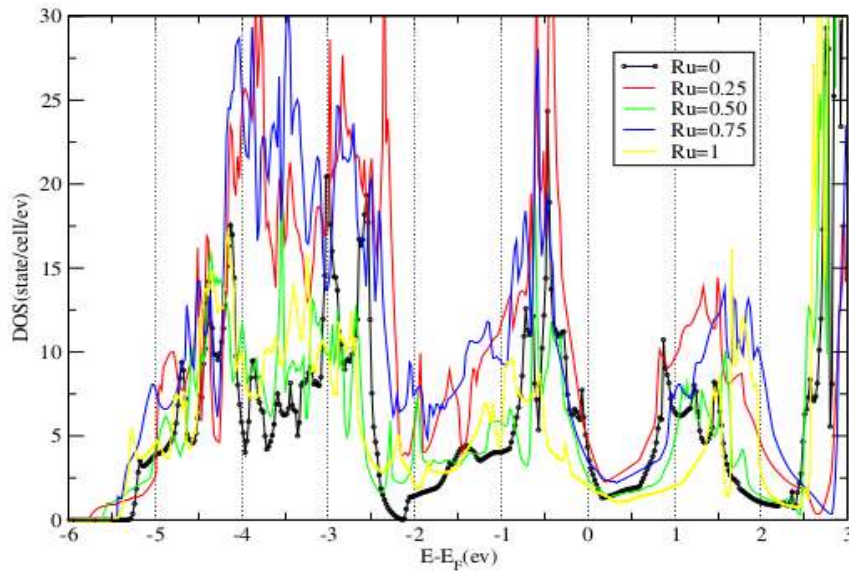


Figure 2: Comparison of the total DOS for La1111(the Fermi level E_F is at zero energy)

The DOS(state/cell/ev) for Ru=0.50 is 2.47. With this value we can predict the value of T_c . Applying

McMillan equation,

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

Where $\theta_D = 319k$, and $\mu^* = N(E_F)/(1+N(E_F))$, as suggested by [14]. Hence for $\lambda = 0.50$, $T_c = 0.02k$, and for $\lambda = 0.70$, $T_c = 39k$. This indicates that the compound can be superconductor only under a strong pairing potential.

The Fermi surface for LaFeAsO and 50% Ru substitution is shown in Fig. 3(a). From the band structure we can see that there are bands that cross the Fermi level and this yields multi-sheet Fermi surfaces. The FS includes electron-like cylinders in the corners of the Brillouin zone and the hole-like cylinders along the Γ -Z line. All Fermi surfaces for electron and hole are cylinder like, that confirms the two-dimensional character of electronic states, already reported for pnictides. We found that, as already reported for LaFeAsO, the FS includes three holes and two electron cylinders. As a result of substitution the hole cylinders is more affected than the electron cylinder.

We shifted the electron-like cylinder from M point to the gamma point to compare with the size of the hole cylinders, to see the nesting between the electrons and holes like-cylinders in the parent compound. The resulting figure(Fig.3(b)) shows that the gap between the hole and electron-like cylinders is increased. In 0.5 substitution the last hole cylinder nearly close with the last electron like cylinders and so nesting may happen.

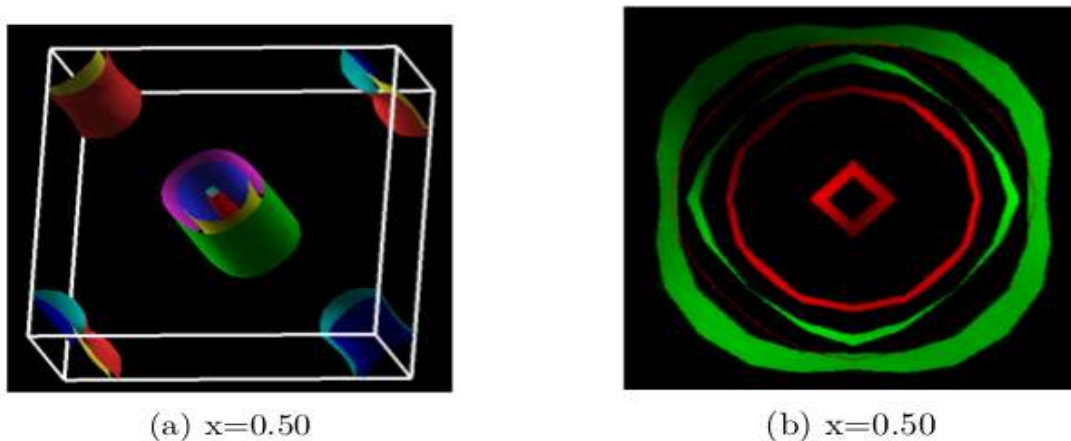


Figure 3: Fermi surface for LaF $e_{1-x}Ru_x$ AsO, x = 0.50 and shifted Fermi surface(b)



4. CONCLUSION

In conclusion we used a first principle method to investigate the effect of Ru on band structure, density of state(DOS) and Fermi surface on $\text{LaFe}_{1-x}\text{Ru}_x\text{ASO}$ compounds. The result shows that Ru substitutions change the hole band than electron bands at M. Superconductivity in such system may not be explained by pair breaking effect of Ru. Shifting the electron like cylinder from M point to gamma helps to see and compare the size of the cylinders and the nesting. The nesting is slightly detected in 0.50Ru. Calculation for T_c indicates that super conductivity can be achieved only for a strong pairing potential, which cannot be explained by BCS type pairing.

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