Density functional study of Co and Te substitution on superconductivity of FeSe

M. A. Afrassa*, A. K. Wordofa

Adama Science and Technology University, Adama, Ethiopia

*mesfin.asfaw@astu.edu.et

Abstract

In this work we present the effect of Cobalt (Co) substitution on iron (Fe) and Selenium (Se) site, and tellurium (Te) substitution on Se site of FeSe($Fe_{0.5}Co_{0.5}Se$, $FeSe_{0.5}Co_{0.5}$, $FeSe_{0.5}Te_{0.5}$). We applied density functional theory (DFT) as implemented in Quantum ESPRESSO. All calculations were done for the space group P4/nmm with non-spin polarized orbitals with lattice parameters a=b=3.765[a.u], c=5.51[a.u]. We found that Co and Te substitution changes the bands and DOS of FeSe. In $FeSe_{0.5}Co_{0.5}$ a number of bands are near the Fermi level and the electron bands are completely changed; this may indicate that Co substitution at Se site is possibly electron doping. Whereas in $Fe_{0.5}Co_{0.5}Se$, a deep electron band is observed at M. The flat band from gamma to Z direction is observed to be below E_F. The DOS result show that $Fe_{0.5}Co_{0.5}Se$ has lowest value (2.299 state/cell/eV) compare to $FeSe_{0.5}Co_{0.5}$(11.324 state/cell/eV) and $FeSe_{0.5}Te_{0.5}$(3.6327). This suggests that $FeSe_{0.5}Co_{0.5}$ is a good candidate for high Tc. Te substitution at Se site increase DOS and Co substitution on Fe site reduces DOS, in agreement to experimental report in enhancing and suppressing Tc respectively.

Keywords:: Superconductivity, Band structure, DOS.

1. Introduction

In Physics one of the challenging phenomena since its discovery 1911, is Superconductivity. Many materials have been reported that shows superconducting phenomena. These include Uranum based compounds, Cu-oxides and Iron based compounds. From the history of superconductivity, we observed that these classes of materials are very rich in various discoveries. But in all findings there had not been reported a superconductor at room temperature and this makes the field very difficult.

In 2008 a new class of material that contains iron was reported. Based on the elemental composition this class of materials are grouped in to 1111-family (e.g. LaFeAsO), 122-family ($BaFeAs_2$), 111-family (LiFeAs), and 11-family (e.g. FeSe)[1]. FeSe is the simplest crystal structure iron-based superconductor where the critical temperature raises from 8k-36.7k under pressure [2].

Experimental report indicated that Tellurium (Te) substitution for Se in FeSe enhances Tc [3-5]. Density functional calculations on FeSe and FeTe indicated that there is a possibility of increasing Tc by either substitution. In fact different experimental and theoretical methods have been employed to raise Tc and to understand the theory of superconductivity. Electronic structure calculation is one of the commonly used methods to understand some properties of the superconducting material. For example, it was reported that first principle study on FeSe indicates phonon-mediated superconductivity [6], and superconductivity under pressure [7]. The study on electronic structure of FeSe is well reviewed in reference[8].But the theory behind the superconductivity of materials is not well understood. The mechanism in which the superconductivity of material is governed differs even for materials of the same family.

The superconductivity of FeSe has been studying by doping different element. For example, sulfur(S) doping up to 20% increase superconducting critical temperature (Tc), whereas Co doping at iron (Fe) site suppressed Tc[9]. It was reported that 50% Te substitution on Se site of FeSe enhance Tc but there is no report on 50% Co substitution. In this work we compare the band structure and DOS for Co and Te substitution on FeSe compound. That is $Fe_{0.5}Co_{0.5}Se$, $FeSe_{0.5}Co_{0.5}$, and $FeSe_{0.5}Te_{0.5}$. The calculations were done by Density functional theory (DFT) as implemented in Quantum ESPRESSO.

The result can possibly explain experimental reports and suggest a better candidate.

2. Computational details

In this work the calculations are performed employing density functional theory (DFT) as implemented in Quantum ESPRESSO (QE) code. The energy convergence is checked with respect to the cutoff energies and k-point sampling. We used lattice parameters of a=b=3.765[a.u], c=5.51[a.u] [10]. The bands are plotted along the high symmetry direction in the conventional tetragonal-TET Brillouin zone, the lattice following the path $\Gamma - X - M - \Gamma - Z - R - A - Z$ [40]. The DOS calculations were performed using tetrahedron method.

3. Result and Discussion

In this research we present comparison result on the effect of Cobalt (Co) and Tellurium (Te). We did the calculation by substituting Co at iron (Fe) site ($Fe_{0.5}Co_{0.5}$ Se) and at Selenium (Se) site ($FeSe_{0.5}Co_{0.5}$). We also did by substituting Te at Se site ($FeSe_{0.5}Te_{0.5}$). We particularly simulated the band structure and density of electron state (DOS). We reproduced the known band structure for the parent compound FeSe. The band structure is calculated in the space group P4/nmm with non-spin polarized orbitals.

The electronic band structure along the high symmetric direction in the Brillouin zone and the density of state for Co and Te substitution at Fe and Se site of FeSe is shown in the figure 1- 6. From Figure 1, Figure 2, and Figure 3, one can see that the band structure has similar nature with that of most iron based superconductors. As we see from the band structure, Tellurium (Te=0.5) substituted band structure (Figure 2) shows a different properties compared to the parent compound (FeSe). The electron band at M is at higher energy compared to the Γ point. When we compare the height of hole bands at Γ point the $FeSe_{0.5}Te_{0.5}$ is a bit higher than that of the FeSe.

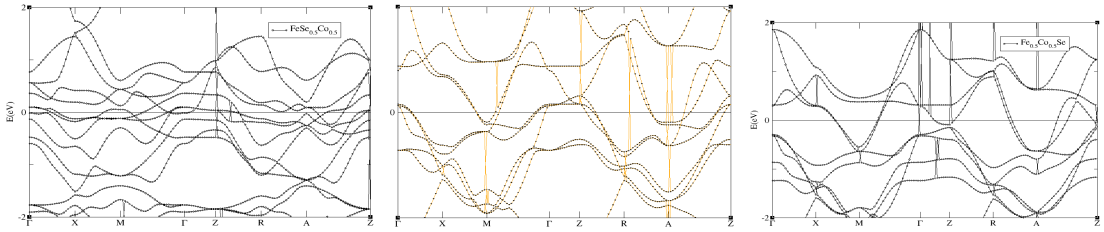

Figure 1: band structure of FeSe0.5Co0.5 Figure 2: band structure of FeSe0.5Te0.5 Figure 3: band structure of Fe Co0.5Se0.5

In $FeSe_{0.5}Te_{0.5}$, it is observed that a number of hole bands are crossing the Fermi level indicating that the superconductivity of the materials is due to hole doping. Sharp bands are seen in $Fe_{0.5}Co_{0.5}Se$ that might shows the compound is in less superconducting state compared to others. In all figures from Γ-Z, there is a flat band which may explain the nature of superconductivity.

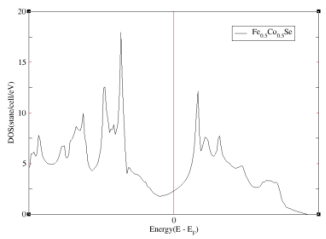

Figure 4: DOS of $FeSe_{0.5}Te_{0.5}$

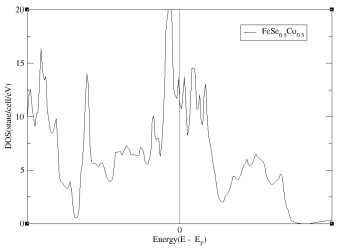

Figure 5: DOS of $Fe_{0.5}Co_{0.5}Se$

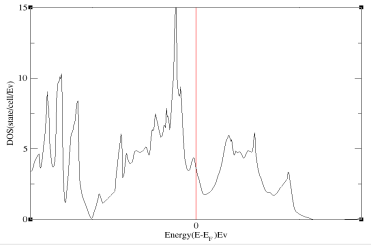

Figure 6: DOS of $FeSe_{0.5}Co_{0.5}$

The calculated total DOS, Fermi energy and total energy are summarized in the table 1 as shown below.

Table 1: Fermi energy, Total energy, and DOS of $FeSe_{0.5}Te_{0.5}$, $FeSe_{0.5}Co_{0.5}$ and $Fe_{0.5}Co_{0.5}Se$

	$FeSe_{0.5}Te_{0.5}$	$FeSe_{0.5}Co_{0.5}$	$Fe_{0.5}Co_{0.5}Se$
Fermi Energy	10.9467	9.2681	9.8252
Total Energy(ET)	-750.674	-1057.812	-1062.476
Density of state(DOS)	3.6327	11.324	2.299

When Co and Te are substituted on Se site, the DOS around the Fermi level decreasing between -0.012 – 0.026 where as in the case of Co substitution on Fe site DOS around the Fermi level, in the energy range -0.193-0.334, is increasing. So we think that $Fe_{0.5}Co_{0.5}Se$ is a good candidate for further study. From the table 1, the highest DOS is for $FeSe_{0.5}Co_{0.5}$ and so the highest Tc is expected. Experimental report indicated that Co substitution has a suppressing effect at Fe site. In this work we found that Co substituted at Se site has a positive effect.

Conclusion

In this work we present a DFT calculation as implemented in QE. Electronic band structure along the high symmetric direction in the Brillouin zone and the density of state for Co and Te substitution at Fe and Se site of FeSe is discussed. The general properties of the band structure are similar with most of the Iron-Based superconductors that shows multi band nature. The bands are affected in the presence of Te and Co at x=0.5. There is a flat band from Γ to Z direction in all compounds ($Fe_{0.5}Co_{0.5}Se$, $FeSe_{0.5}Co_{0.5}$ and $FeSe_{0.5}Te_{0.5}$). At Γ point the hole bands increasing in the energy in $FeSe_{0.5}Co_{0.5}$. It was experimentally reported that in $FeSe_{0.5}Te_{0.5}$ due to the reduced Fermi surface nesting, a possible SDW state becomes more unstable than in FeSe. This may be an indication for the enhancement of high T_C in agreement with our result. This can lead to higher values of Tc. But from our calculation the effect of enhancement is high $FeSe_{0.5}Co_{0.5}$. From our calculation we noticed that the increment of DOS at Fermi level with all compared to the parent compound but $FeSe_{0.5}Co_{0.5}$ has the highest. We concluded that substitution of Co and Te has effect but $FeSe_{0.5}Co_{0.5}$ is a better candidate for further investigation.

References

[1] G. R. Stewart, Review of Modern Physics 83, (2011).

[2] P. Cheng, *et al*., Euro. Phys. Lett.**85**, 67003(2009).

[3] M. H. Fang, *et al*., Phys. Rev. **B 78** -224503 (2008).
[4] K. W. Yeh *et al*., Europhys. Lett. **84**-37002 (2008).
[*5] A. Subedi et al., Phys. Rev. B 78 -134514 (2008).*
[6] Alexander P. Koufos and Dimitrios A. Papaconstantopoulos, Phys. Rev. B 89, 035150 (2014)
[7] M. A. Afrassa, and Habtamu Beyene, Advances in Physics Theories and Applications, 77, 2019
[8] Xu Liu, J. Phys.: Condens. Matter 27 (2015) 183201
[9] Yoshikazu et al, J. Phys. Soc. Jpn. 78, 074712 (2009)
[10] A.S. Panfilov *et al.,* Fiz. Nizk. Temp. 40, 793–800 (2014)