

# Electronic and Superconductivity Properties of FeSe Superconductor

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## Abstract

We have investigated theoretically electronic and superconducting properties of FeSe superconductor. The calculated specific heat effective mass is found  $m^*/m_{band} = 2.15$ . This result is comparable with angle resolved photoemission spectroscopy data with the other Fe-pnictides compound. The electron-phonon coupling constant is found  $\lambda = 0.7$  for this superconductor. This result is also comparable with the results of linearized augmented plane wave method. It is observed that the FeSe system is more correlated system compared to the Fe element.

**Keywords:** FeSe Superconductors; Specific Heat; Effective Mass; Electron-phonon coupling constant.

## 1. Introduction

The discovery of superconductivity in Fe-pnictides [1] compounds has attracted tremendous interest the research activity in strongly correlated electron system. PbO type-FeSe phase has been reported to be a superconductor with transition temperature,  $T_c \sim 8$  K [2]. The newly discovered superconductor FeSe has been subjected to theoretical investigation by Subedi and his colleagues [3]. On the other hand the compounds  $\text{FeSe}_{1-x}\text{Te}_x$  ( $x = 0-1$ ), where Te substitution has an effect on superconductivity, have been investigated experimentally [4-5]. It was found that  $T_c$  increases with Te doping, reaching a maximum  $T_c \sim 15$  K at about 50-70% substitution, and then decreases with more Te doping. Recently a systematic theoretical examination of the effect of Te doping on electronic properties in  $\text{FeSe}_{1-x}\text{Te}_x$  system are discussed in [6].

The electronic properties namely the band effective mass  $m^*/m_{band}$  is not established well for Fe and Fe-pnictides compound such as FeSe compound.

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The experimental mass enhancement  $m^*/m_{band} = 1.3-2.1$  is observed in LaOFeP compound within the angle resolved photoemission spectroscopy (ARPES) data [7]. It is also comparable to the ARPES data [8] as well as the experimental data obtained by the low temperature specific heat data 1.4-2.1 [9] of Fe element.

However, it is significant lower than the renormalization seen in most transition metal oxides including the cuprate high temperature superconductors [10-11] and is not clear for the FeSe system. Moreover the experimental estimation mass enhancement is found  $m^*/m_{band} = 6-20$  for  $\text{FeSe}_{0.42}\text{Te}_{0.58}$  compound from the ARPES study [12].

On the hand electron-phonon coupling constant play an important role in superconductivity according to the McMillan equation. At ambient conditions, the electron-phonon coupling constant is found for FeSe compound  $\lambda = 0.603 - 0.65$  [13] by inverting the McMillan equation using the measured Debye temperature  $\theta_D$ . Other computational papers [3, 14] found this value of approximately  $\lambda = 0.15$  using linear response theory. It is not clear the source of discrepancy between these calculations. The effective mass enhancement and electron-phonon coupling constant for FeSe compound are not established well. It is therefore important to fully study the electronic structure of FeSe compound, and its implication to specific heat effective carrier mass as well as electron-phonon coupling constant.

We already performed the electronic (band and density of state (DOS)) and elastic properties (transverse  $v_t$ , longitudinal  $v_l$  wave velocity, and  $\theta_D$ ) calculations of  $\text{FeSe}_{1-x}\text{Te}_x$  [6,15] compounds using plane wave pseudopotential method (PWPP) within the frame work of the density functional theory [DFT] [16] implemented in CASTEP code [17]. The exchange correlation term is considered by the local density approximation (LDA). We also performed tight binding linear muffin-tin-orbitals method (TB-LMTO) with atomic sphere approximation (ASA) [18] in order to understand the basic electronic structure of FeSe compound [19]. We used these DOS and Debye temperature  $\theta_D$  for calculating the effective mass and electron phonon coupling constant  $\lambda$ .

In this work we studied the Sommerfeld coefficient and specific heat effective mass for FeSe compound. Finally we calculated the electron-phonon coupling constant  $\lambda$  for FeSe superconductor by inverting the McMillan equation using Debye temperature  $\theta_D$  and experimental critical temperature  $T_c$ . We discussed the results of effective mass and electron-phonon coupling constant in both the PWPP and LMTO methods.

## 2. Results and Discussions

### 2.1 Electronic properties of FeSe compound

In order to explain the electronic properties, we have taken the calculated value of DOS from our calculations [6, 19]. We obtained the DOS values in the PWPP and LMTO methods 1.49 and 1.81  $\text{eV}^{-1}$  on a per Fe both spins basis, respectively [6, 19]. This result is comparable to the 1.41 [20] using SPRKKR code. We can evaluate the Sommerfeld constant  $\gamma$  from density of state. The value of  $N(E_F)$  is directly proportional to the Sommerfeld constant [21]

$$\gamma = \frac{1}{3} \pi^2 N(E_F) K_B^2. \quad (1)$$

Here  $N(E_F)$  is the density of state in the Fermi level.  $K_B$  is the Boltzmann constant. We can calculate the Sommerfeld constant  $\gamma$  by using the formula (1). We obtained the  $\gamma$  values 3.51 [6] and 4.26 (mJ/molK<sup>2</sup>) in the PWPP and LMTO methods, respectively. On the other hand the experimental Sommerfeld constant for 9.17mJ/mol K<sup>2</sup> obtained low temperature specific heat [2]. The experimental estimations of  $\gamma$  for FeSe compound is quite larger than the calculated results. This is due to the electron-phonon interactions. The electron-phonon interactions are not included in the band structure calculations. The calculated electronic specific heat  $\gamma_{theor}$  can be compared with the available experimental data on the electronic specific heat coefficient  $\gamma_{exp}$ . The differences between  $\gamma_{theor}$  and  $\gamma_{exp}$  are usually attributed to the renormalization of one-electron effective masses due to the electron-phonon interaction. Therefore, we obtain the general expression of effective mass [21]

$$\frac{\gamma_{exp}}{\gamma_{theor}} = \frac{m^*}{m_{band}}. \quad (2)$$

We can calculate the specific heat effective mass from eq. (2), and obtain  $m^*/m_{band} = 2.61$  in PWPP method [6]. On the other hand we obtain  $m^*/m_{band} = 2.15$  in LMTO method. A sheet dependent mass enhancement  $m^*/m_{band} = 1.3-2.1$  is observed in 1111 Fe-pnictides of the form LaOFeP within the ARPES. The specific heat effective mass of FeSe compound is larger than the ARPES value of LaOFeP compound in PWPP method [6]. The LMTO method value is comparable with the ARPES data.

**Table 1:** The effective mass enhancement of different elements.

	LaOFeP	FeSe	Fe
$m^*/m$	1.3-2.1[7]	2.61[6]	1.4-2.1[9]
		2.15 <sup>a</sup>	

<sup>a</sup>This with LMTO method

## 2.2 Superconductivity properties of FeSe compound

The DOS calculations are used to calculate superconductivity parameters. We can calculate the electron-ion matrix element known as the Hopfield parameter,  $\eta_i$ [22], using the following formula [23] for each atom

$$\eta_i = N(E_F) \langle I^2 \rangle_i. \quad (3)$$

Where  $N(E_F)$  is the total DOS per spin at  $E_F$ .  $\langle I^2 \rangle_i$  is the electron-ion matrix element for each atom type, which is calculated by the Gaspari and Gyorffy theory [23]. It is given by the following equation

$$\langle I^2 \rangle_i = \frac{E_F}{\pi^2 N^2(E_F)} \sum_{l=0}^2 \frac{2(l+1) \sin^2(\delta_{l+1}^i - \delta_l^i) N_{l+1}^i N_l^i}{N_{l+1}^{(1),i} N_l^{(1),i}} \quad (4)$$

Where  $N_l^i$  are the per spin angular momenta ( $l$ ) components of the DOS at  $E_F$  for atom type  $i$ ,  $N_l^{(1),i}$  are the so-called free-scatterer DOS for atom type  $i$ , and  $\delta_l^i$  are scattering phase shifts calculated at the muffin-tin radius and at  $E_F$  for atom type  $i$ . Free-scatterer DOS are calculated by

$$N_l^{(1)} = \frac{\sqrt{E_F}}{\pi} (2l+1) \int_0^{R_S} r^2 u_l^2(r, E_F) dr, \quad (5)$$

and scattering phase shifts are calculated by

$$\tan \delta_l(R_S, E_F) = \frac{j_l(kR_S) - j_l(kR_S)L_l(k, R_S)}{n_l'(kR_S) - n_l'(kR_S)L_l(k, R_S)}, \quad (6)$$

where  $R_S$  is the muffin-tin radius,  $j_l$  are spherical Bessel functions,  $\eta_l$  are spherical Neumann functions,  $L_l = \frac{u_l'}{u_l}$  is the logarithmic derivative of the radial wave function,  $u_l$ , One can evaluate at  $R_S$  for different energies,  $k = \sqrt{E_F}$ . The  $u_l$  can compute by solving the radial wave equation at each  $k$  point in the Brillouin zone.

The Hopfield parameter is then used to calculate the electron-phonon coupling constant, which is obtained using the following equation from McMillan's strong-coupling theory [24]

$$\lambda = \sum_{i=1}^2 \frac{\eta_i}{M_i \langle \omega^2 \rangle}, \quad (7)$$

where  $M_i$  is the atomic mass of atom type  $i$ , and  $\langle \omega^2 \rangle$  is the average of the squared phonon frequency taken from the calculated Debye temperature of Chandra and his colleagues [15]. The Debye temperature is related to the phonon frequency by

$$\langle \omega^2 \rangle = \frac{1}{2} \theta_D^2. \quad (8)$$

The Debye temperature is proportional to the mean sound velocity  $v_m$  [25]:

$$\theta_D = \frac{h}{K_B} \sqrt[3]{\frac{3n}{4\pi V_0}} v_m, \quad (9)$$

where  $h$  is Planck's constant, the volume of unit cell of FeSe system is  $V_0 = 71.766 \text{ \AA}^3$  and  $n$  is the number of atoms in unit cell,  $v_m$  is the average wave velocity and can be obtained from the transverse  $v_t$  and longitudinal wave velocity  $v_l$ , respectively [25]

$$v_m = \left[ \frac{1}{3} \left( \frac{2}{v_t^3} + \frac{1}{v_l^3} \right) \right]^{1/3}. \quad (10)$$

We have taken  $v_t$  and  $v_l$  values from [14], and obtained the values of  $v_m$  as well as  $\theta_D$ . The estimated values of Debye temperature is 285 K [15]. We used this value for calculation of electron-phonon coupling constant. The McMillan equation for critical superconductivity transition temperature is given by the [24]

$$T_c = \frac{\theta_D}{1.45} \exp \left[ \frac{-1.04(1+\lambda)}{\lambda - \mu^*(1+\lambda)} \right]. \quad (11)$$

We have also taken the experimental  $T_c = 8\text{K}$  for FeSe from Ref. [3]. The  $\mu^*$  is the Coulomb pseudopotential, given by the Bennemann-Garland equation [26]

$$\mu^* = 0.13 \frac{N(E_F)}{1+N(E_F)}. \quad (12)$$

From the above expressions (7) and (11) we can determine the coupling constant  $\lambda$  into two ways. One method is first find the value Hopfield parameter  $\eta_i$  and phonon frequency by conversion of Debye temperatures. The last one is from direct conversion of superconducting critical temperature  $T_c$  and Debye temperature. In our calculation we have chosen the last one for determine the coupling constant. Our calculated Debye temperature is 285 K [15]. The critical transition temperature  $T_c$  is given 8 K for FeSe superconductor [3]. The calculated electron phonon- coupling constant is 0.7. This is comparable to the pressure dependent value 0.61-0.71 [27]. At ambient conditions, our electron-phonon coupling constant calculation  $\lambda$  is consistent with the value calculated by Ksenofontov and his colleagues [13],  $\lambda = 0.65$ , by inverting the McMillan equation using the measured  $\theta_D$ . Other calculations based on the linear response theory [3, 14] find values of approximately  $\lambda = 0.15$ . It is not clear to the source of discrepancy between the band calculations and linear response theory. Other iron-based superconducting material, LaFeAsO, electron-phonon coupling constants of approximately 0.2 [28, 29] have been reported. The LaFeAsO element is known to be on the verge of magnetic instability. This suggests that spin fluctuations are important in this material.

**Table 2:** The electron-phonon coupling constant of different elements.

	FeSe	LaFeAsO
$\lambda$	0.7 <sup>a</sup>	0.2 [28, 29]
		0.61-0.71[27]
		0.65[13]
		0.15[3]

### 3. Conclusions

In the present work we investigated electronic and superconductivity properties theoretically based on the first-principles DFT total energy calculations in PWPP and LMTO methods. The specific heat effective mass enhancement factor of FeSe compound is found to be 2.61 in FeSe compound in the PWPP and 2.15 in the LMTO methods, respectively. It is comparable to a sheet dependent mass enhancement  $m^*/m_{band} = 1.3-2.1$  is observed in Fe-pnictides of the form LaOFeP. The effective mass of FeSe compound is larger than in the Fe compound. It indicates that FeSe compound is more correlated compare to the Fe element. The calculated electron-phonon coupling constant is 0.7. This is comparable to the pressure dependent value 0.61-0.71. At ambient conditions, our electron-phonon coupling constant calculation  $\lambda = 0.603$  is consistent with the value calculated by Ksenofontov and his colleagues  $\lambda = 0.65$ , by inverting the McMillan equation using the measured  $\theta_D$ . Other calculations based on the linear response theory find values of approximately  $\lambda = 0.15$ . It is not clear the source of discrepancy between the band calculations and the linear response theory.

### 4. Recommendations

We have performed these calculations in the non-magnetic cases for FeSe compound. The calculations using the ferromagnetic, antiferromagnetic, and other magnetic orders should be considered for further study, but are beyond the scope of this paper.

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