

# Theoretical Study on the Effect of Multiband Structure on Critical Temperature and Electronic Specific Heat in SmOFeAs Iron Pnictide Superconductor

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# Abstract

In the present theoretical work, superconducting order parameter ( $\Delta$ ) and electronic specific heat ( $C_{es}$ ) of SmOFeAs iron pnictide (IP) superconductor has been studied using multiband (MB) model of IP superconductors. Attempt has been made to use the MB structure of IP superconductors and expressions for critical temperature ( $T_c$ ) and  $C_{es}$  are obtained, calculations being made for one, two and three bands of SmOFeAs. It has been found that MB results are close to the experimental value of  $T_c$  for this compound.  $C_{es}$  calculations show jump of  $1.5 \times 10^{-5}$  eV/atom K,  $4 \times 10^{-5}$  eV/atom K and  $4 \times 10^{-5}$ eV/atom K for one, two and three band models respectively. The study brings out the importance of MB structure in IPs, highlighting the fact that increasing the number of bands, increases  $T_c$ . The specific heat jump ( $\Delta C$ ) does not correspond to the BCS value, thereby proving that IPs are unconventional in nature.

# **Keywords**

Electronic Specific Heat, Iron Pnictide Superconductor, Multiband, Superconducting Order Parameter

# **1. Introduction**

The year 2006 [1] witnessed a major breakthrough in the field of superconductivity with the discovery of a new class of iron based superconductors called IPs. Further increase in  $T_c$  in the same class of SCs was witnessed in the year 2008 [2]. Researchers all over the world were amused at the discovery made by Hideo Hosono [3] and coworkers in the course of exploration of magnetic semiconductors. These transition metal based superconductors having general formula LnOFeAs (Ln = La, Ce, Sm, Gd, Nd, Pr) are layered structures with alternate LnO & FeAs layers, superconductivity believed to be present because of the FeAs layers. The structure orientation of Fe atoms shows it to be surrounded by four arsenic atoms resulting in a distorted tetrahedral geometry. The iron atoms are seen to make a square lattice and arsenic atoms are placed at the centre of each square being displaced above & below the Fe planes. IPs are second in class after the cuprates [4] to have high  $T_c$  of around 55 Kas shown by experimental studies of Ren and Chen [5] [6] and theoretical study by Mebrahtu [7]. Interest in this newly class of discovered materials was generated not only because of its high  $T_{o}$ but also because iron, being the most magnetic material [8] that could have been destructive for superconductivity, showed high values of  $T_{c}$ . Within a span of ten years, the quantum of research in this field is high because of the extraordinary properties exhibited by these compounds. It has been shown that in the normal state, these compounds are semi-metals [9] (upon doping [10] or application of pressure [11] [12] [13] [14] is seen to increase  $T_c$  in IPs). Several experimentation in this field is trying to study minutely various properties associated with them. Angle resolved photoemission experiments [15] have demonstrated that IPs are MB [16] [17] in nature. Iron has five bands at the Fermi surface and all the five d-bands of iron are relevant in studying the superconducting properties of these compounds as opposed to the single band of cuprates [18] [19] and BCS [20] superconductors or the two band MgB<sub>2</sub> [21] [22] [23]. Previous theories have found that MB nature [24] of IPs makes them a significant class in the vast area of superconductivity and that MB structure serves as an important ingredient for high  $T_c$  [25] for this class of compounds. The four unpaired d electrons of iron are seen to hybridise [26] with the three unpaired p electrons of arsenic, resulting in bands found at the Fermi surface due to overlapping orbitals [27] [28]. Raghu et al. has discussed that a minimal two band model [29] is needed for the superconducting IPs. Several others have also studied two bandsuperconductivity [30] [31] [32] [33]. Three band superconductivities [34] have also been studied using different theories like Eliashberg theory [35], Ginzburg Landau theory [36], etc.

Over the years, the MB property of IPs is exploited in understanding these materials in a better way. Earlier, also it has been found that interband interactions lead to higher  $T_c$  in cuprate SCs [37]. Since IPs are also MB SCs with nesting present at the Fermi surface, therefore it is desirable to investigate the role of interband and intraband interactions on various superconducting properties. Several properties of IPs are investigated to understand the mechanism of this special class of high temperature superconductors (HTS). The electronic specific heat of IPs is studied using electron-Cooper pair interaction by Mukubwa [38]. Mohamed *et al.* have explained pressure effect for HTS using pressure dependent Schrodinger equation and string theory [39]. With this motivation in mind,  $T_c$  and  $C_{es}$  of SmOFeAs compound [40] [41] [42] [43] is investigated using a MB

model, employing Green's function technique and the results are compared with experimental values.

#### 2. Mathematical Technique and Formulation

In the present theoretical work, the two thermodynamical properties which is  $\Delta$  and  $C_{es}$  of SmOFeAs are investigated as a function of the number of bands. The model Hamiltonian uses itinerant nature of electrons. It is described as:

$$H = \sum_{mk\sigma} E_{mk\sigma} C^{+}_{mk\sigma} C_{mk\sigma} - \sum_{mkk'} V_{mm} C^{+}_{mk\uparrow} C^{+}_{m-k\downarrow} C_{m-k\downarrow} C_{mk'\uparrow}$$

$$- V_{mn} \sum_{kk'\atop m\neq n} C^{+}_{mk\uparrow} C^{+}_{m-k\downarrow} C_{n-k'\downarrow} C_{nk'\uparrow}$$
(1)

In Equation (1), the first term represents energy of itinerant electrons. The second term denotes the intraband interaction term.  $V_{mm}$  is the intraband interaction potential. The third term is the interband interaction term. It represents tunnelling between the bands.  $V_{mn}$  is the interband interaction potential. m, n is band index, k is wave vector and  $\sigma$  is spin index for fermions.

Considering the two Green's functions

$$G_{\substack{\uparrow\uparrow\\rs\,qq}} = \left\langle \left\langle C_{rq\uparrow}, C_{sq\uparrow}^{+} \right\rangle \right\rangle \tag{2a}$$

$$G_{\downarrow\uparrow}_{rs-qq} = \left\langle \left\langle C^+_{r-q\downarrow}, C^+_{sq\uparrow} \right\rangle \right\rangle$$
(2b)

Here *r* and *s* are the band index and *q* denotes wave vector.

Using the first Green function (2a), the equation of motion is expressed as:

$$\left(\omega - E_{rq\uparrow}\right)G_{\uparrow\uparrow}_{rs\,q\,q} = \frac{1}{2\pi}\delta_{rs} - V_{rr}\Delta_{rr}G_{\downarrow\uparrow}_{rs-qq} - \sum_{n} V_{rn}\gamma_{\downarrow\downarrow}G_{\uparrow\uparrow}_{nsqq} - \sum_{n} V_{rn}\Delta_{nn}G_{\downarrow\uparrow}_{rs-qq}$$
(3)

Using the second Green function (2b), the second equation of motion is written as:

$$\left(\omega + E_{r-q\downarrow}\right)G_{\downarrow\uparrow}_{rs-qq} = -V_{rr}\Delta_{rr}G_{\uparrow\uparrow}_{rs\,qq} - V_{rm}\sum_{\substack{m\\m\neq r}}\Delta_{mm}G_{\uparrow\uparrow}_{rs\,qq} + V_{rm}\sum_{\substack{m\\m\neq r}}\gamma_{\uparrow\uparrow}G_{\downarrow\uparrow}_{ms-qq}$$
(4)

where the OPs are defined as:

$$\begin{split} \Delta_{rr} &= \sum_{k'} \left\langle C_{r-k'\downarrow}, C_{rk'\uparrow} \right\rangle \\ \Delta_{nn} &= \sum_{k'} \left\langle C_{n-k'\downarrow}, C_{nk'\uparrow} \right\rangle \\ \gamma_{\downarrow\downarrow} &= \sum_{k'} \left\langle C_{r-q\downarrow}^+, C_{n-k'\downarrow} \right\rangle \end{split}$$

is number factor representing number of charge per unit volume.

#### 2.1. One Band Model (OBM)

Using the two equations of Motion (3) and (4) and substituting r = s = 1, calculations are done for OBM using  $E_{1q\uparrow} = E_{1-q\downarrow}$  and  $G_1 = G_{\substack{\uparrow\uparrow\\11qq}}$  and  $G_2 = G_{\substack{\downarrow\uparrow\\11-aa}}$ 

 $\Delta$  is defined as:

$$\Delta_{11} = \sum_{K} V_{11} \left\langle C_{1k\uparrow}^{+}, C_{1-k\downarrow}^{+} \right\rangle$$
(5)

The correlation function (CF)  $\langle C_{1k\uparrow}^+, C_{1-k\downarrow}^+ \rangle$  is related to  $G_2$  as:

$$\left\langle C_{1k\uparrow}^{+}, C_{1-k\downarrow}^{+} \right\rangle = -\frac{1}{i} \int_{-\infty}^{\infty} \frac{G_{2}\left(\omega + i\varepsilon\right) - G_{2}\left(\omega - i\varepsilon\right)}{\mathrm{e}^{\frac{\omega}{kT}} - \eta} \tag{6}$$

where,  $\eta = -1$  for fermions, *k* is Boltzmann constant and *T* is absolute temperature in kelvin.

The expression of  $\Delta$  is obtained as:

$$\Delta_{11} = \frac{V_{11}^2 \Delta_{11}}{2\sqrt{E_{1q\uparrow}^2 + (V_{11}\Delta_{11})^2}} \tanh \frac{\sqrt{E_{1q\uparrow}^2 + (V_{11}\Delta_{11})^2}}{2kT}$$
(7)

Converting summation into integration with cut off energy  $\pm \hbar \omega_D$  from the Fermi level and substituting  $T \to T_C$  as  $\Delta \to 0$ :

$$1 = N_0 \int_0^{\hbar\omega_D} \frac{V_{11}}{2E_{1q\uparrow}} \tanh \frac{E_{1q\uparrow}}{2kT_C} dE_{1q\uparrow}$$
(8)

 $T_c$  can be expressed as:

$$1 = N_0 V_{11} \int_{0}^{\hbar\omega_D} \frac{1}{2\sqrt{E_{1q\uparrow}^2 + \overline{\Delta}_{11}^2}} \tanh \frac{\sqrt{E_{1q\uparrow}^2 + \overline{\Delta}_{11}^2}}{2kT} dE_{1q\uparrow}$$
(9)

Here  $\overline{\Delta}_{11} = V_{11}\Delta_{11}$ For OBM,  $C_{es}$  is defined as:

$$C_{es}^{1} = \frac{\partial}{\partial T} \frac{1}{N} \sum 2E_{1q\uparrow} \left\langle c_{1k\uparrow}^{+}, c_{1k\uparrow} \right\rangle$$
(10)

CF  $\langle C_{1k\uparrow}^+, C_{1k\uparrow}^- \rangle$  is related to  $G_1$  as:

$$\left\langle C_{1k\uparrow}^{+}, C_{1k\uparrow}^{-} \right\rangle = \frac{-1}{i} \int_{-\infty}^{\infty} \frac{G_{1}(\omega + iE) - G_{1}(\omega - iE)}{e^{\frac{\omega}{kT}} - \eta}$$
(11)

*C<sub>es</sub>* for OBM comes out as:

$$C_{es}^{1} = \frac{1}{2NkT^{2}} \sum E_{1q\uparrow}^{2} \operatorname{sech}^{2} \left( \frac{\sqrt{E_{1q\uparrow}^{2} + (V_{11}\Delta_{11})^{2}}}{2kT} \right)$$
(12)

Converting summation into integration,

$$C_{es}^{1} = \frac{1}{NkT^{2}} \int_{0}^{\hbar\omega_{D}} E_{1q\uparrow}^{2} \operatorname{sech}^{2} \left( \frac{\sqrt{E_{1q\uparrow}^{2} + (V_{11}\Delta_{11})^{2}}}{2kT} \right)$$
(13)

#### 2.2. Two Band Model (TBM)

Using the two equations of Motion (3) and (4) and substituting the four conditions: r = 1, s = 1; r = 1, s = 2; r = 2, s = 2 and r = 2, s = 1, calculations are done

for TBM using  $G_1 = G_{\uparrow\uparrow}$ ,  $G_2 = G_{\downarrow\uparrow}$ ,  $G_3 = G_{\uparrow2qq}$ ,  $G_4 = G_{\downarrow2qq}$ ,  $G_5 = G_{\uparrow\uparrow}$ ,  $G_6 = G_{\downarrow\uparrow\uparrow}$ ,  $E_{1q\uparrow} = E_{1-q\downarrow}^{11qq}$  and  $E_{2q\uparrow}^{11-qq} = E_{2-q\downarrow}^{-11qq}$ Similarly for TBM, the following results are obtained:

$$\left\langle C_{1k\uparrow}^{+}, C_{1-k\downarrow}^{+} \right\rangle = \frac{V_{11}\Delta_{11} + V_{12}\Delta_{22}}{2\sqrt{E_{1q\uparrow}^{2} + \left(V_{11}\Delta_{11} + V_{12}\Delta_{22}\right)^{2}}} \tanh \frac{\sqrt{E_{1q\uparrow}^{2} + \left(V_{11}\Delta_{11} + V_{12}\Delta_{22}\right)^{2}}}{2kT} \quad (14)$$

The second CF is obtained as:

$$\left\langle C_{2k\uparrow}^{+}, C_{2-k\downarrow}^{+} \right\rangle = \frac{V_{21}\Delta_{11} + V_{22}\Delta_{22}}{2\sqrt{E_{2q\uparrow}^{2} + \left(V_{21}\Delta_{11} + V_{22}\Delta_{22}\right)^{2}}} \tanh \frac{\sqrt{E_{2q\uparrow}^{2} + \left(V_{21}\Delta_{11} + V_{22}\Delta_{22}\right)^{2}}}{2kT}$$
(15)

 $C_{es}^{21}$  comes out as:

$$C_{es}^{21} = \frac{1}{2NkT^2\Delta_1\Delta_2}\sum E_{1q\uparrow}^2 \operatorname{sech}^2\left(\frac{\sqrt{E_{1q\uparrow}^2 + \Delta_1^2}}{2kT}\right)$$
(16)

Converting summation into integration,

$$C_{es}^{21} = \frac{1}{NkT^2 \Delta_1 \Delta_2} \int_0^{\hbar\omega_D} E_{1q\uparrow}^2 \operatorname{sech}^2 \left( \frac{\sqrt{E_{1q\uparrow}^2 + \Delta_1^2}}{2kT} \right)$$
(17)

 $C_{es}$  for the second band corresponding to  $G_5$  is defined as:

$$C_{es}^{22} = \frac{\partial}{\partial T} \frac{1}{N} \sum 2E_{2q\uparrow} \left\langle c_{2k\uparrow}^{+}, c_{2k\uparrow} \right\rangle$$
(18)

CF  $\langle C_{2k\uparrow}^+, C_{2k\uparrow}^- \rangle$  is related to  $G_5$  as:

$$\left\langle C_{2k\uparrow}^{+}, C_{2k} \right\rangle = \frac{\frac{-1}{i} \int_{-\infty}^{\infty} G_{5} \left( \omega + iE \right) - G_{5} \left( \omega - iE \right)}{e^{\frac{\omega}{kT}} - \eta}$$
(19)

 $C_{es}^{22}$  is calculated as:

$$C_{es}^{22} = \frac{1}{2NkT^2} \sum E_{2q\uparrow}^2 \operatorname{sech}^2 \left( \frac{\sqrt{E_{2q\uparrow}^2 + \Delta_2^2}}{2kT} \right)$$
(20)

Converting summation into integration,

$$C_{es}^{22} = \frac{1}{NkT^2} \int_{0}^{h\omega_D} E_{2q\uparrow}^2 \operatorname{sech}^2 \left( \frac{\sqrt{E_{2q\uparrow}^2 + \Delta_2^2}}{2kT} \right)$$
(21)

#### 2.3. Three Band Model (THBM)

Using the two equations of Motion (3) and (4) and substituting the following eight conditions,

*r* = 1, *s* = 1; *r* = 1, *s* = 2; *r* = 1, *s* = 3; *r* = 2, *s* = 1; *r* = 2, *s* = 2; *r* = 2, *s* = 3; *r* = 3, *s* = 1; r = 3, s = 2 and r = 3, s = 3, using the ten Green's functions  $G_1$  to  $G_{10}$  and making following substitutions:

$$E_{1q\uparrow} = E_{1-q\downarrow}, E_{21q\uparrow} = E_{2-q\downarrow}, E_{3q\uparrow} = E_{3-q\downarrow}$$

For the first band,

$$\left\langle C_{1k\uparrow}^{+}, C_{1-k\downarrow}^{+} \right\rangle = \frac{V_{11}\Delta_{11} + V_{12}\Delta_{22} + V_{13}\Delta_{33}}{2\sqrt{\Delta_{1}^{2} + \left(E_{1q\uparrow}^{+} + \frac{V_{12}V_{31}}{V_{32}}\gamma_{\uparrow\uparrow}\right)^{2}}} \tanh \frac{\sqrt{\Delta_{1}^{2} + \left(E_{1q\uparrow}^{+} + \frac{V_{12}V_{31}}{V_{32}}\gamma_{\uparrow\uparrow}\right)^{2}}}{2kT}$$
(22)

For the second band,  $\Delta$  is obtained as:

$$\Delta_{22} = \frac{V_{21}\Delta_{11} + V_{22}\Delta_{22} + V_{23}\Delta_{33}}{2\sqrt{E_{2q\uparrow}^2 + (V_{21}\Delta_{11} + V_{22}\Delta_{22} + V_{23}\Delta_{33})^2}} \times \tanh \frac{\sqrt{E_{2q\uparrow}^2 + (V_{21}\Delta_{11} + V_{22}\Delta_{22} + V_{23}\Delta_{33})^2}}{2kT}$$
(23)

For the third band, CF related to  $G_{10}$  is written as:

$$\left\langle C_{3k\uparrow}^{+}, C_{3-k\downarrow}^{+} \right\rangle = -\frac{1}{i} \int_{-\infty}^{\infty} \frac{G_{10} \left( \omega + i\varepsilon \right) - G_{10} \left( \omega - i\varepsilon \right)}{\mathrm{e}^{\frac{\omega}{KT}} - \eta}$$
(24)

The corresponding  $\Delta_{33} = V_{33} \langle C_{3k\uparrow}^+, C_{3-k\downarrow}^+ \rangle$  comes out to be:

$$\Delta_{33} = \frac{V_{31}\Delta_{11} + V_{32}\Delta_{22} + V_{33}\Delta_{33}}{2\sqrt{\left(V_{31}\Delta_{11} + V_{32}\Delta_{22} + V_{33}\Delta_{33}\right)^2 + \left(E_{3q\uparrow} + \frac{V_{32}V_{13}}{V_{12}}\gamma_{\uparrow\uparrow}\right)^2}} \\ \times \tanh \frac{\sqrt{\left(V_{31}\Delta_{11} + V_{32}\Delta_{22} + V_{33}\Delta_{33}\right)^2 + \left(E_{1q\uparrow} + \frac{V_{32}V_{13}}{V_{12}}\gamma_{\uparrow\uparrow}\right)^2}}{2kT}$$
(25)

For THBM, expression for  $C_{es}^{31}$  is:

$$C_{es}^{31} = \frac{1}{2NkT^2} \sum E_{1q\uparrow} \left( E_{1q\uparrow} + \frac{V_{12}V_{31}}{V_{32}} \gamma \right) \operatorname{sech}^2 \left( \frac{\sqrt{\left( E_{1q\uparrow} + \frac{V_{12}V_{31}}{V_{32}} \gamma \right)^2 + \Delta_1^2}}{2KT} \right)$$
(26)

Converting summation into integration gives:

$$C_{es}^{31} = \int_{0}^{\hbar\omega_{D}} \frac{1}{NkT^{2}} E_{1q\uparrow} \left( E_{1q\uparrow} + \frac{V_{12}V_{31}}{V_{32}}\gamma \right) \operatorname{sech}^{2} \left( \frac{\sqrt{\left( E_{1q\uparrow} + \frac{V_{12}V_{31}}{V_{32}}\gamma \right)^{2} + \Delta_{1}^{2}}}{2KT} \right)$$
(27)

 $C_{es}^{32}$  is calculated as:

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$$C_{es}^{32} = \frac{1}{2NkT^2} \sum E_{2q\uparrow}^2 \operatorname{sech}^2 \left( \frac{\sqrt{E_{2q\uparrow} + \Delta_2^2}}{2kT} \right)$$
(28)

Converting summation into integration,

$$C_{es}^{32} = \frac{1}{NkT^2} \int_0^{\hbar\omega_D} E_{2q\uparrow}^2 \operatorname{sech}^2\left(\frac{\sqrt{E_{2q\uparrow} + \Delta_2^2}}{2kT}\right)$$
(29)

 $C_{es}$  for the third band corresponding to  $G_9$  is:

$$C_{es}^{33} = \frac{\partial}{\partial T} \frac{1}{N} \sum 2E_{3q\uparrow} \left\langle c_{3k\uparrow}^{+}, c_{3k\uparrow} \right\rangle$$
(30)

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$$C_{es}^{33} = \frac{1}{2NkT^2} \sum E_{3q\uparrow} \sqrt{\xi^2 - \Delta_3^2} \operatorname{sech}^2 \frac{\sqrt{\left(E_{3q\uparrow} + \frac{V_{32}V_{13}}{V_{12}}\gamma\right)^2 + \Delta_3^2}}{2kT}$$
(31)

Converting summation into integration,

$$C_{es}^{33} = \frac{1}{NkT^2} \int_{0}^{\hbar\omega_D} E_{3q\uparrow} \left( E_{3q\uparrow} + \frac{V_{32}V_{13}}{V_{12}}\gamma \right) \operatorname{sech}^2 \frac{\sqrt{\left( E_{3q\uparrow} + \frac{V_{32}V_{13}}{V_{12}}\gamma \right)^2 + \Delta_3^2}}{2kT} \quad (32)$$

# 3. Results and Discussion

In this section, the numerical results obtained for  $T_c$  and  $C_{es}$  of MB SmOFeAs are presented. The results are investigated as a function of the number of bands, expressions being obtained for one, two and three band models, highlighting the MB nature of the superconducting compound.

#### 3.1. Variation of $\Delta$ with *T*

 $\Delta$  is a measure of the binding energy of Cooper pair. Its variation is studied with T as a function of the number of bands.

**Figure 1** shows the combined variation of  $\Delta_{11}$ ,  $\Delta_{22}$  and  $\Delta_{33}$  with *T* for OB, TB and THBMs illustrating the rise in  $T_c$  with increasing number of bands. It is seen that with increasing T,  $\Delta$  decreases and at  $T = T_{o} \Delta = 0$ . This is the usual behaviour of  $\Delta$  vs T and hence justified. T<sub>c</sub> for OBM comes out to be 11 K; for TBM,  $T_c$  is 45 K and for THBM it is 57 K. During calculations, the values of  $\hbar\omega_D =$ 0.05 eV,  $N = 10^{27}$  eV/atom,  $N_o V_{11} = 0.24$ .  $N_o V_{12} = 0.12$ ,  $N_o V_{13} = 0.06$ . The highest value of  $T_c$  is seen to be 57 K which is very well in agreement with experimental results [5].

#### 3.2. Variation of Ces with T

 $C_{es}$  is the amount of heat per unit mass required to raise the temperature by one unit. Its variation is studied with T as a function of the number of bands.

Using Equation (13), the variation of  $C_{es}^1$  with T for OBM shows that initially the SH for SC is less than the SH for normal state (NS), it then suddenly



**Figure 1.**  $\Delta_{11}$ ,  $\Delta_{22}$  and  $\Delta_{33}$  (meV) versus T(K) for OB, TB and THBM.



**Figure 2.**  $C_{es}^1$  (eV/atom-K) versus T(K) for OBM.

increases and then drags down at a particular T which is the  $T_c$  of the system which is 11 K as seen in the **Figure 2**. At  $T_c$  the curve shows a jump  $\Delta C$  of  $1.5 \times 10^{-5}$  eV/atom K which is contrary as seen in the BCS model [44].  $\Delta C^{/\gamma}T_c$  is calculated as 1.101 for the model which is also not in accordance with BCS model [45], thus signifying that IPs are unconventional SCs [46] [47].

**Figure 3** shows the combined graph of the variation of  $C_{es}^{21}$  and  $C_{es}^{22}$  with *T* for TBM illustrating that initially the SH of SC is less than the SH for NS, it then suddenly increases at 7 K and then drags down at the  $T_c$  for the system, observed at 45 K.  $\Delta C$  is  $4 \times 10^{-5}$  eV/atom K and  $\Delta C/\gamma T_c$  is calculated as 0.718 for the model. Both these values are not in accordance with BCS model, thereby showing that IPs are unconventional SCs.



**Figure 3.**  $C_{es}^{21}$  and  $C_{es}^{22}$  (eV/atom-K) versus T(K) for TBM.



**Figure 4.** SH  $C_{es}^{31}$ ,  $C_{es}^{32}$  and  $C_{es}^{33}$  (eV/atom-K) versus T(K) for THBM.

**Figure 4** shows the combined graph of the variation of  $C_{es}^{31}$ ,  $C_{es}^{32}$  and  $C_{es}^{33}$  with *T* for THBM illustrating that initially the SH of SC is less than the SH for NS, it then suddenly increases and then drags down at the *T<sub>c</sub>* for the system observed at 57 K.  $\Delta C$  is  $4 \times 10^{-5}$  eV/atom K and  $\Delta C/^{\gamma}T_{c}$  is calculated as 0.567 for the model. Both these values are not in accordance with BCS model proving IPs to be unconventional in nature. The value of Sommerfeld coefficient<sup> $\gamma$ </sup> for the compound SmOFeAs is 119.4 mJ/mol K<sup>2</sup> [45].

# 4. Conclusion

The present study has been undertaken to get some information regarding the

behaviour of  $T_c$  and electronic specific heat for superconducting SmOFeAs. It is seen that upon increasing the number of bands has shown an increase in  $T_c$  which is very well in agreement with experimental results, thereby proving that interband interactions play an important role in enhancing the  $T_c$ . Thus this study also supports that MB structures are helpful to stabilize superconductivity and for obtaining high  $T_c$  in this class of compounds. This appears reasonable as interband interactions are already found to enhance  $T_c$  [25]. The specific heat calculations reveal that IPs are governed by a mechanism other than the BCS one [46]. The sharp peak observed in the specific heat curve is attributed to AFM ordering of Sm<sup>3+</sup> magnetic ions in the system which is otherwise not seen in the lanthanum compound that has non-magnetic La<sup>3+</sup> ions [47]. The theoretical model is restricted uptil three bands as suggested by Ummarino [35] that a simple THBM in strong-coupling regime [48] [49] [50] can reproduce in a quantitative way the experimental  $T_c$ .

# **Conflicts of Interest**

The authors declare no conflicts of interest regarding the publication of this paper.

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