



**ELECTRICAL-AND-THERMOELECTRIC LAWS, RELATIONS, AND COEFFICIENTS IN n(p)-TYPE DEGENERATE GaP(1-x)Te(x)-CRYSTALLINE ALLOY, ENHANCED BY OUR STATIC DIELECTRIC CONSTANT LAW AND ELECTRICAL CONDUCTIVITY (VII)**

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### ABSTRACT

In the  $n^+(p^+) - p(n) X(x) \equiv \text{GaP}_{1-x}\text{Te}_x$  - crystalline alloy,  $0 \leq x \leq 1$ , the electrical-and-thermoelectric laws, relations, and various coefficients, enhanced by our static dielectric constant law given in Equations (1a, 1b), being due to the effects of the size of donor (acceptor) d(a)-radius  $r_{d(a)}$  and the x-concentration, by our electrical conductivity-formula given in Eq. (14), and finally by our accurate Fermi energy given in Eq. (11), are now investigated, basing on the same physical model and mathematical treatment method, as those used in our recent works (Van Cong, 2024, 2025). It should be noted here that, for  $x=0$ , these obtained numerical results may be reduced to those given in the n(p)-type degenerate GaP-crystal. Then,

some remarkable results could be cited in the following. In Tables 5n(5p) given Appendix 1, for a given impurity density N and with increasing temperature T, and then in Tables 6n(6p) given Appendix 1, for a given T and with decreasing N, the reduced Fermi-energy  $\xi_{n(p)}$  decreases, and other thermoelectric coefficients are in variations, as indicated by the arrows by: (increase: ↗, decrease: ↘). Further, one notes in these Tables that, for any given x and  $r_{d(a)}$ , with increasing T (or with decreasing N) one obtains: (i) for  $\xi_{n(p)} \approx 1.8138$ , while the numerical results of the Seebeck coefficient S present a same minimum

$(S)_{\min.} \left( \simeq -1.563 \times 10^{-4} \frac{V}{K} \right)$ , those of the figure of merit ZT show a same maximum  $(ZT)_{\max.} = 1$ , (ii) for  $\xi_{n(p)} = 1$ , the numerical results of S, ZT, the Mott figure of merit  $(ZT)_{Mott}$ , the first Van-Cong coefficient VC1, and the Thomson coefficient  $T_s$ , present the same results:  $-1.322 \times 10^{-4} \frac{V}{K}$ , 0.715, 3.290,  $1.105 \times 10^{-4} \frac{V}{K}$ , and  $1.657 \times 10^{-4} \frac{V}{K}$ , respectively, and finally (iii) for  $\xi_n \simeq 1.8138$ ,  $(ZT)_{Mott} = 1$ . It seems that these same results could represent **a new law in the thermoelectric properties, obtained in the degenerate case.**

**KEYWORDS:** Electrical conductivity, Seebeck coefficient (S), Figure of merit (ZT), First Van-Cong coefficient (VC1), Second Van-Cong coefficient (VC2), Thomson coefficient ( $T_s$ ), Peltier coefficient (Pt).

## INTRODUCTION

In the  $n^+(p^+) - p(n) X(x) \equiv GaP_{1-x}Te_x$ - crystalline alloy,  $0 \leq x \leq 1$ , the electrical-and-thermoelectric laws, relations, and various coefficients, enhanced by our static dielectric constant law,  $\epsilon(r_{d(a)}, x)$ ,  $r_{d(a)}$  being the donor (acceptor) d(a)-radius, given in Equations (1a, 1b) and new electrical conductivity, in Eq. (14), and also by our accurate Fermi energy,  $E_{Fn(Fp)}$ , given in Eq. (11), are now investigated, by basing on the same physical model and mathematical treatment method, as those used in our recent works (Van Cong, 2024, 2025). It should be noted here that for  $x=0$ , these obtained numerical results may be reduced to those given in the n(p)-type degenerate GaP-crystal (Van Cong, and Van Cong et al., 1980-2023; Hyun et al. 1998; Kim et al., 2015). Then, some remarkable results could be noted in the following.

(1) The generalized Mott criterium in the metal-insulator transition (MIT) is expressed in Equations (3, 5, 6), stating that the critical impurity density  $N_{CDn(CDp)}$  is just the density of electrons (holes), localized in the exponential conduction (valence)-band tail (EBT),  $N_{CDn(CDp)}^{EBT}$ , obtained with a precision of the order of  $2.92 \times 10^{-7}$ , as given in our recent work (Van Cong, 2024), and the effective electron (hole)-density can be defined by:  $N^* \equiv N - N_{CDn(CDp)} \simeq N - N_{CDn(CDp)}^{EBT}$ , N being the total impurity density, as that observed in the compensated crystals.

(2) The ratio of the inverse effective screening length  $k_{sn(sp)}$  to Fermi wave number  $k_{Fn(kp)}$  at 0 K,  $R_{sn(sp)}(N^*)$ , defined in Eq. (7), is valid at any  $N^*$ .

(3) The Fermi energy for any N and T,  $E_{Fn(Fp)}$ , determined in Eq. (11) with a precision of the order of  $2.11 \times 10^{-4}$  (Van Cong and Debiais, 1993), and it is present in all the expressions of electrical-and-thermoelectric coefficients.

(4) Our expressions for the electrical conductivity,  $\sigma$ , and for the Seebeck coefficient, S, determined respectively in Equations (14, 19) are the basic expressions, used to determine all the following electrical-and-thermoelectric coefficients.

(5) In Tables 5n(5p) given Appendix 1, for a given impurity density  $N$  and with increasing temperature T, and further in Tables 6n(6p) given Appendix 1, for a given  $T$  and with decreasing N, the reduced Fermi-energy  $\xi_{n(p)}$  decreases, and other thermoelectric coefficients are in variations, as indicated by the arrows by: (increase: ↗, decrease: ↘). Furthermore, one notes in these Tables that, for any given x and  $r_{d(a)}$ , with increasing T (or with decreasing N) one obtains: (i) for  $\xi_{n(p)} \simeq 1.8138$ , while the numerical results of the Seebeck coefficient S present a same minimum  $(S)_{min} (\simeq -1.563 \times 10^{-4} \frac{V}{K})$ , those of the figure of merit ZT show a same maximum  $(ZT)_{max} = 1$ , (ii) for  $\xi_{n(p)} = 1$ , the numerical results of S, ZT, the Mott figure of merit  $(ZT)_{Mott}$ , the first Van-Cong coefficient VC1, and the Thomson coefficient  $Ts$ , present the same results:  $-1.322 \times 10^{-4} \frac{V}{K}$ , 0.715, 3.290,  $1.105 \times 10^{-4} \frac{V}{K}$ , and  $1.657 \times 10^{-4} \frac{V}{K}$ , respectively, and finally (iii) for  $\xi_n \simeq 1.8138$ ,  $(ZT)_{Mott} = 1$ . It seems that these same results could represent **a new law in the thermoelectric properties, obtained in the degenerate case**.

## OUR STATIC DIELECTRIC CONSTANT LAW AND GENERALIZED MOTT CRITERIUM IN THE METAL-INSULATOR TRANSITION

First of all, in the  $n^+(p^+) - p(n) X(x)$ - crystalline alloy at T=0 K, we denote the donor (acceptor) d(a)-radius by  $r_{d(a)}$ , the corresponding intrinsic one by:  $r_{do(ao)} = r_{Sb(Ga)}$ , the unperturbed relative effective electron (hole) mass in conduction (valence) bands by:  $m_{c(v)}(x)/m_o$ , the unperturbed relative static dielectric constant by:  $\epsilon_o(x)$ , and the intrinsic band gap by:  $E_{go}(x)$ . Then, their values are reported in Table 1 in Appendix 1.

Therefore, we can define the effective donor (acceptor)-ionization energy in absolute values as:

$$E_{do(ao)}(x) = \frac{13600 \times [m_c(v)(x)/m_0]}{[\varepsilon_0(x)]^2} \text{ meV}, \text{ and then, the isothermal bulk modulus, by:}$$

$$B_{do(ao)}(x) \equiv \frac{E_{do(ao)}(x)}{\left(\frac{4\pi}{3}\right) \times (r_{do(ao)})^3}.$$

### Our Static Dielectric Constant Law

Here, the changes in all the energy-band-structure parameters, expressed in terms of the effective relative dielectric constant  $\varepsilon(r_{d(a)}, x)$ , developed as follows.

At  $r_{d(a)} = r_{do(ao)}$ , the needed boundary conditions are found to be, for the impurity-atom volume  $V = (4\pi/3) \times (r_{d(a)})^3$ ,  $V_{do(ao)} = (4\pi/3) \times (r_{do(ao)})^3$ , for the pressure  $p$ ,  $p_o = 0$ , and for the deformation potential energy (or the strain energy)  $\alpha$ ,  $\alpha_o = 0$ . Further, the two important equations, used to determine the  $\alpha$ -variation,  $\Delta \alpha \equiv \alpha - \alpha_o = \alpha$ , are defined by:

$$\frac{dp}{dv} = -\frac{B}{V} \text{ and } p = -\frac{d\alpha}{dv}, \text{ giving rise to: } \frac{d}{dv} \left( \frac{d\alpha}{dv} \right) = \frac{B}{V}. \text{ Then, by an integration, one gets:}$$

$$[\Delta\alpha(r_{d(a)}, x)]_{n(p)} = B_{do(ao)}(x) \times (V - V_{do(ao)}) \times \ln \left( \frac{V}{V_{do(ao)}} \right) = E_{do(ao)}(x) \times \left[ \left( \frac{r_{d(a)}}{r_{do(ao)}} \right)^3 - 1 \right] \times \ln \left( \frac{r_{d(a)}}{r_{do(ao)}} \right)^3 \geq 0.$$

Furthermore, we also showed that, as  $r_{d(a)} > r_{do(ao)}$  ( $r_{d(a)} < r_{do(ao)}$ ), the compression (dilatation) gives rise to the increase (the decrease) in the energy gap  $E_{eno(ep)}(r_{d(a)}, x)$ , and the effective donor (acceptor)-ionization energy  $E_{d(a)}(r_{d(a)}, x)$  in absolute values, obtained in the effective Bohr model, which is represented respectively by:  $\pm [\Delta\alpha(r_{d(a)}, x)]_{n(p)}$ ,

$$E_{eno(epo)}(r_{d(a)}, x) - E_{eo}(x) = E_{d(a)}(r_{d(a)}, x) - E_{do(ao)}(x) = E_{do(ao)}(x) \times \left[ \left( \frac{\varepsilon_0(x)}{\varepsilon(r_{d(a)})} \right)^2 - 1 \right] = + [\Delta\alpha(r_{d(a)}, x)]_{n(p)},$$

for  $r_{d(a)} \geq r_{do(ao)}$ , and for  $r_{d(a)} \leq r_{do(ao)}$ ,

$$E_{eno(epo)}(r_{d(a)}, x) - E_{eo}(x) = E_{d(a)}(r_{d(a)}, x) - E_{do(ao)}(x) = E_{do(ao)}(x) \times \left[ \left( \frac{\varepsilon_0(x)}{\varepsilon(r_{d(a)})} \right)^2 - 1 \right] = - [\Delta\alpha(r_{d(a)}, x)]_{n(p)}.$$

Therefore, one obtains the expressions for relative dielectric constant  $\varepsilon(r_{d(a)}, x)$  and energy band gap  $E_{gn(gp)}(r_{d(a)}, x)$ , as:

(i)-for  $r_{d(a)} \geq r_{do(ao)}$ , since  $\varepsilon(r_{d(a)}, x) = \frac{\varepsilon_0(x)}{\sqrt{1 + \left[ \left( \frac{r_{d(a)}}{r_{do(ao)}} \right)^3 - 1 \right] \times \ln \left( \frac{r_{d(a)}}{r_{do(ao)}} \right)^3}} \leq \varepsilon_0(x)$ , being a **new  $\varepsilon(r_{d(a)}, x)$ -law**,

$$E_{gno(gp)}(r_{d(a)}, x) - E_{go}(x) = E_{d(a)}(r_{d(a)}, x) - E_{do(ao)}(x) = E_{do(ao)}(x) \times \left[ \left( \frac{r_{d(a)}}{r_{do(ao)}} \right)^3 - 1 \right] \times \ln \left( \frac{r_{d(a)}}{r_{do(ao)}} \right)^3 \geq 0, \quad (1a)$$

according to the increase in both  $E_{gn(gp)}(r_{d(a)}, x)$  and  $E_{d(a)}(r_{d(a)}, x)$ , with increasing  $r_{d(a)}$  and for a given  $x$ , and

(ii)-for  $r_{d(a)} \leq r_{do(ao)}$ , since  $\varepsilon(r_{d(a)}, x) = \frac{\varepsilon_0(x)}{\sqrt{1 - \left[ \left( \frac{r_{d(a)}}{r_{do(ao)}} \right)^3 - 1 \right] \times \ln \left( \frac{r_{d(a)}}{r_{do(ao)}} \right)^3}} \geq \varepsilon_0(x)$ , with a condition, given by:  $\left[ \left( \frac{r_{d(a)}}{r_{do(ao)}} \right)^3 - 1 \right] \times \ln \left( \frac{r_{d(a)}}{r_{do(ao)}} \right)^3 < 1$ , being a **new  $\varepsilon(r_{d(a)}, x)$ -law**,

$$E_{gno(gp)}(r_{d(a)}, x) - E_{go}(x) = E_{d(a)}(r_{d(a)}, x) - E_{do(ao)}(x) = -E_{do(ao)}(x) \times \left[ \left( \frac{r_{d(a)}}{r_{do(ao)}} \right)^3 - 1 \right] \times \ln \left( \frac{r_{d(a)}}{r_{do(ao)}} \right)^3 \leq 0, \quad (1b)$$

corresponding to the decrease in both  $E_{gn(gp)}(r_{d(a)}, x)$  and  $E_{d(a)}(r_{d(a)}, x)$ , with decreasing  $r_{d(a)}$  and for a given  $x$ .

It should be noted that, in the following, all the electrical-and-thermoelectric properties strongly depend on this **new  $\varepsilon(r_{d(a)}, x)$ -law**.

Furthermore, the effective Bohr radius  $a_{Bn(Bp)}(r_{d(a)}, x)$  is defined by:

$$a_{Bn(Bp)}(r_{d(a)}, x) \equiv \frac{\varepsilon(r_{d(a)}, x) \times \hbar^2}{m_{c(v)}(x) \times m_0 \times q^2} = 0.53 \times 10^{-8} \text{ cm} \times \frac{\varepsilon(r_{d(a)}, x)}{m_{c(v)}(x)}. \quad (2)$$

### Generalized Mott Criterium in the MIT

Now, it is interesting to remark that the critical total donor (acceptor)-density in the MIT at  $T=0$  K,  $N_{CDn(NDp)}(r_{d(a)}, x)$ , was given by the Mott's criterium, with an empirical parameter,  $M_{n(p)}$ , as:

$$N_{CDn(CDp)}(r_{d(a)}, x)^{1/3} \times a_{Bn(Bp)}(r_{d(a)}, x) = M_{n(p)}, \quad M_{n(p)} = 0.25, \quad (3)$$

depending thus on our new  $\varepsilon(r_{d(a)}, x)$ -law.

This excellent one can be explained from the definition of the reduced effective Wigner-Seitz (WS) radius  $r_{sn(sp)}$ , characteristic of interactions, by:

$$r_{sn(sp)}(N, r_{d(a)}, x) \equiv \left(\frac{3}{4\pi N}\right)^{1/3} \times \frac{1}{a_{Bn(Bp)}(r_{d(a)}, x)} = 1.1723 \times 10^8 \times \left(\frac{1}{N}\right)^{1/3} \times \frac{m_c(v)(x) \times m_o}{\varepsilon(r_{d(a)}, x)}, \quad (4)$$

being equal to, in particular, at  $N=N_{CDn(CDp)}(r_{d(a)}, x)$ :  $r_{sn(sp)}(N_{CDn(CDp)}(r_{d(a)}, x), r_{d(a)}, x) = 2.4813963$ , for any  $(r_{d(a)}, x)$ -values. Then, from Eq. (4), one also has :

$$N_{CDn(CDp)}(r_{d(a)}, x)^{1/3} \times a_{Bn(Bp)}(r_{d(a)}, x) = \left(\frac{3}{4\pi}\right)^{\frac{1}{3}} \times \frac{1}{2.4813963} = 0.25 = (WS)_{n(p)} = M_{n(p)} \quad (5)$$

explaining thus the existence of the Mott's criterium.

Furthermore, by using  $M_{n(p)} = 0.25$ , according to the empirical Heisenberg parameter  $H_{n(p)} = 0.47137$ , as those given in our previous work (Van Cong, 2024), we have also showed that  $N_{CDn(CDp)}$  is just the density of electrons (holes) localized in the exponential conduction (valence)-band tail,  $N_{CDn(CDp)}^{EBT}$ , with a precision of the order of  $2.92 \times 10^{-7}$ .

It shoud be noted that the values of  $M_{n(p)}$  and  $H_{n(p)}$  could be chosen so that those of  $N_{CDn(CDp)}$  and  $N_{CDn(CDp)}^{EBT}$  are found to be in good agreement with their experimental results.

Therefore, the density of electrons (holes) given in parabolic conduction (valence) bands can be defined, as that given in compensated materials:

$$N^*(N, r_{d(a)}, x) \equiv N - N_{CDn(NDp)}(r_{d(a)}, x) = N^*, \text{ for a presentation simplicity.} \quad (6)$$

In summary, as observed in Table 4 of our previous paper (Van Cong, 2024), one remarks that, for a given  $x$  and an increasing  $r_{d(a)}$ ,  $\varepsilon(r_{d(a)}, x)$  decreases, while  $E_{gno(gpo)}(r_{d(a)}, x)$ ,  $N_{CDn(NDp)}(r_{d(a)}, x)$  and  $N_{CDn(CDp)}^{EBT}(r_{d(a)}, x)$  increase, affecting strongly all electrical-and-thermoelectric properties, as those observed in following Sections.

## PHYSICAL MODEL

In the  $n^+(p^+) - p(n)$   $\mathbf{X}(\mathbf{x})$ - crystalline alloy, if denoting the Fermi wave number by:

$$k_{Fn(Fp)}(N^*) \equiv \left( \frac{3\pi^2 N^*}{\epsilon_c(v)} \right)^{\frac{1}{3}}, \text{ the reduced effective Wigner-Seitz (WS) radius } r_{sn(sp)},$$

characteristic of interactions, being given in Eq. (4), in which  $N$  is replaced by  $N^*$ , is now defined by:

$$\gamma \times r_{sn(sp)}(N^*) \equiv \frac{k_{Fn(Fp)}^{-1}}{a_{Bn(Bp)}} < 1,$$

being proportional to  $N^{*-1/3}$ . Here,  $\gamma = (4/9\pi)^{1/3}$ ,  $k_{Fn(Fp)}^{-1}$  means the averaged distance between ionized donors (acceptors), and  $a_{Bn(Bp)}(r_{d(a)}, x)$  is determined in Eq. (2).

Then, the ratio of the inverse effective screening length  $k_{sn(sp)}$  to Fermi wave number  $k_{Fn(kp)}$  at 0 K is defined by:

$$R_{sn(sp)}(N^*) \equiv \frac{k_{sn(sp)}}{k_{Fn(Fp)}} = \frac{k_{Fn(Fp)}^{-1}}{k_{sn(sp)}^{-1}} = R_{snWS(spWS)} + [R_{snTF(spTF)} - R_{snWS(spWS)}] e^{-r_{sn(sp)}} < 1, \quad (7)$$

being valid at any  $N^*$ .

Here, these ratios,  $R_{snTF(spTF)}$  and  $R_{snWS(spWS)}$ , can be determined as follows.

First, for  $N \gg N_{CDn(NDp)}(r_{d(a)}, x)$ , according to the **Thomas-Fermi (TF)-approximation**, the ratio  $R_{snTF(spTF)}(N^*)$  is reduced to

$$R_{snTF(spTF)}(N^*) \equiv \frac{k_{snTF(spTF)}}{k_{Fn(Fp)}} = \frac{k_{Fn(Fp)}^{-1}}{k_{snTF(spTF)}^{-1}} = \sqrt{\frac{4\gamma r_{sn(sp)}}{\pi}} \ll 1, \quad (8)$$

being proportional to  $N^{*-1/6}$ .

Secondly, for  $N \ll N_{CDn(NDp)}(r_{d(a)})$ , according to the **Wigner-Seitz (WS)-approximation**, the ratio  $R_{snWS(snWS)}$  is respectively reduced to

$$R_{sn(sp)WS}(N^*) \equiv \frac{k_{sn(sp)WS}}{k_{Fn}} = 0.5 \times \left( \frac{s}{2\pi} - \gamma \frac{d[r_{sn(sp)}^2 \times E_{CE}(N^*)]}{dr_{sn(sp)}} \right), \quad (9)$$

where  $E_{CE}(N^*)$  is the majority-carrier correlation energy (CE), being determined by:

$$E_{CE}(N^*) = \frac{-0.87553}{0.0908 + r_{sn(sp)}} + \frac{\frac{0.87553}{0.0908 + r_{sn(sp)}} + \left( \frac{2[1 - \ln(2)]}{\pi^2} \right) \times \ln(r_{sn(sp)}) - 0.093288}{1 + 0.03847728 \times r_{sn(sp)}^{1.67878876}}.$$

Furthermore, in the highly degenerate case, the physical conditions are found to be given by:

$$\frac{k_{Fn(Fp)}^{-1}}{a_{Fn(Fp)}} < \frac{\eta_{n(p)}}{E_{Fn(Fp)}} \equiv \frac{1}{A_{n(p)}} < \frac{k_{Fn(Fp)}^{-1}}{k_{sn(sp)}^{-1}} \equiv R_{sn(sp)} < 1, \quad \eta_{n(p)}(N^*) \equiv \frac{\sqrt{2\pi N^*}}{\varepsilon(r_{d(a)})} \times q^2 k_{sn(sp)}^{-1/2}, \quad (10)$$

which gives:  $A_{n(p)}(N^*) = \frac{E_{Fn(Fp)}(N^*)}{\eta_{n(p)}(N^*)}$ .

## FERMI ENERGY AND FERMI-DIRAC DISTRIBUTION FUNCTION

### Fermi Energy

Here, for a presentation simplicity, we change all the sign of various parameters, given in the  $p^+ - X(x)$ -crystalline alloy in order to obtain the same one, as given in the  $n^+ - X(x)$ -crystalline alloy, according to the reduced Fermi energy  $E_{Fn(Fp)}$ ,  $\xi_{n(p)}(N, r_{d(a)}, x, T) \equiv \frac{E_{Fn(Fp)}(N, r_{d(a)}, x, T)}{k_B T} > 0 (< 0)$ , obtained respectively in the degenerate (non-degenerate) case.

For any  $(N, r_{d(a)}, x, T)$ , the reduced Fermi energy  $\xi_{n(p)}(N, r_{d(a)}, x, T)$  or the Fermi energy  $E_{Fn(Fp)}(N, r_{d(a)}, x, T)$ , obtained in our previous paper (Van Cong, Debiais, and Doan Khanh, 1991- 1993), obtained with a precision of the order of  $2.11 \times 10^{-4}$ , is found to be given by:

$$\xi_{n(p)}(u) \equiv \frac{E_{Fn(Fp)}(u)}{k_B T} = \frac{G(u) + A u^B F(u)}{1 + A u^B} \equiv \frac{V(u)}{W(u)}, \quad A = 0.0005372 \text{ and } B = 4.82842262, \quad (11)$$

where  $u$  is the reduced electron density,  $u(N, r_{d(a)}, x, T) \equiv \frac{N^*}{N_{c(v)}(T, x)}$ ,

$$N_{c(v)}(T, x) = 2g_{c(v)} \times \left(\frac{m_{c(v)}(x) \times m_0 \times k_B T}{2\pi\hbar^2}\right)^{\frac{3}{2}} \text{ (cm}^{-3}\text{)}, \quad g_{c(v)} = 1, \quad F(u) = au^{\frac{2}{3}} \left(1 + bu^{-\frac{4}{3}} + cu^{-\frac{8}{3}}\right)^{-\frac{2}{3}},$$

$$a = [3\sqrt{\pi}/4]^{2/3}, \quad b = \frac{1}{8} \left(\frac{\pi}{a}\right)^2, \quad c = \frac{62.3739855}{1920} \left(\frac{\pi}{a}\right)^4, \quad \text{and } G(u) \simeq \ln(u) + 2^{-\frac{3}{2}} \times u \times e^{-du},$$

$$d = 2^{3/2} \left[\frac{1}{\sqrt{27}} - \frac{3}{16}\right] > 0.$$

So, in the non-degenerate case ( $u \ll 1$ ), one has:  $E_{Fn(Fp)}(u) = k_B T \times G(u) \simeq k_B T \times \ln(u)$  as  $u \rightarrow 0$ , the limiting non-degenerate condition, and in the very degenerate case ( $u \gg 1$ ),

one gets:  $E_{Fn(Fp)}(u \gg 1) = k_B T \times F(u) = k_B T \times au^{\frac{2}{3}} \left(1 + bu^{-\frac{4}{3}} + cu^{-\frac{8}{3}}\right)^{-\frac{2}{3}} \simeq \frac{\hbar^2 \times k_{Fn(Fp)}^2(N^*)}{2 \times m_{c(v)}(x) \times m_0}$

as  $u \rightarrow \infty$ , the limiting degenerate condition. In other words,  $\xi_{n(p)} \equiv \frac{E_{Fn(Fp)}}{k_B T}$  is accurate, and it also verifies the correct limiting conditions.

In particular, at T=0K, since  $u^{-1} = 0$ , Eq. (11) is reduced to:  $E_{Fn(Fp)}(N^*) \equiv \frac{\hbar^2 \times k_{Fn(Fp)}^2(N^*)}{2 \times m_c(v) \times m_0}$ , being proportional to  $(N^*)^{2/3}$ , and also equal to 0 at  $N^* = 0$ , according to the MIT.

In the following, it should be noted that all the electrical-and-thermoelectric properties strongly depend on such the accurate expression of  $\xi_{n(p)}(N, r_{d(a)}, x, T)$ .

### Fermi-Dirac Distribution Function (FDDF)

The Fermi-Dirac distribution function (FDDF) is given by:  $f(E) \equiv (1 + e^\gamma)^{-1}$ ,  $\gamma \equiv (E - E_{Fn(Fp)})/(k_B T)$ .

So, the average of  $E^p$ , calculated using the FDDF-method, as developed in our previous work (Van Cong, 2018, 2025) is found to be given by:

$$\langle E^p \rangle_{FDDF} \equiv G_p(E_{Fn(Fp)}) \times E_{Fn(Fp)}^p \equiv \int_{-\infty}^{\infty} E^p \times \left(-\frac{\partial f}{\partial E}\right) dE, \quad -\frac{\partial f}{\partial E} = \frac{1}{k_B T} \times \frac{e^\gamma}{(1+e^\gamma)^2}.$$

Further, one notes that, at 0 K,  $-\frac{\partial f}{\partial E} = \delta(E - E_{Fn(Fp)})$ ,  $\delta(E - E_{Fn(Fp)})$  being the Dirac delta ( $\delta$ )-function. Therefore,  $G_p(E_{Fn(Fp)}) = 1$ .

Then, at low T, by a variable change  $\gamma \equiv (E - E_{Fn(Fp)})/(k_B T)$ , one has:

$$G_p(E_{Fn(Fp)}) \equiv 1 + E_{Fn(Fp)}^{-p} \times \int_{-\infty}^{\infty} \frac{e^\gamma}{(1+e^\gamma)^2} \times (k_B T \gamma + E_{Fn(Fp)})^p d\gamma = 1 + \sum_{\mu=1,2,\dots}^p C_p^\beta \times (k_B T)^\beta \times E_{Fn(Fp)}^{-\beta} \times I_\beta,$$

where  $C_p^\beta \equiv p(p-1)\dots(p-\beta+1)/\beta!$  and the integral  $I_\beta$  is given by:

$$I_\beta = \int_{-\infty}^{\infty} \frac{\gamma^\beta \times e^\gamma}{(1+e^\gamma)^2} d\gamma = \int_{-\infty}^{\infty} \frac{\gamma^\beta}{(e^{\gamma/2} + e^{-\gamma/2})^2} d\gamma, \text{ vanishing for odd values of } \beta. \text{ Then, for even}$$

values of  $\beta = 2n$ , with  $n=1, 2, \dots$ , one obtains:

$$I_{2n} = 2 \int_0^{\infty} \frac{\gamma^{2n} \times e^\gamma}{(1+e^\gamma)^2} d\gamma.$$

Now, using an identity  $(1 + e^\gamma)^{-2} \equiv \sum_{s=1}^{\infty} (-1)^{s+1} s \times e^{\gamma(s-1)}$ , a variable change:  $s\gamma = -t$ , the Gamma function:  $\int_0^{\infty} t^{2n} e^{-t} dt \equiv \Gamma(2n+1) = (2n)!$ , and also the definition of the Riemann's zeta function:  $\zeta(2n) \equiv 2^{2n-1} \pi^{2n} |B_{2n}| / (2n)!$ ,  $B_{2n}$  being the Bernoulli numbers, one finally gets:  $I_{2n} = (2^{2n} - 2) \times \pi^{2n} \times |B_{2n}|$ . So, from above Eq. of  $\langle E^p \rangle_{FDDF}$ , we get in the degenerate case the following ratio:

$$G_p(E_{Fn(Fp)}) \equiv \frac{\langle E^p \rangle_{FDDF}}{E_{Fn(Fp)}^p} = 1 + \sum_{n=1}^p \frac{p(p-1)\dots(p-2n+1)}{(2n)!} \times (2^{2n} - 2) \times |B_{2n}| \times y^{2n} \equiv G_{p \geq 1}(y), \quad (12)$$

$$\text{where } y \equiv \frac{\pi}{\xi_{n(p)}(N^*, T)} = \frac{\pi k_B T}{E_{Fn(Fp)}(N^*, T)}.$$

Then, some usual results of  $G_{p \geq 1}(y)$  are given in Table 2 in Appendix 1, being needed to determine all the following electrical-and-thermoelectric properties.

## ELECTRICAL-AND-THERMOELECTRIC PROPERTIES

Here, if denoting, for majority electrons (holes), the electrical conductivity by  $\sigma(N, r_{d(a)}, x, T)$  expressed in  $\text{ohm}^{-1} \times \text{cm}^{-1}$ , the thermal conductivity by  $\kappa(N, r_{d(a)}, x, T)$  in  $\frac{\text{W}}{\text{cm} \times \text{K}}$ , and the Lorenz number L defined by:

$L = \frac{\pi^2}{3} \times \left(\frac{k_B}{q}\right)^2 = 2.4429637 \left(\frac{\text{W} \times \text{ohm}}{\text{K}^2}\right) = 2.4429637 \times 10^{-8} (\text{V}^2 \times \text{K}^{-2})$ , then the well-known Wiedemann-Frank law states that the ratio,  $\frac{\kappa}{\sigma}$ , is proportional to the temperature T(K), as:

$$\frac{\kappa(N, r_{d(a)}, x, T)}{\sigma(N, r_{d(a)}, x, T)} = L \times T. \quad (13)$$

We now determine the general form of  $\sigma$  in the following.

First of all, it is expressed in terms of the kinetic energy of the electron (hole),  $E_k \equiv \frac{\hbar^2 \times k^2}{2 \times m_{Cn(Cp)} \times m_0}$ , or the wave number k, as:

$$\sigma(k) \equiv \frac{q^2 \times k}{\pi \times \hbar} \times \frac{k}{k_{sn(sp)}} \times [k \times a_{Bn(Bp)}] \times \left(\frac{E_k}{n_{n(p)}}\right)^{1/2},$$

which is thus proportional to  $E_k^2$ .

Then, for  $E \geq 0$ , we obtain:  $\langle E^2 \rangle_{FDDF} \equiv G_2(y = \frac{\pi k_B T}{E_{Fn(Fp)}}) \times E_{Fn(Fp)}^2$ , and  $G_2(y) = (1 + \frac{y^2}{3}) \equiv G_2(N, r_{d(a)}, x, T)$ , with  $y \equiv \frac{\pi}{\xi_{n(p)}} = \xi_{n(p)}(N, r_{d(a)}, x, T)$  for a presentation simplicity. Therefore, one obtains (Van Cong, 2025):

$$\begin{aligned} \sigma(N, r_{d(a)}, x, T) &\equiv \left[ \frac{q^2}{\pi \times \hbar} \times \frac{k_{Fn(Fp)}(N^*)}{R_{sn(sp)}(N^*)} \times [k_{Fn(Fp)}(N^*) \times a_{Bn(Bp)}(r_{d(a)})] \times \sqrt{A_{n(p)}(N^*)} \right] \times \\ &\left[ G_2(N, r_{d(a)}, x, T) \times \left( \frac{E_{Fn(Fp)}(N, r_{d(a)}, x, T)}{E_{Fn(Fp)}(N^*)} \right)^2 \right] \left( \frac{1}{\text{ohm} \times \text{cm}} \right), \\ \frac{q^2}{\pi \times \hbar} &= 7.7480735 \times 10^{-5} \text{ ohm}^{-1}, \quad A_{n(p)}(N^*) = \frac{E_{Fn(Fp)}(N^*)}{n_{n(p)}(N^*)}, \quad R_{sn(sp)}(N^*) \equiv \frac{k_{sn(sp)}}{k_{Fn(Fp)}}, \end{aligned} \quad (14)$$

which can be used to define the resistivity as:  $\rho(N, r_{d(a)}, x, T) \equiv 1/\sigma(N, r_{d(a)}, x, T)$ , noting again that  $N^* \equiv N - N_{CDn(NDp)}(r_{d(a)}, x)$ . This  $\sigma(N, r_{d(a)}, x, T)$ -result is an essential one in this paper, being used to determine other electrical-and-thermoelectric properties.

In Eq. (14), one notes that at  $T = 0$  K,  $\sigma(N, r_{d(a)}, x, T = 0K)$  is proportional to  $E_{Fn(Fp)}^2$ , or to  $(N^*)^{4/3}$ . Thus,  $\sigma(N = N_{CDn(NDp)}, r_{d(a)}, x, T = 0K) = 0$  at  $N^* = 0$ , at which the metal-insulator transition (MIT) occurs.

### Electrical Coefficients

The relaxation time  $\tau$  is related to  $\sigma$  by (Van Cong, 2025):

$$\tau(N, r_{d(a)}, x, T) \equiv \sigma(N, r_{d(a)}, x, T) \times \frac{m_{c(v)}(x) \times m_0}{q^2 \times N^*}. \text{ Therefore, the mobility } \mu \text{ is given by:}$$

$$\mu(N, r_{d(a)}, x, T) \equiv \mu(N^*, r_{d(a)}, T) = \frac{q \times \tau(N, r_{d(a)}, x, T)}{m_{c(v)}(x) \times m_0} = \frac{\sigma(N, r_{d(a)}, x, T)}{q \times N^*} \left( \frac{cm^2}{V \times s} \right). \quad (15)$$

Here, at  $T = 0$  K,  $\mu(N^*, r_{d(a)}, T)$  is thus proportional to  $(N^*)^{1/3}$ , since  $\sigma(N^*, r_{d(a)}, T = 0K)$  is proportional to  $(N^*)^{4/3}$ . Thus,  $\mu(N^* = 0, r_{d(a)}, T = 0K) = 0$  at  $N^* = 0$ , at which the metal-insulator transition (MIT) occurs.

Then, since  $\tau$  and  $\sigma$  are both proportional to  $E_{Fn(Fp)}(N^*, T)^2$ , as given above, the Hall factor is defined by:

$$r_H(N, r_{d(a)}, x, T) \equiv \frac{(\tau^2)_{FDDF}}{[(\tau)_{FDDF}]^2} = \frac{G_4(y)}{[G_2(y)]^2}, \quad y \equiv \frac{\pi}{\xi_{n(p)}(N, r_{d(a)}, x, T)} = \frac{\pi k_B T}{E_{Fn(Fp)}(N, r_{d(a)}, x, T)}, \text{ and therefore,}$$

the Hall mobility yields:

$$\mu_H(N, r_{d(a)}, x, T) \equiv \mu(N, r_{d(a)}, x, T) \times r_H(N^*, T) \left( \frac{cm^2}{V \times s} \right), \quad (16)$$

noting that, at  $T=0K$ , since  $r_H(N, r_{d(a)}, x, T) = 1$ , one then gets:

$$\mu_H(N, r_{d(a)}, x, T) \equiv \mu(N, r_{d(a)}, x, T).$$

### Our generalized Einstein relation

Our generalized Einstein relation is found to be defined as:

$$\frac{D(N, r_{d(a)}, x, T)}{\mu(N, r_{d(a)}, x, T)} \equiv \frac{N^*}{q} \times \frac{dE_{Fn(Fp)}}{dN^*} \equiv \frac{k_B \times T}{q} \times \left( u \frac{d\xi_{n(p)}(u)}{du} \right) = \sqrt{\frac{3 \times L}{\pi^2}} \times T \times \left( u \frac{d\xi_{n(p)}(u)}{du} \right), \quad \frac{k_B}{q} = \sqrt{\frac{3 \times L}{\pi^2}}$$

where  $D(N, r_{d(a)}, x, T)$  is the diffusion coefficient,  $\xi_{n(p)}(u)$  is defined in Eq. (11), and the mobility  $\mu(N, r_{d(a)}, x, T)$  is determined in Eq. (15). Then, by differentiating this function

$\xi_{n(p)}(u)$  with respect to  $u$ , one thus obtains  $\frac{d\xi_{n(p)}(u)}{du}$ . Therefore, Eq. (17) can also be rewritten as:

$$\frac{D(N, r_{d(a)}, x, T)}{\mu(N, r_{d(a)}, x, T)} = \frac{k_B \times T}{q} \times u \frac{V'(u) \times W(u) - V(u) \times W'(u)}{W^2(u)},$$

where  $W'(u) = ABu^{B-1}$  and  $V'(u) = u^{-1} + 2^{-\frac{s}{2}}e^{-du}(1 - du) + \frac{2}{s}Au^{B-1}F(u)\left[\left(1 + \frac{sB}{2}\right) + \frac{4}{s} \times \frac{bu^{-\frac{4}{s}+2cu^{-\frac{8}{s}}}}{1+bu^{-\frac{4}{s}+cu^{-\frac{8}{s}}}}\right]$ .

One remarks that: (i) as  $u \rightarrow 0$ , one has:  $W^2 \approx 1$  and  $u[V' \times W - V \times W'] \approx 1$ , and therefore:  $\frac{D_{n(p)}(u)}{\mu} \approx \frac{k_B \times T}{q}$ , and (ii) as  $u \rightarrow \infty$ , one has:  $W^2 \approx A^2u^{2B}$  and  $u[V' \times W - V \times W'] \approx \frac{2}{s}au^{2/3}A^2u^{2B}$ , and therefore, in this **highly degenerate case** and at  $T=0K$ , the **above generalized Einstein relation** is reduced to the **usual Einstein one**:  $\frac{D(N, r_{d(a)}, x, T=0 K)}{\mu(N, r_{d(a)}, x, T=0 K)} \approx \frac{2}{3}E_{Fno(Fpo)}(N^*)/q$ . In other words, **Eq. (17) verifies the correct limiting conditions**.

Furthermore, in the present degenerate case ( $u \gg 1$ ), Eq. (17) gives:

$$\frac{D(N, r_{d(a)}, x, T)}{\mu(N, r_{d(a)}, x, T)} \approx \frac{2}{3} \times \frac{E_{Fno(Fpo)}(u)}{q} \times \left[ 1 + \frac{4}{3} \times \frac{\left( bu^{-\frac{4}{s}+2cu^{-\frac{8}{s}}} \right)}{\left( 1+bu^{-\frac{4}{s}+cu^{-\frac{8}{s}}} \right)} \right], \quad (18)$$

where  $a = [3\sqrt{\pi}/4]^{2/3}$ ,  $b = \frac{1}{8}\left(\frac{\pi}{a}\right)^2$  and  $c = \frac{62.3739855}{1920}\left(\frac{\pi}{a}\right)^4$ .

In Tables 3n(3p) given in Appendix 1, for given  $x$ ,  $N > N_{CDn}$  and  $T=4.2$  K and  $77$  K, and from Equations (14, 15, 16, 17), the numerical results of the coefficients:  $\sigma$ ,  $\mu$ ,  $\mu_H$  and  $D$  are found to be decreased with increasing  $r_{d(a)}$ , respectively.

### Thermoelectric Coefficients

First of all, from Eq. (14), obtained for  $\sigma(N, r_{d(a)}, x, T)$ , the well-known Mott definition for the thermoelectric power or for the Seebeck coefficient,  $S$ , is found to be given by:

$$S(N, r_{d(a)}, x, T) \equiv \frac{-\pi^2}{3} \times \frac{k_B}{q > 0} \times k_B T \times \left. \frac{\partial \ln \sigma(E)}{\partial E} \right|_{E=E_{Fn(Fp)}} = \frac{-\pi^2}{3} \times \frac{k_B}{q} \times \frac{\partial \ln \sigma(\xi_{n(p)})}{\partial \xi_{n(p)}}.$$

Then, using Eq. (11), for the degenerate case,  $\xi_{n(p)} \geq 0$ , one gets, by putting

$$F_S(N, r_{d(a)}, x, T) \equiv \left[ 1 - \frac{y^2}{3 \times G_2(y = \frac{\pi}{\xi_{n(p)}})} \right],$$

$$S(N, r_{d(a)}, x, T) \equiv \frac{-\pi^2}{3} \times \frac{k_B}{q} \times \frac{2F_{SB}(N^*, T)}{\xi_{n(p)}} = -\sqrt{\frac{3 \times L}{\pi^2}} \times \frac{2 \times \xi_{n(p)}}{\left(1 + \frac{s \times \xi_{n(p)}^2}{\pi^2}\right)} = -2\sqrt{L} \times \frac{\sqrt{(ZT)_{Mott}}}{1+(ZT)_{Mott}} \left(\frac{V}{K}\right) < 0, \quad (ZT)_{Mott} = \frac{\pi^2}{3 \times \xi_{n(p)}^2}, \quad (19)$$

according to:

$$\frac{\partial S}{\partial \xi_{n(p)}} = \sqrt{\frac{3 \times L}{\pi^2}} \times 2 \times \frac{\frac{s \times \xi_{n(p)}^2}{\pi^2} - 1}{\left(1 + \frac{s \times \xi_{n(p)}^2}{\pi^2}\right)^2} = \sqrt{\frac{3 \times L}{\pi^2}} \times 2 \times \frac{(ZT)_{Mott} \times [1 - (ZT)_{Mott}]}{[1 + (ZT)_{Mott}]^2}.$$

Here, one notes that: (i) as  $\xi_{n(p)} \rightarrow +\infty$  or  $\xi_{n(p)} \rightarrow +0$ , one has a same limiting value of S:  $S \rightarrow -0$ , (ii) at  $\xi_{n(p)} = \sqrt{\frac{\pi^2}{3}} \simeq 1.8138$ , since  $\frac{\partial S}{\partial \xi_{n(p)}} = 0$ , one therefore gets: a minimum  $(S)_{min.} = -\sqrt{L} \simeq -1.563 \times 10^{-4} \left(\frac{V}{K}\right)$ , and (iii) at  $\xi_{n(p)} = 1$  one obtains:  $S \simeq -1.322 \times 10^{-4} \left(\frac{V}{K}\right)$ .

Further, the figure of merit, ZT, is found to be defined by:

$$ZT(N, r_{d(a)}, x, T) \equiv \frac{S^2 \times \sigma \times T}{\kappa} = \frac{S^2}{L} = \frac{4 \times (ZT)_{Mott}}{[1 + (ZT)_{Mott}]^2}. \quad (20)$$

Here, one notes that: (i)  $\frac{\partial(ZT)}{\partial \xi_{n(p)}} = 2 \times \frac{S}{L} \times \frac{\partial S}{\partial \xi_{n(p)}}$ ,  $S < 0$ , (ii) at  $\xi_{n(p)} = \sqrt{\frac{\pi^2}{3}} \simeq 1.8138$ , since  $\frac{\partial(ZT)}{\partial \xi_{n(p)}} = 0$ , one gets: a maximum  $(ZT)_{max.} = 1$ , and  $(ZT)_{Mott} = 1$ , and (iii) at  $\xi_{n(p)} = 1$ , one obtains:  $ZT \simeq 0.715$  and  $(ZT)_{Mott} = \frac{\pi^2}{3} \simeq 3.290$ .

Finally, the first Van-Cong coefficient, VC1, can be defined by:

$$VC1(N, r_{d(a)}, x, T) \equiv -N^* \times \frac{ds}{dN^*} \left(\frac{V}{K}\right) = N^* \times \frac{\partial s}{\partial \xi_{n(p)}} \times -\frac{\partial \xi_{n(p)}}{\partial N^*}, \quad \text{being equal to } 0 \quad \text{for } \xi_{n(p)} = \sqrt{\frac{\pi^2}{3}}, \quad (21)$$

and the second Van-Cong coefficient, VC2, as:

$$VC2(N, r_{d(a)}, x, T) \equiv T \times VC1(V), \quad (22)$$

the Thomson coefficient, Ts, by:

$$Ts(N, r_{d(a)}, x, T) \equiv T \times \frac{ds}{dT} \left(\frac{V}{K}\right) = T \times \frac{\partial s}{\partial \xi_{n(p)}} \times \frac{\partial \xi_{n(p)}}{\partial T}, \quad \text{being equal to } 0 \text{ for } \xi_{n(p)} = \sqrt{\frac{\pi^2}{3}}, \quad (23)$$

and the Peltier coefficient,  $P_t$ , as:

$$P_t(N, r_{d(a)}, x, T) \equiv T \times S(V). \quad (24)$$

One notes here that in next Tables 5n(p) and 6n(p) given in Appendix 1, obtained with such given physical conditions  $N$ (or  $T$ ) for the decreasing  $\xi_{n(p)}$ , since  $VC1(N, r_{d(a)}, x, T)$  and  $Ts(N, r_{d(a)}, x, T)$  are expressed in terms of  $\frac{-ds}{dn^*}$  and  $\frac{ds}{dT}$ , one has:  $[VC1, Ts] < 0$  for  $\xi_{n(p)} > \sqrt{\frac{\pi^2}{3}}$ ,

$[VC1, Ts] = 0$  for  $\xi_{n(p)} = \sqrt{\frac{\pi^2}{3}}$ , and  $[VC1, Ts] > 0$  for  $\xi_{n(p)} < \sqrt{\frac{\pi^2}{3}}$ , stating also that for

$$\xi_{n(p)} = \sqrt{\frac{\pi^2}{3}}:$$

(i)  $S$ , determined in Eq. (19), thus presents a same minimum  
 $(S)_{min.} = -\sqrt{L} \simeq -1.563 \times 10^{-4} \left(\frac{V}{K}\right)$ ,

(ii)  $ZT$ , determined in Eq. (20), therefore presents a same maximum:  $(ZT)_{max.} = 1$ , since the variations of  $ZT$  are expressed in terms of  $[VC1, Ts] \times S$ ,  $S < 0$ .

Furthermore, it is interesting to remark that the (VC2)-coefficient is related to our generalized Einstein relation (17) by:

$$\frac{k_B}{q} \times VC2(N, r_{d(a)}, x, T) \equiv -\frac{\partial S}{\partial \xi_{n(p)}} \times \frac{D(N, r_{d(a)}, x, T)}{\mu(N, r_{d(a)}, x, T)} \left(\frac{V^2}{K}\right), \quad \frac{k_B}{q} = \sqrt{\frac{3 \times L}{\pi^2}}, \quad (25)$$

according, in this work, with the use of our Eq. (21), to:

$$VC2(N, r_{d(a)}, x, T) \equiv -\frac{D(N, r_{d(a)}, x, T)}{\mu(N, r_{d(a)}, x, T)} \times 2 \times \frac{(ZT)_{Mott} \times [1 - (ZT)_{Mott}]}{[1 + (ZT)_{Mott}]^2} (V).$$

Of course, our relation (25) is reduced to:  $\frac{D}{\mu}$ ,  $VC1$  and  $VC2$ , being determined respectively by Equations (17, 21, 22).

Now, in the degenerate n(p)-type  $X(x)$  – alloy, and for  $N > N_{CDn(CDp)}$ , and for  $T=3K$  (80K), the numerical results of various thermoelectric coefficients are reported in Tables 4n(4p) in Appendix 1, noting that their variations with increasing  $r_{d(a)}$  are represented by the arrows: ↗ (increase), and ↘ (decrease), respectively.

Then, in Tables 5n(5p) given Appendix 1 for a given  $N$  and with increasing  $T$ , and in Tables 6n(6p) given Appendix 1 for a given  $T$  and with decreasing  $N$ , the reduced Fermi-energy

$\xi_{n(p)}$  decreases, and various thermoelectric coefficients are in variations, as indicated by the arrows as: (increase: ↗, decrease: ↘).

## CONCLUDING REMARKS

Here, some concluding remarks can be given as follows.

(1) In the  $n^+(p^+) - p(n) X(x) \equiv GaP_{1-x}Te_x$ - crystalline alloy,  $0 \leq x \leq 1$ , the electrical-and-thermoelectric laws, relations, and various coefficients are found to be enhanced by our static dielectric constant law,  $\epsilon(r_{d(a)}, x)$ , being decreased with increasing  $r_{d(a)}$ , as given in Equations (1a, 1b) and also in Table 2 of our recent work (2024), by our new electrical conductivity, as given in Eq. (14), and in particular by our accurate Fermi energy,  $E_{Fn(Fp)}$ , as given in Eq. (11), which exists in all the electrical-and-thermoelectric formula.

(2) The generalized Mott criterium in the MIT is expressed in Equations (3, 5, 6), stating that the critical impurity density  $N_{CDn(CDp)}$  is just the density of electrons (holes), localized in the exponential conduction (valence)-band tail,  $N_{CDn(CDp)}^{EBT}$ , obtained with a precision of the order of  $2.92 \times 10^{-7}$ , as given in our previous work (2024), and the effective electron (hole)-density can be defined by:  $N^* \equiv N - N_{CDn(CDp)} \simeq N - N_{CDn(CDp)}^{EBT}$ , as that observed in the compensated crystals.

(3) The ratio of the inverse effective screening length  $k_{sn(sp)}$  to Fermi wave number  $k_{Fn(kp)}$  at 0 K,  $R_{sn(sp)}(N^*)$ , defined in Eq. (7), is valid for any density  $N^*$ .

(4) In Tables 5n(5p) given Appendix 1, for a given impurity density  $N$  and with increasing temperature  $T$ , and then in Tables 6n(6p) given Appendix 1, for a given  $T$  and with decreasing  $N$ , the reduced Fermi-energy  $\xi_{n(p)}$  decreases, and other thermoelectric coefficients are in variations, as indicated by the arrows by: (increase: ↗, decrease: ↘). One remarks in these Tables that, for any given  $x$  and  $r_{d(a)}$ , with increasing  $T$  (or with decreasing  $N$ ) one obtains: (i) for  $\xi_{n(p)} \simeq 1.8138$ , while the numerical results of the Seebeck coefficient  $S$  present a same minimum  $(S)_{min.} = -\sqrt{L} \simeq -1.563 \times 10^{-4} \left(\frac{V}{K}\right)$ , those of the figure of merit ZT show a same maximum  $(ZT)_{max.} = 1$ , (ii) for  $\xi_{n(p)} = 1$ , the numerical results of  $S$ , ZT, the Mott figure of merit  $(ZT)_{Mott}$ , the Van-Cong coefficient VC1, and the Thomson coefficient  $Ts$ , present the same results:  $-1.322 \times 10^{-4} \frac{V}{K}$ ,  $0.715$ ,  $3.290$ ,  $1.105 \times 10^{-4} \frac{V}{K}$ ,

and  $1.657 \times 10^{-4} \frac{V}{K}$ , respectively, and finally (iii) for  $\xi_n \simeq 1.8138$ ,  $(ZT)_{Mott} = 1$ . It seems that these same results could represent a new law given for the thermoelectric properties, obtained in the degenerate case.

(5) Finally, our electrical-and-thermoelectric relation is given in Eq. (25) by:

$$\frac{k_B}{q} \times VC2(N, r_{d(a)}, x, T) \equiv -\frac{\partial S}{\partial \xi_{n(p)}} \times \frac{D(N, r_{d(a)}, x, T)}{\mu(N, r_{d(a)}, x, T)} \left( \frac{V^2}{K} \right), \quad \frac{k_B}{q} = \sqrt{\frac{3 \times L}{\pi^2}}, \quad \text{according, in this work, to:}$$

$$VC2(N, r_{d(a)}, x, T) \equiv -\frac{D(N, r_{d(a)}, x, T)}{\mu(N, r_{d(a)}, x, T)} \times 2 \times \frac{(ZT)_{Mott} \times [1 - (ZT)_{Mott}]}{[1 + (ZT)_{Mott}]^2} (V), \quad \text{being reduced to: } \frac{D}{\mu},$$

VC1 and VC2, determined respectively in Equations (17, 21, 22). This should be a new result.

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**APPENDIX 1: Tables**

**Table 1:** The values of energy-band-structure parameters are given in the following.

In the  $\text{GaP}_{1-x}\text{Te}_x$ -crystalline alloy, in which  $r_{d0(ao)} = r_{P(\text{Ga})} = 0.110 \text{ nm}$  ( $0.126 \text{ nm}$ ), we have:  
 $g_{c(v)}(x) = 1 \times x + 1 \times (1 - x)$ ,  $m_{c(v)}(x)/m_0 = 0.209 (0.4) \times x + 0.13 (0.5) \times (1 - x)$ ,  
 $\varepsilon_0(x) = 12.3 \times x + 11.1 \times (1 - x)$ ,  $E_{go}(x) = 1.796 \times x + 1.796 \times (1 - x)$ .

**Table 2:** Expressions for  $G_{p=1}(y \equiv \frac{\pi}{\xi_{n(p)}})$ , due to the Fermi-Dirac distribution function, noting that  $G_{p=1}(y \equiv \frac{\pi k_B T}{E_F n(F_p)} = \frac{\pi}{\xi_{n(p)}}) = 1$ , used to determine the electrical-and-thermoelectric coefficients.

|  |                       |   |             |  |                                |              |
|--|-----------------------|---|-------------|--|--------------------------------|--------------|
| $G_{3/2}(y)$                                 | $G_2(y)$              | $G_{5/2}(y)$                              | $G_3(y)$    | $G_{7/2}(y)$                                 | $G_4(y)$                       | $G_{9/2}(y)$ |
| $(1 + \frac{y^2}{8} + \frac{7y^4}{640})$     | $(1 + \frac{y^2}{3})$ | $(1 + \frac{5y^2}{8} - \frac{7y^4}{384})$ | $(1 + y^2)$ | $(1 + \frac{35y^2}{24} + \frac{49y^4}{384})$ | $(1 + 2y^2 + \frac{7y^4}{15})$ |              |
| $(1 + \frac{21y^2}{8} + \frac{147y^4}{128})$ |                       |   |             |  |                                |              |

**Table 3n:** Here, one notes that, for given  $x$ ,  $N > N_{CDN}$  and  $T(=4.2 \text{ K} \text{ and } 77 \text{ K})$ , the functions:  $\sigma, \mu, \mu_H, D$ , expressed respectively in  $(\frac{10^2}{\text{ohm} \times \text{cm}}, \frac{10^3 \times \text{cm}^2}{\text{V} \times \text{s}}, \frac{10^3 \times \text{cm}^2}{\text{V} \times \text{s}}, \frac{10 \times \text{cm}^2}{\text{s}})$ , decrease with increasing  $r_d$ .

| Donor<br>$r_d$ (nm) | P     | As    | Sb    | Sn |
|---------------------|-------|-------|-------|----|
| 0.110               | 0.118 | 0.136 | 0.140 |    |

For  $x=0$ , the values of  $(\sigma, \mu, \mu_H, D)$  at 4.2K

| N ( $10^{18} \text{ cm}^{-3}$ ) |                          |                          |                          |                          |
|---------------------------------|--------------------------|--------------------------|--------------------------|--------------------------|
| 3                               | 6.57, 1.447, 1.448, 5.42 | 6.34, 1.403, 1.404, 5.23 | 4.62, 1.080, 1.081, 3.89 | 4.16, 0.997, 0.997, 3.53 |
| 10                              | 17.0, 1.082, 1.082, 9.28 | 16.5, 1.049, 1.049, 8.99 | 12.6, 0.813, 0.813, 6.90 | 11.6, 0.753, 0.753, 6.36 |
| 40                              | 50.7, 0.795, 0.795, 17.3 | 49.0, 0.768, 0.768, 16.7 | 37.2, 0.585, 0.585, 12.7 | 34.3, 0.540, 0.540, 11.7 |
| 70                              | 79.8, 0.714, 0.714, 22.6 | 77.1, 0.689, 0.689, 21.8 | 57.9, 0.519, 0.519, 16.4 | 53.3, 0.478, 0.478, 15.1 |

For  $x=0.5$ , the values of  $(\sigma, \mu, \mu_H, D)$  at 4.2K

| N ( $10^{18} \text{ cm}^{-3}$ ) |                          |                          |                          |                          |
|---------------------------------|--------------------------|--------------------------|--------------------------|--------------------------|
| 3                               | 5.36, 1.248, 1.249, 3.45 | 5.15, 1.210, 1.211, 3.32 | 3.56, 0.936, 0.937, 2.39 | 3.12, 0.866, 0.867, 2.13 |
| 10                              | 14.4, 0.927, 0.927, 6.04 | 13.9, 0.899, 0.899, 5.85 | 10.5, 0.699, 0.699, 4.45 | 9.60, 0.648, 0.648, 4.09 |
| 40                              | 42.9, 0.675, 0.675, 11.2 | 41.5, 0.653, 0.653, 10.9 | 31.5, 0.499, 0.499, 8.29 | 29.0, 0.462, 0.462, 7.64 |
| 70                              | 67.4, 0.604, 0.604, 14.6 | 65.1, 0.583, 0.583, 14.1 | 49.0, 0.441, 0.441, 10.7 | 45.1, 0.407, 0.407, 9.83 |

For  $x=1$ , the values of  $(\sigma, \mu, \mu_H, D)$  at 4.2K

| N ( $10^{18} \text{ cm}^{-3}$ ) |                          |                          |                          |                          |
|---------------------------------|--------------------------|--------------------------|--------------------------|--------------------------|
| 3                               | 4.45, 1.117, 1.119, 2.38 | 4.25, 1.084, 1.086, 2.29 | 2.70, 0.847, 0.849, 1.56 | 2.26, 0.789, 0.791, 1.35 |
| 10                              | 12.5, 0.823, 0.824, 4.29 | 12.1, 0.799, 0.799, 4.15 | 8.97, 0.623, 0.623, 3.13 | 8.14, 0.578, 0.578, 2.86 |
| 40                              | 37.6, 0.594, 0.594, 8.02 | 36.4, 0.575, 0.575, 7.75 | 27.6, 0.442, 0.442, 5.91 | 25.4, 0.409, 0.409, 5.45 |
| 70                              | 59.0, 0.530, 0.530, 10.4 | 57.0, 0.512, 0.512, 10.1 | 43.0, 0.389, 0.389, 7.61 | 39.5, 0.359, 0.359, 7.00 |

For  $x=0$ , the values of  $(\sigma, \mu, \mu_H, D)$  at 77 K

| N ( $10^{18} \text{ cm}^{-3}$ ) |                          |                          |                          |                          |
|---------------------------------|--------------------------|--------------------------|--------------------------|--------------------------|
| 3                               | 7.10, 1.566, 1.829, 5.75 | 6.86, 1.518, 1.776, 5.56 | 5.03, 1.176, 1.389, 4.14 | 4.54, 1.088, 1.291, 3.77 |
| 10                              | 17.3, 1.098, 1.136, 9.39 | 16.7, 1.065, 1.102, 9.10 | 12.8, 0.825, 0.854, 6.98 | 11.8, 0.764, 0.792, 6.43 |
| 40                              | 50.8, 0.797, 0.801, 17.4 | 49.1, 0.770, 0.774, 16.8 | 37.3, 0.587, 0.590, 12.7 | 34.4, 0.542, 0.545, 11.7 |
| 70                              | 79.9, 0.714, 0.716, 22.6 | 77.2, 0.690, 0.692, 21.9 | 58.0, 0.520, 0.521, 16.4 | 53.3, 0.478, 0.479, 15.1 |

For  $x=0.5$ , the values of  $(\sigma, \mu, \mu_H, D)$  at 77 K

| N ( $10^{18} \text{ cm}^{-3}$ ) |                          |                          |                          |                          |
|---------------------------------|--------------------------|--------------------------|--------------------------|--------------------------|
| 3                               | 6.16, 1.435, 1.848, 3.85 | 5.93, 1.394, 1.799, 3.71 | 4.19, 1.101, 1.465, 2.72 | 3.71, 1.030, 1.391, 2.45 |
| 10                              | 14.7, 0.952, 1.008, 6.12 | 14.3, 0.923, 0.978, 5.97 | 10.8, 0.718, 0.762, 4.55 | 9.87, 0.666, 0.707, 4.18 |
| 40                              | 43.1, 0.678, 0.684, 11.3 | 41.7, 0.656, 0.662, 10.9 | 31.6, 0.501, 0.506, 8.32 | 29.1, 0.463, 0.468, 7.67 |
| 70                              | 67.5, 0.605, 0.607, 14.7 | 65.2, 0.584, 0.587, 14.2 | 49.1, 0.442, 0.444, 10.7 | 45.2, 0.407, 0.409, 9.85 |

For  $x=1$ , the values of ( $\sigma, \mu, \mu_H, D$ ) at 77 K

| N ( $10^{19} \text{ cm}^{-3}$ ) |                          |                          |                          |                          |
|---------------------------------|--------------------------|--------------------------|--------------------------|--------------------------|
| 3                               | 5.53, 1.390, 2.007, 2.93 | 5.31, 1.354, 1.965, 2.84 | 3.51, 1.102, 1.730, 2.20 | 2.98, 1.040, 1.708, 2.08 |
| 10                              | 13.0, 0.858, 0.935, 4.43 | 12.6, 0.832, 0.908, 4.28 | 9.38, 0.651, 0.714, 3.24 | 8.51, 0.605, 0.665, 2.96 |
| 40                              | 37.8, 0.598, 0.607, 8.05 | 36.6, 0.579, 0.587, 7.79 | 27.8, 0.445, 0.451, 5.94 | 25.6, 0.411, 0.417, 5.47 |
| 70                              | 59.2, 0.531, 0.535, 10.4 | 57.1, 0.514, 0.517, 10.1 | 43.1, 0.390, 0.393, 7.63 | 39.7, 0.360, 0.362, 7.02 |

**Table 3p:** Here, one notes that, for given  $x$ ,  $N > N_{CDP}$  and  $T = 4.2 \text{ K}$  and  $77 \text{ K}$ , the functions:  $\sigma, \mu, \mu_H, D$ , expressed respectively in  $\left( \frac{10^3}{\text{ohm} \times \text{cm}}, \frac{10^2 \times \text{cm}^2}{\text{V} \times \text{s}}, \frac{10^2 \times \text{cm}^2}{\text{V} \times \text{s}}, \frac{10 \times \text{cm}^2}{\text{s}} \right)$ , decrease with increasing  $r_a$ .

| Acceptor   | Ga    | Mg    | In    | Cd    |
|------------|-------|-------|-------|-------|
| $r_a$ (nm) | 0.126 | 0.140 | 0.144 | 0.148 |

For  $x=0$ , the values of ( $\sigma, \mu, \mu_H, D$ ) at 4.2K

| N ( $10^{19} \text{ cm}^{-3}$ ) |                          |                          |                          |                          |
|---------------------------------|--------------------------|--------------------------|--------------------------|--------------------------|
| 3                               | 1.27, 3.892, 3.894, 1.41 | 1.11, 3.699, 3.701, 1.26 | 1.00, 3.596, 3.598, 1.17 | 0.88, 3.491, 3.494, 1.07 |
| 5                               | 2.15, 3.330, 3.331, 1.90 | 1.93, 3.123, 3.124, 1.73 | 1.80, 3.006, 3.007, 1.63 | 1.65, 2.879, 2.880, 1.52 |
| 8                               | 3.34, 2.959, 2.959, 2.45 | 3.03, 2.755, 2.755, 2.24 | 2.85, 2.639, 2.639, 2.12 | 2.64, 2.510, 2.510, 1.99 |
| 10                              | 4.08, 2.815, 2.815, 2.75 | 3.71, 2.614, 2.614, 2.53 | 3.50, 2.498, 2.499, 2.39 | 3.26, 2.371, 2.371, 2.24 |

For  $x=0.5$ , the values of ( $\sigma, \mu, \mu_H, D$ ) at 4.2K

| N ( $10^{19} \text{ cm}^{-3}$ ) |                          |                          |                          |                          |
|---------------------------------|--------------------------|--------------------------|--------------------------|--------------------------|
| 3                               | 1.78, 4.614, 4.616, 2.07 | 1.59, 4.331, 4.333, 1.89 | 1.48, 4.171, 4.173, 1.78 | 1.35, 3.997, 3.999, 1.65 |
| 5                               | 2.86, 4.055, 4.056, 2.73 | 2.60, 3.775, 3.776, 2.50 | 2.44, 3.616, 3.616, 2.37 | 2.27, 3.439, 3.439, 2.21 |
| 8                               | 4.34, 3.663, 3.664, 3.49 | 3.96, 3.393, 3.393, 3.20 | 3.74, 3.238, 3.238, 3.03 | 3.49, 3.066, 3.066, 2.84 |
| 10                              | 5.28, 3.507, 3.507, 3.92 | 4.83, 3.241, 3.241, 3.59 | 4.56, 3.089, 3.089, 3.40 | 4.26, 2.919, 2.920, 3.19 |

For  $x=1$ , the values of ( $\sigma, \mu, \mu_H, D$ ) at 4.2K

| N ( $10^{19} \text{ cm}^{-3}$ ) |                          |                          |                          |                          |
|---------------------------------|--------------------------|--------------------------|--------------------------|--------------------------|
| 3                               | 2.40, 2.682, 2.684, 3.06 | 2.18, 5.291, 5.292, 2.80 | 2.05, 2.067, 2.069, 2.65 | 1.90, 4.820, 4.821, 2.48 |
| 5                               | 3.78, 5.090, 5.091, 3.99 | 3.45, 4.713, 4.713, 3.66 | 3.26, 4.496, 4.497, 3.47 | 3.04, 4.256, 4.257, 3.25 |
| 8                               | 5.70, 4.659, 4.660, 5.10 | 5.21, 4.297, 4.297, 4.67 | 4.93, 4.089, 4.089, 4.43 | 4.61, 3.857, 3.857, 4.15 |
| 10                              | 6.92, 4.484, 4.484, 5.73 | 6.33, 4.128, 4.129, 5.25 | 5.99, 3.924, 3.924, 4.97 | 5.61, 3.697, 3.697, 4.66 |

For  $x=0$ , the values of ( $\sigma, \mu, \mu_H, D$ ) at 77K

| N ( $10^{19} \text{ cm}^{-3}$ ) |                          |                          |                          |                          |
|---------------------------------|--------------------------|--------------------------|--------------------------|--------------------------|
| 3                               | 1.38, 4.229, 4.983, 1.50 | 1.21, 4.061, 4.866, 1.36 | 1.11, 3.981, 4.839, 1.27 | 0.99, 3.920, 4.868, 1.17 |
| 5                               | 2.23, 3.445, 3.706, 1.96 | 2.00, 3.238, 3.497, 1.78 | 1.87, 3.121, 3.382, 1.68 | 1.72, 2.996, 3.261, 1.57 |
| 8                               | 3.39, 3.008, 3.118, 2.48 | 3.08, 2.802, 2.908, 2.27 | 2.90, 2.684, 2.789, 2.15 | 2.69, 2.555, 2.658, 2.01 |
| 10                              | 4.12, 2.848, 2.923, 2.78 | 3.76, 2.645, 2.717, 2.55 | 3.54, 2.529, 2.599, 2.41 | 3.30, 2.401, 2.469, 2.26 |

For  $x=0.5$ , the values of ( $\sigma, \mu, \mu_H, D$ ) at 77K

| N ( $10^{19} \text{ cm}^{-3}$ ) |                          |                          |                          |                          |
|---------------------------------|--------------------------|--------------------------|--------------------------|--------------------------|
| 3                               | 1.88, 4.873, 5.457, 2.16 | 1.69, 4.590, 5.172, 1.97 | 1.57, 4.432, 5.019, 1.86 | 1.44, 4.264, 4.862, 1.73 |
| 5                               | 2.93, 4.156, 4.386, 2.78 | 2.66, 3.873, 4.094, 2.55 | 2.51, 3.711, 3.628, 2.41 | 2.33, 3.533, 3.746, 2.26 |
| 8                               | 4.40, 3.709, 3.813, 3.52 | 4.01, 3.436, 3.534, 3.23 | 3.79, 3.279, 3.374, 3.06 | 3.54, 3.106, 3.197, 2.87 |
| 10                              | 5.33, 3.538, 3.611, 3.94 | 4.87, 3.271, 3.339, 3.62 | 4.60, 3.117, 3.183, 3.43 | 4.30, 2.947, 3.010, 3.22 |

For  $x=1$ , the values of ( $\sigma, \mu, \mu_H, D$ ) at 77K

| N ( $10^{19} \text{ cm}^{-3}$ ) |                          |                          |                          |                          |
|---------------------------------|--------------------------|--------------------------|--------------------------|--------------------------|
| 3                               | 2.50, 5.904, 6.406, 3.15 | 2.27, 5.505, 5.988, 2.89 | 2.14, 5.277, 5.751, 2.73 | 1.98, 5.026, 5.492, 2.56 |
| 5                               | 3.85, 5.183, 5.396, 4.05 | 3.52, 4.801, 5.001, 3.71 | 3.32, 4.581, 4.775, 3.52 | 3.10, 4.338, 4.525, 3.30 |
| 8                               | 5.76, 4.703, 4.803, 5.13 | 5.26, 4.338, 4.431, 4.71 | 4.98, 4.128, 4.217, 4.46 | 4.66, 3.895, 3.980, 4.19 |

10 6.97, 4.515, 4.586, 5.76 6.38, 4.157, 4.223, 5.28 6.03, 3.952, 4.014, 5.00 5.64, 3.723, 3.783, 4.69

**Table 4n:** In the lightly degenerate n-type  $\text{X}(\text{x})$  – alloy, and for  $T=3\text{K}$  and  $80\text{K}$ , the numerical results of various thermoelectric coefficients are reported. Further, their variations with increasing  $r_{d(a)}$  are represented by the arrows:  $\nearrow$  (increase), and  $\searrow$  (decrease).

| Donor  | P          | As      | Sb      | Sn      |
|--|------------|---------|---------|---------|
| <b>For <math>x=0</math> and <math>N=3 \times 10^{18} \text{ cm}^{-3}</math>,</b>       |            |         |         |         |
| $\xi_n(T=3\text{K})$   | $\searrow$ | 217.111 | 216.464 | 208.752 |
| $\xi_n(T=80\text{K})$  | $\searrow$ | 8.298   | 8.274   | 7.991   |
| $\kappa_{(T=3\text{K})} \left( \frac{10^{-5} \times W}{\text{cm}^2 \times K} \right)$  | $\searrow$ | 4.812   | 4.644   | 3.386   |
| $\kappa_{(T=80\text{K})} \left( \frac{10^{-5} \times W}{\text{cm}^2 \times K} \right)$ | $\searrow$ | 1.396   | 1.348   | 0.989   |
| $-S_{(T=3\text{K})} \left( \frac{10^{-6} \times V}{K} \right)$                         | $\searrow$ | 2.611   | 2.619   | 2.716   |
| $-S_{(T=80\text{K})} \left( \frac{10^{-5} \times V}{K} \right)$                        | $\searrow$ | 6.521   | 6.538   | 6.748   |
| $-VC1_{(T=3\text{K})} \left( \frac{10^{-6} \times V}{K} \right)$                       | $\searrow$ | 1.740   | 1.746   | 1.810   |
| $-VC1_{(T=80\text{K})} \left( \frac{10^{-5} \times V}{K} \right)$                      | $\searrow$ | 3.799   | 3.806   | 3.889   |
| $-VC2_{(T=3\text{K})} \left( \frac{10^{-6} \times V}{K} \right)$                       | $\searrow$ | 5.222   | 5.237   | 5.431   |
| $-VC2_{(T=80\text{K})} \left( \frac{10^{-5} \times V}{K} \right)$                      | $\searrow$ | 3.039   | 3.045   | 3.111   |
| $-Ts_{(T=3\text{K})} \left( \frac{10^{-6} \times V}{K} \right)$                        | $\searrow$ | 2.611   | 2.619   | 2.715   |
| $-Ts_{(T=80\text{K})} \left( \frac{10^{-5} \times V}{K} \right)$                       | $\searrow$ | 5.699   | 5.709   | 5.834   |
| $-Pt_{(T=3\text{K})}(10^{-6} \times V)$  | $\searrow$ | 7.834   | 7.857   | 8.148   |
| $-Pt_{(T=80\text{K})}(10^{-3} \times V)$   | $\searrow$ | 5.217   | 5.231   | 5.398   |
| $ZT_{(T=3\text{K})}(10^{-4})$  | $\nearrow$ | 2.791   | 2.808   | 3.019   |
| $ZT_{(T=80\text{K})}(10^{-1})$   | $\nearrow$ | 1.741   | 1.750   | 1.864   |
| <b>For <math>x=0.5</math> and <math>N=3 \times 10^{18} \text{ cm}^{-3}</math>,</b>     |            |         |         |         |
| $\xi_n(T=3\text{K})$   | $\searrow$ | 160.564 | 159.608 | 148.081 |
| $\xi_n(T=80\text{K})$  | $\searrow$ | 6.233   | 6.198   | 5.780   |
| $\kappa_{(T=3\text{K})} \left( \frac{10^{-5} \times W}{\text{cm}^2 \times K} \right)$  | $\searrow$ | 3.927   | 3.775   | 2.610   |
| $\kappa_{(T=80\text{K})} \left( \frac{10^{-5} \times W}{\text{cm}^2 \times K} \right)$ | $\searrow$ | 1.217   | 1.172   | 0.828   |
| $-S_{(T=3\text{K})} \left( \frac{10^{-6} \times V}{K} \right)$                         | $\searrow$ | 3.531   | 3.552   | 3.828   |
| $-S_{(T=80\text{K})} \left( \frac{10^{-5} \times V}{K} \right)$                        | $\searrow$ | 8.387   | 8.426   | 8.931   |
| $-VC1_{(T=3\text{K})} \left( \frac{10^{-6} \times V}{K} \right)$                       | $\searrow$ | 2.353   | 2.367   | 2.551   |
| $-VC1_{(T=80\text{K})} \left( \frac{10^{-5} \times V}{K} \right)$                      | $\searrow$ | 4.411   | 4.421   | 4.545   |
| $-VC2_{(T=3\text{K})} \left( \frac{10^{-6} \times V}{K} \right)$                       | $\searrow$ | 7.059   | 7.101   | 7.653   |
| $-VC2_{(T=80\text{K})} \left( \frac{10^{-5} \times V}{K} \right)$                      | $\searrow$ | 3.529   | 3.537   | 3.636   |
| $-Ts_{(T=3\text{K})} \left( \frac{10^{-6} \times V}{K} \right)$                        | $\searrow$ | 3.529   | 3.551   | 3.827   |
| $-Ts_{(T=80\text{K})} \left( \frac{10^{-5} \times V}{K} \right)$                       | $\searrow$ | 6.616   | 6.632   | 6.817   |
| $-Pt_{(T=3\text{K})}(10^{-5} \times V)$  | $\searrow$ | 1.059   | 1.065   | 1.148   |
| $-Pt_{(T=80\text{K})}(10^{-3} \times V)$   | $\searrow$ | 6.709   | 6.741   | 7.144   |
| $ZT_{(T=3\text{K})}(10^{-4})$  | $\nearrow$ | 5.103   | 5.164   | 5.999   |
| $ZT_{(T=80\text{K})}(10^{-1})$   | $\nearrow$ | 2.879   | 2.906   | 3.265   |

**For x=1 and N=3 × 10<sup>18</sup> cm<sup>-3</sup>,**

|  |   |         |         |         |        |
|--|---|---------|---------|---------|--------|
| $\xi_n(T=3K)$  | ↘ | 123.803 | 122.518 | 106.781 | 99.466 |
| $\xi_n(T=80K)$   | ↘ | 4.888   | 4.839   | 4.215   | 3.893  |
| $\kappa_{(T=3K)} \left( \frac{10^{-5} \times W}{cm \times K} \right)$  | ↘ | 3.258   | 3.113   | 1.979   | 1.656  |
| $\kappa_{(T=80K)} \left( \frac{10^{-8} \times W}{cm \times K} \right)$ | ↘ | 1.095   | 1.050   | 0.693   | 0.585  |
| $-S_{(T=3K)} \left( \frac{10^{-6} \times V}{K^4} \right)$              | ↘ | 4.579   | 4.627   | 5.308   | 5.698  |
| $-S_{(T=80K)} \left( \frac{10^{-4} \times V}{K} \right)$               | ↘ | 1.020   | 1.027   | 1.135   | 1.197  |
| $-VC1_{(T=3K)} \left( \frac{10^{-5} \times V}{K} \right)$              | ↘ | 3.051   | 3.083   | 3.536   | 3.795  |
| $-VC1_{(T=80K)} \left( \frac{10^{-5} \times V}{K} \right)$             | ↘ | 4.915   | 4.946   | 5.564   | 6.001  |
| $-VC2_{(T=3K)} \left( \frac{10^{-6} \times V}{K} \right)$              | ↘ | 9.152   | 9.248   | 10.608  | 11.386 |
| $-VC2_{(T=80K)} \left( \frac{10^{-3} \times V}{K} \right)$             | ↘ | 3.932   | 3.957   | 4.451   | 4.801  |
| $-Ts_{(T=3K)} \left( \frac{10^{-6} \times V}{K} \right)$               | ↘ | 4.576   | 4.624   | 5.304   | 5.693  |
| $-Ts_{(T=80K)} \left( \frac{10^{-5} \times V}{K} \right)$              | ↘ | 7.372   | 7.420   | 8.347   | 9.001  |
| $-Pt_{(T=3K)} (10^{-5} \times V)$                                      | ↗ | 1.374   | 1.388   | 1.592   | 1.709  |
| $-Pt_{(T=80K)} (10^{-3} \times V)$                                     | ↗ | 8.157   | 8.219   | 9.080   | 9.573  |
| $ZT_{(T=3K)} (10^{-4})$  | ↗ | 8.582   | 8.763   | 11.534  | 13.292 |
| $ZT_{(T=80K)} (10^{-1})$   | ↗ | 4.255   | 4.320   | 5.274   | 5.861  |

**Table 4p:** In the lightly degenerate p-type X(x) – alloy, in which N=2 × 10<sup>19</sup> cm<sup>-3</sup>, and for T=3K and 80K, the numerical results of various thermoelectric coefficients are reported. Further, their variations with increasing  $r_d(a)$  are represented by the arrows: ↗ (increase), and ↘ (decrease).

| Acceptor   |   | Ga      | Mg      | In      | Cd     |
|--|---|---------|---------|---------|--------|
| <b>For x=0,</b>  |   |         |         |         |        |
| $\xi_n(T=3K)$  | ↘ | 134.452 | 119.021 | 107.417 | 90.933 |
| $\xi_n(T=80K)$   | ↘ | 5.283   | 4.706   | 4.241   | 3.483  |
| $\kappa_{(T=3K)} \left( \frac{10^{-5} \times W}{cm \times K} \right)$  | ↘ | 5.576   | 4.510   | 3.828   | 2.983  |
| $\kappa_{(T=80K)} \left( \frac{10^{-8} \times W}{cm \times K} \right)$ | ↘ | 1.824   | 1.535   | 1.338   | 1.054  |
| $-S_{(T=3K)} \left( \frac{10^{-6} \times V}{K} \right)$                | ↘ | 4.216   | 4.763   | 5.277   | 6.233  |
| $-S_{(T=80K)} \left( \frac{10^{-5} \times V}{K} \right)$               | ↘ | 9.601   | 10.490  | 11.301  | 12.806 |
| $-VC1_{(T=3K)} \left( \frac{10^{-6} \times V}{K} \right)$              | ↘ | 2.809   | 3.173   | 3.515   | 4.151  |
| $-VC1_{(T=80K)} \left( \frac{10^{-5} \times V}{K} \right)$             | ↘ | 4.716   | 5.044   | 5.530   | 6.430  |
| $-VC2_{(T=3K)} \left( \frac{10^{-6} \times V}{K} \right)$              | ↘ | 8.428   | 9.519   | 10.545  | 12.452 |
| $-VC2_{(T=80K)} \left( \frac{10^{-3} \times V}{K} \right)$             | ↘ | 3.772   | 4.035   | 4.424   | 5.144  |
| $-Ts_{(T=3K)} \left( \frac{10^{-6} \times V}{K} \right)$               | ↘ | 4.214   | 4.760   | 5.273   | 6.226  |
| $-Ts_{(T=80K)} \left( \frac{10^{-5} \times V}{K} \right)$              | ↘ | 7.073   | 7.567   | 8.295   | 9.646  |
| $-Pt_{(T=3K)} (10^{-5} \times V)$                                      | ↘ | 1.265   | 1.429   | 1.583   | 1.870  |
| $-Pt_{(T=80K)} (10^{-3} \times V)$                                     | ↘ | 7.681   | 8.392   | 9.041   | 10.245 |
| $ZT_{(T=3K)} (10^{-4})$  | ↗ | 7.277   | 9.285   | 11.398  | 15.902 |
| $ZT_{(T=80K)} (10^{-1})$   | ↗ | 3.773   | 4.505   | 5.228   | 6.713  |

**For  $x=0.5$ ,**

|  |   |         |         |         |         |
|--|---|---------|---------|---------|---------|
| $\xi_n(T=3K)$  | ↘ | 182.288 | 172.784 | 165.867 | 156.440 |
| $\xi_n(T=80K)$   | ↘ | 7.023   | 6.676   | 6.425   | 6.083   |
| $\kappa_{(T=3K)} \left( \frac{10^{-5} \times W}{cm \times K} \right)$  | ↘ | 8.592   | 7.518   | 6.861   | 6.086   |
| $\kappa_{(T=80K)} \left( \frac{10^{-5} \times W}{cm \times K} \right)$ | ↘ | 2.579   | 2.285   | 2.108   | 1.900   |
| $-S_{(T=3K)} \left( \frac{10^{-6} \times V}{K} \right)$                | ↘ | 3.110   | 3.281   | 3.418   | 3.624   |
| $-S_{(T=80K)} \left( \frac{10^{-5} \times V}{K} \right)$               | ↘ | 7.569   | 7.908   | 8.173   | 8.560   |
| $-VC1_{(T=3K)} \left( \frac{10^{-5} \times V}{K} \right)$              | ↘ | 2.073   | 2.187   | 2.278   | 2.415   |
| $-VC1_{(T=80K)} \left( \frac{10^{-5} \times V}{K} \right)$             | ↘ | 4.178   | 4.281   | 4.355   | 4.455   |
| $-VC2_{(T=3K)} \left( \frac{10^{-6} \times V}{K} \right)$              | ↘ | 6.218   | 6.560   | 6.834   | 7.245   |
| $-VC2_{(T=80K)} \left( \frac{10^{-5} \times V}{K} \right)$             | ↘ | 3.342   | 3.425   | 3.484   | 3.564   |
| $-Ts_{(T=3K)} \left( \frac{10^{-6} \times V}{K} \right)$               | ↘ | 3.109   | 3.280   | 3.417   | 3.622   |
| $-Ts_{(T=80K)} \left( \frac{10^{-5} \times V}{K} \right)$              | ↘ | 6.267   | 6.421   | 6.532   | 6.682   |
| $-Pt_{(T=3K)} (10^{-5} \times V)$                                      | ↘ | 0.933   | 0.984   | 1.025   | 1.087   |
| $-Pt_{(T=80K)} (10^{-3} \times V)$                                     | ↘ | 6.055   | 6.327   | 6.539   | 6.848   |
| $ZT_{(T=3K)} (10^{-4})$  | ↗ | 3.959   | 4.407   | 4.780   | 5.375   |
| $ZT_{(T=80K)} (10^{-1})$   | ↗ | 2.345   | 2.560   | 2.734   | 2.999   |

**For  $x=1$ ,**

|  |   |         |         |         |         |
|--|---|---------|---------|---------|---------|
| $\xi_n(T=3K)$  | ↘ | 227.487 | 221.389 | 217.004 | 211.105 |
| $\xi_n(T=80K)$   | ↘ | 8.679   | 8.455   | 8.294   | 8.077   |
| $\kappa_{(T=3K)} \left( \frac{10^{-5} \times W}{cm \times K} \right)$  | ↘ | 12.095  | 10.879  | 10.154  | 9.320   |
| $\kappa_{(T=80K)} \left( \frac{10^{-5} \times W}{cm \times K} \right)$ | ↘ | 3.484   | 3.147   | 2.947   | 2.717   |
| $-S_{(T=3K)} \left( \frac{10^{-6} \times V}{K} \right)$                | ↘ | 2.492   | 2.561   | 2.613   | 2.686   |
| $-S_{(T=80K)} \left( \frac{10^{-5} \times V}{K} \right)$               | ↘ | 6.259   | 6.411   | 6.524   | 6.683   |
| $-VC1_{(T=3K)} \left( \frac{10^{-5} \times V}{K} \right)$              | ↘ | 1.661   | 1.707   | 1.741   | 1.790   |
| $-VC1_{(T=80K)} \left( \frac{10^{-5} \times V}{K} \right)$             | ↘ | 3.690   | 3.754   | 3.800   | 3.864   |
| $-VC2_{(T=3K)} \left( \frac{10^{-6} \times V}{K} \right)$              | ↘ | 4.984   | 5.121   | 5.224   | 5.370   |
| $-VC2_{(T=80K)} \left( \frac{10^{-5} \times V}{K} \right)$             | ↘ | 2.952   | 3.003   | 3.040   | 3.091   |
| $-Ts_{(T=3K)} \left( \frac{10^{-6} \times V}{K} \right)$               | ↘ | 2.492   | 2.560   | 2.612   | 2.685   |
| $-Ts_{(T=80K)} \left( \frac{10^{-5} \times V}{K} \right)$              | ↘ | 5.534   | 5.630   | 5.700   | 5.795   |
| $-Pt_{(T=3K)} (10^{-5} \times V)$                                      | ↘ | 0.748   | 0.768   | 0.784   | 0.806   |
| $-Pt_{(T=80K)} (10^{-3} \times V)$                                     | ↘ | 5.007   | 5.129   | 5.219   | 5.346   |
| $ZT_{(T=3K)} (10^{-4})$  | ↗ | 2.542   | 2.684   | 2.794   | 2.952   |
| $ZT_{(T=80K)} (10^{-1})$   | ↗ | 1.604   | 1.682   | 1.742   | 1.828   |

**Table 5n:** Here, for a given  $N$  and with increasing  $T$ , the reduced Fermi-energy  $\xi_n$  decreases, and other thermoelectric coefficients are in variations, as indicated by the arrows as: (increase: ↗, decrease: ↘). One notes here that with increasing  $T$ : (i) for  $\xi_n \approx 1.8138$ , while the numerical results of  $S$  present a same minimum ( $S$ )<sub>min</sub> ( $\approx -1.563 \times 10^{-4} \frac{V}{K}$ ), those of ZT show a same maximum ( $ZT$ )<sub>max</sub> = 1, (ii) for  $\xi_n = 1$ , those of  $S$ , ZT, ( $ZT$ )<sub>Mott</sub>, VC1, and  $T_s$  present the same results:  $-1.322 \times 10^{-4} \frac{V}{K}$ , 0.715, 3.290,  $1.105 \times 10^{-4} \frac{V}{K}$ , and  $1.657 \times 10^{-4} \frac{V}{K}$ , respectively, and (iii) for  $\xi_n \approx 1.8138$ , ( $ZT$ )<sub>Mott</sub> = 1.

For x=0,

In the degenerate P- X(x) – alloy, for  $N = 2 \times N_{CD0} (r_p) = 3.3719916 \times 10^{17} \text{ cm}^{-3}$ , one gets:

|                             |        |                  |        |                  |         |
|-----------------------------|--------|------------------|--------|------------------|---------|
| T(K)                        | 43.85  | <b>44.769183</b> | 45.7   | <b>60.920214</b> | 60.945  |
| $\xi_n$                     | 1.877  | <b>1.8138</b>    | 1.752  | <b>1</b>         | 0.999   |
| $S (10^{-4} \frac{V}{K})$   | -1.562 | <b>-1.563</b>    | -1.562 | <b>-1.322</b>    | -1.321  |
| ZT                          | 0.999  | <b>1</b>         | 0.999  | <b>0.715</b>     | 0.714   |
| $(ZT)_{Mott}$               | 0.933  | <b>1</b>         | 1.071  | <b>3.290</b>     | 3.296   |
| $VC1 (10^{-4} \frac{V}{K})$ | -0.059 | <b>0</b>         | 0.061  | <b>1.105</b>     | 1.106   |
| $VC2 (10^{-4} \frac{V}{K})$ | 2.590  | <b>0</b>         | 2.778  | <b>67.313</b>    | 67.440  |
| $T_s (10^{-4} \frac{V}{K})$ | -0.089 | <b>0</b>         | 0.091  | <b>1.657</b>     | 1.660   |
| Pt ( $10^{-2} V$ )          | -6.850 | <b>-6.997</b>    | -7.139 | <b>-8.0518</b>   | -8.0510 |

In the degenerate As- X(x) – alloy, for  $N = 2 \times N_{CD0} (r_{As}) = 3.6247868 \times 10^{17} \text{ cm}^{-3}$ , one gets:

|                             |        |                  |        |                  |         |
|-----------------------------|--------|------------------|--------|------------------|---------|
| T(K)                        | 45.98  | <b>46.979655</b> | 47.99  | <b>63.928142</b> | 63.955  |
| $\xi_n$                     | 1.880  | <b>1.8138</b>    | 1.750  | <b>1</b>         | 0.999   |
| $S (10^{-4} \frac{V}{K})$   | -1.562 | <b>-1.563</b>    | -1.562 | <b>-1.322</b>    | -1.321  |
| ZT                          | 0.999  | <b>1</b>         | 0.999  | <b>0.715</b>     | 0.714   |
| $(ZT)_{Mott}$               | 0.931  | <b>1</b>         | 1.074  | <b>3.290</b>     | 3.296   |
| $VC1 (10^{-4} \frac{V}{K})$ | -0.061 | <b>0</b>         | 0.063  | <b>1.105</b>     | 1.107   |
| $VC2 (10^{-4} \frac{V}{K})$ | -2.814 | <b>0</b>         | 3.018  | <b>70.637</b>    | 70.774  |
| $T_s (10^{-4} \frac{V}{K})$ | -0.092 | <b>0</b>         | 0.094  | <b>1.657</b>     | 1.660   |
| Pt ( $10^{-2} V$ )          | -7.182 | <b>-7.343</b>    | -7.496 | <b>-8.4494</b>   | -8.4485 |

In the degenerate Sb- X(x) – alloy, for  $N = 2 \times N_{CD0} (r_{Sb}) = 6.6108594 \times 10^{17} \text{ cm}^{-3}$ , one gets:

|                             |         |                  |         |                  |          |
|-----------------------------|---------|------------------|---------|------------------|----------|
| T(K)                        | 68.64   | <b>70.128324</b> | 71.63   | <b>95.427976</b> | 95.468   |
| $\xi_n$                     | 1.879   | <b>1.8138</b>    | 1.750   | <b>1</b>         | 0.999    |
| $S (10^{-4} \frac{V}{K})$   | -1.562  | <b>-1.563</b>    | -1.562  | <b>-1.322</b>    | -1.321   |
| ZT                          | 0.999   | <b>1</b>         | 0.999   | <b>0.715</b>     | 0.714    |
| $(ZT)_{Mott}$               | 0.931   | <b>1</b>         | 1.074   | <b>3.290</b>     | 3.296    |
| $VC1 (10^{-4} \frac{V}{K})$ | -0.061  | <b>0</b>         | 0.063   | <b>1.105</b>     | 1.107    |
| $VC2 (10^{-4} \frac{V}{K})$ | -4.190  | <b>0</b>         | 4.485   | <b>105.443</b>   | 105.647  |
| $T_s (10^{-4} \frac{V}{K})$ | -0.091  | <b>0</b>         | 0.094   | <b>1.657</b>     | 1.660    |
| Pt ( $10^{-2} V$ )          | -10.722 | <b>-10.961</b>   | -11.189 | <b>-12.613</b>   | -12.6114 |

In the degenerate Sn- X(x) – alloy, for  $N = 2 \times N_{CD0} (r_{Sn}) = 7.9274126 \times 10^{17} \text{ cm}^{-3}$ , one gets:

|                             |         |                  |         |                  |         |
|-----------------------------|---------|------------------|---------|------------------|---------|
| T(K)                        | 77.47   | <b>79.154538</b> | 80.85   | <b>107.71051</b> | 107.82  |
| $\xi_n$                     | 1.880   | <b>1.8138</b>    | 1.750   | <b>1</b>         | 0.998   |
| $S (10^{-4} \frac{V}{K})$   | -1.562  | <b>-1.563</b>    | -1.562  | <b>-1.322</b>    | -1.320  |
| ZT                          | 0.999   | <b>1</b>         | 0.999   | <b>0.715</b>     | 0.713   |
| $(ZT)_{Mott}$               | 0.931   | <b>1</b>         | 1.074   | <b>3.290</b>     | 3.306   |
| $VC1 (10^{-4} \frac{V}{K})$ | -0.061  | <b>0</b>         | 0.063   | <b>1.105</b>     | 1.109   |
| $VC2 (10^{-4} \frac{V}{K})$ | -4.742  | <b>0</b>         | 5.064   | <b>119.014</b>   | 119.574 |
| $T_s (10^{-4} \frac{V}{K})$ | -0.092  | <b>0</b>         | 0.094   | <b>1.657</b>     | 1.663   |
| Pt ( $10^{-2} V$ )          | -12.101 | <b>-12.372</b>   | -12.629 | <b>-14.236</b>   | -14.232 |

For x=0.5,

In the degenerate P- X(x) – alloy, for  $N = 2 \times N_{CD0} (r_p) = 6.3822952 \times 10^{17} \text{ cm}^{-3}$ , one gets:

|      |       |                  |        |                  |        |
|------|-------|------------------|--------|------------------|--------|
| T(K) | 51.42 | <b>52.538752</b> | 53.665 | <b>71.492753</b> | 71.562 |
|------|-------|------------------|--------|------------------|--------|

|  |        |               |        |                |         |
|--|--------|---------------|--------|----------------|---------|
| $\xi_m$                                  | 1.880  | <b>1.8138</b> | 1.750  | <b>1</b>       | 0.998   |
| $S \left( 10^{-4} \frac{V}{K} \right)$   | -1.562 | <b>-1.563</b> | -1.562 | <b>-1.322</b>  | -1.320  |
| ZT                                       | 0.999  | <b>1</b>      | 0.999  | <b>0.715</b>   | 0.713   |
| $(ZT)_{Mott}$                            | 0.931  | <b>1</b>      | 1.074  | <b>3.290</b>   | 3.305   |
| $VC1 \left( 10^{-4} \frac{V}{K} \right)$ | -0.061 | <b>0</b>      | 0.063  | <b>1.105</b>   | 1.109   |
| $VC2 \left( 10^{-4} \frac{V}{K} \right)$ | -3.149 | <b>0</b>      | 3.364  | <b>78.995</b>  | 79.350  |
| $T_s \left( 10^{-4} \frac{V}{K} \right)$ | -0.092 | <b>0</b>      | 0.094  | <b>1.657</b>   | 1.663   |
| Pt ( $10^{-3} V$ )                       | -8.032 | <b>-8.212</b> | -8.382 | <b>-9.4492</b> | -9.4469 |

In the degenerate As-  $X(x)$  – alloy, for  $N = 2 \times N_{CDn}(r_{As}) = 6.8607702 \times 10^{17} \text{ cm}^{-3}$ , one gets:

|  |        |                  |        |                  |         |
|--|--------|------------------|--------|------------------|---------|
| T(K)                                     | 53.96  | <b>55.132846</b> | 56.315 | <b>75.022696</b> | 75.097  |
| $\xi_m$                                  | 1.880  | <b>1.8138</b>    | 1.750  | <b>1</b>         | 0.998   |
| $S \left( 10^{-4} \frac{V}{K} \right)$   | -1.562 | <b>-1.563</b>    | -1.562 | <b>-1.322</b>    | -1.320  |
| ZT                                       | 0.999  | <b>1</b>         | 0.999  | <b>0.715</b>     | 0.713   |
| $(ZT)_{Mott}$                            | 0.931  | <b>1</b>         | 1.074  | <b>3.290</b>     | 3.305   |
| $VC1 \left( 10^{-4} \frac{V}{K} \right)$ | -0.061 | <b>0</b>         | 0.063  | <b>1.105</b>     | 1.109   |
| $VC2 \left( 10^{-4} \frac{V}{K} \right)$ | -3.301 | <b>0</b>         | 3.531  | <b>82.896</b>    | 83.276  |
| $T_s \left( 10^{-4} \frac{V}{K} \right)$ | -0.092 | <b>0</b>         | 0.094  | <b>1.657</b>     | 1.663   |
| Pt ( $10^{-3} V$ )                       | -8.428 | <b>-8.617</b>    | -8.796 | <b>-9.9158</b>   | -9.9132 |

In the degenerate Sb-  $X(x)$  – alloy, for  $N = 2 \times N_{CDn}(r_{Sb}) = 1.2512622 \times 10^{18} \text{ cm}^{-3}$ , one gets:

|  |         |                  |         |                  |         |
|--|---------|------------------|---------|------------------|---------|
| T(K)                                     | 80.55   | <b>82.298904</b> | 84.062  | <b>111.98924</b> | 112.1   |
| $\xi_m$                                  | 1.880   | <b>1.8138</b>    | 1.750   | <b>1</b>         | 0.998   |
| $S \left( 10^{-4} \frac{V}{K} \right)$   | -1.562  | <b>-1.563</b>    | -1.562  | <b>-1.322</b>    | -1.320  |
| ZT                                       | 0.999   | <b>1</b>         | 0.999   | <b>0.715</b>     | 0.713   |
| $(ZT)_{Mott}$                            | 0.931   | <b>1</b>         | 1.074   | <b>3.290</b>     | 3.305   |
| $VC1 \left( 10^{-4} \frac{V}{K} \right)$ | -0.061  | <b>0</b>         | 0.063   | <b>1.105</b>     | 1.109   |
| $VC2 \left( 10^{-4} \frac{V}{K} \right)$ | -4.923  | <b>0</b>         | 5.266   | <b>123.742</b>   | 124.308 |
| $T_s \left( 10^{-4} \frac{V}{K} \right)$ | -0.092  | <b>0</b>         | 0.094   | <b>1.657</b>     | 1.663   |
| Pt ( $10^{-3} V$ )                       | -12.582 | <b>-12.863</b>   | -13.130 | <b>-14.8016</b>  | -14.798 |

In the degenerate Sn-  $X(x)$  – alloy, for  $N = 2 \times N_{CDn}(r_{Sn}) = 1.5004512 \times 10^{18} \text{ cm}^{-3}$ , one gets:

|  |         |                  |         |                   |          |
|--|---------|------------------|---------|-------------------|----------|
| T(K)                                     | 90.92   | <b>92.891593</b> | 94.89   | <b>126.403371</b> | 126.53   |
| $\xi_m$                                  | 1.879   | <b>1.8138</b>    | 1.750   | <b>1</b>          | 0.998    |
| $S \left( 10^{-4} \frac{V}{K} \right)$   | -1.562  | <b>-1.563</b>    | -1.562  | <b>-1.322</b>     | -1.320   |
| ZT                                       | 0.999   | <b>1</b>         | 0.999   | <b>0.715</b>      | 0.713    |
| $(ZT)_{Mott}$                            | 0.931   | <b>1</b>         | 1.074   | <b>3.290</b>      | 3.305    |
| $VC1 \left( 10^{-4} \frac{V}{K} \right)$ | -0.061  | <b>0</b>         | 0.063   | <b>1.105</b>      | 1.109    |
| $VC2 \left( 10^{-4} \frac{V}{K} \right)$ | -5.550  | <b>0</b>         | 5.970   | <b>139.669</b>    | 140.316  |
| $T_s \left( 10^{-4} \frac{V}{K} \right)$ | -0.091  | <b>0</b>         | 0.094   | <b>1.657</b>      | 1.663    |
| Pt ( $10^{-3} V$ )                       | -14.202 | <b>-14.519</b>   | -14.822 | <b>-16.7068</b>   | -16.7025 |

For  $x=1$ ,

In the degenerate P-  $X(x)$  – alloy, for  $N = 2 \times N_{CDn}(r_p) = 1.0297905 \times 10^{18} \text{ cm}^{-3}$ , one gets:

|         |       |                  |        |                  |       |
|---------|-------|------------------|--------|------------------|-------|
| T(K)    | 57.37 | <b>58.616225</b> | 59.875 | <b>79.762746</b> | 79.84 |
| $\xi_m$ | 1.880 | <b>1.8138</b>    | 1.750  | <b>1</b>         | 0.998 |

|  |        |   |        |   |        |   |          |   |          |
|--|--------|---|--------|---|--------|---|----------|---|----------|
| $S \left( 10^{-4} \frac{V}{K} \right)$   | -1.562 | ↘ | -1.563 | ↗ | -1.562 | ↗ | -1.322   | ↗ | -1.320   |
| ZT                                       | 0.999  | ↗ | 1      | ↘ | 0.999  | ↘ | 0.715    | ↘ | 0.713    |
| $(ZT)_{Mott}$                            | 0.931  | ↗ | 1      | ↗ | 1.074  | ↗ | 3.290    | ↗ | 3.305    |
| $VC1 \left( 10^{-4} \frac{V}{K} \right)$ | -0.061 | ↗ | 0      | ↗ | 0.063  | ↗ | 1.105    | ↗ | 1.109    |
| $VC2 \left( 10^{-4} \frac{V}{K} \right)$ | -3.508 | ↗ | 0      | ↗ | 3.760  | ↗ | 88.133   | ↗ | 88.528   |
| $T_s \left( 10^{-4} \frac{V}{K} \right)$ | -0.092 | ↗ | 0      | ↗ | 0.094  | ↗ | 1.657    | ↗ | 1.663    |
| Pt ( $10^{-3} V$ )                       | -8.961 | ↘ | -9.162 | ↘ | -9.352 | ↘ | -10.5423 | ↗ | -10.5396 |

In the degenerate As- $X(x)$ -alloy, for  $N = 2 \times N_{CDW}(r_{As}) = 1.106993 \times 10^{18} \text{ cm}^{-3}$ , one gets:

|  |        |           |        |            |        |   |          |   |          |
|--|--------|-----------|--------|------------|--------|---|----------|---|----------|
| T(K)                                     | 57.37  | 61.510393 | 59.875 | 83.7010199 | 83.785 |   |          |   |          |
| $\xi_p$                                  | 1.880  | 1.8138    | 1.750  | 1          | 0.998  |   |          |   |          |
| $S \left( 10^{-4} \frac{V}{K} \right)$   | -1.562 | ↘         | -1.563 | ↗          | -1.562 | ↗ | -1.322   | ↗ | -1.320   |
| ZT                                       | 0.999  | ↗         | 1      | ↘          | 0.999  | ↘ | 0.715    | ↘ | 0.713    |
| $(ZT)_{Mott}$                            | 0.931  | ↗         | 1      | ↗          | 1.074  | ↗ | 3.290    | ↗ | 3.305    |
| $VC1 \left( 10^{-4} \frac{V}{K} \right)$ | -0.061 | ↗         | 0      | ↗          | 0.063  | ↗ | 1.105    | ↗ | 1.109    |
| $VC2 \left( 10^{-4} \frac{V}{K} \right)$ | -3.508 | ↗         | 0      | ↗          | 3.760  | ↗ | 92.485   | ↗ | 92.914   |
| $T_s \left( 10^{-4} \frac{V}{K} \right)$ | -0.092 | ↗         | 0      | ↗          | 0.094  | ↗ | 1.657    | ↗ | 1.663    |
| Pt ( $10^{-3} V$ )                       | -8.961 | ↘         | -9.614 | ↘          | -9.352 | ↘ | -11.0628 | ↗ | -11.0599 |

In the degenerate Sb- $X(x)$ -alloy, for  $N = 2 \times N_{CDW}(r_{Sb}) = 2.0189256 \times 10^{18} \text{ cm}^{-3}$ , one gets:

|  |         |           |         |            |         |   |          |   |          |
|--|---------|-----------|---------|------------|---------|---|----------|---|----------|
| T(K)                                     | 89.87   | 91.818907 | 93.79   | 124.943703 | 125.07  |   |          |   |          |
| $\xi_p$                                  | 1.879   | 1.8138    | 1.750   | 1          | 0.998   |   |          |   |          |
| $S \left( 10^{-4} \frac{V}{K} \right)$   | -1.562  | ↘         | -1.563  | ↗          | -1.562  | ↗ | -1.322   | ↗ | -1.320   |
| ZT                                       | 0.999   | ↗         | 1       | ↘          | 0.999   | ↘ | 0.715    | ↘ | 0.713    |
| $(ZT)_{Mott}$                            | 0.931   | ↗         | 1       | ↗          | 1.074   | ↗ | 3.290    | ↗ | 3.305    |
| $VC1 \left( 10^{-4} \frac{V}{K} \right)$ | -0.061  | ↗         | 0       | ↗          | 0.063   | ↗ | 1.105    | ↗ | 1.109    |
| $VC2 \left( 10^{-4} \frac{V}{K} \right)$ | -5.486  | ↗         | 0       | ↗          | 5.888   | ↗ | 138.056  | ↗ | 138.702  |
| $T_s \left( 10^{-4} \frac{V}{K} \right)$ | -0.091  | ↗         | 0       | ↗          | 0.094   | ↗ | 1.657    | ↗ | 1.663    |
| Pt ( $10^{-3} V$ )                       | -14.038 | ↘         | -14.351 | ↘          | -14.650 | ↘ | -16.5138 | ↗ | -16.5095 |

In the degenerate Sn- $X(x)$ -alloy, for  $N = 2 \times N_{CDW}(r_{Sn}) = 2.4209948 \times 10^{18} \text{ cm}^{-3}$ , one gets:

|  |         |            |         |            |         |   |          |   |          |
|--|---------|------------|---------|------------|---------|---|----------|---|----------|
| T(K)                                     | 101.43  | 103.636916 | 105.86  | 141.025204 | 141.162 |   |          |   |          |
| $\xi_p$                                  | 1.880   | 1.8138     | 1.750   | 1          | 0.998   |   |          |   |          |
| $S \left( 10^{-4} \frac{V}{K} \right)$   | -1.562  | ↘          | -1.563  | ↗          | -1.562  | ↗ | -1.322   | ↗ | -1.320   |
| ZT                                       | 0.999   | ↗          | 1       | ↘          | 0.999   | ↘ | 0.715    | ↘ | 0.713    |
| $(ZT)_{Mott}$                            | 0.931   | ↗          | 1       | ↗          | 1.074   | ↗ | 3.290    | ↗ | 3.305    |
| $VC1 \left( 10^{-4} \frac{V}{K} \right)$ | -0.061  | ↗          | 0       | ↗          | 0.063   | ↗ | 1.105    | ↗ | 1.109    |
| $VC2 \left( 10^{-4} \frac{V}{K} \right)$ | -6.212  | ↗          | 0       | ↗          | 6.640   | ↗ | 155.825  | ↗ | 156.525  |
| $T_s \left( 10^{-4} \frac{V}{K} \right)$ | -0.092  | ↗          | 0       | ↗          | 0.094   | ↗ | 1.657    | ↗ | 1.663    |
| Pt ( $10^{-3} V$ )                       | -15.843 | ↘          | -16.198 | ↘          | -16.535 | ↘ | -18.6393 | ↗ | -18.6347 |

**Table 5p:** Here, for a given  $N$  and with increasing  $T$ , the reduced Fermi-energy  $\xi_p$  decreases, and other thermoelectric coefficients are in variations, as indicated by the arrows as: (increase:  $\nearrow$ , decrease:  $\searrow$ ). One notes here that with increasing  $T$ : (i) for  $\xi_p \approx 1.8138$ , while the numerical results of  $S$  present a same minimum ( $S_{min.} \approx -1.563 \times 10^{-4} \frac{V}{K}$ ), those of ZT show a same maximum ( $ZT_{max.} = 1$ ), (ii) for  $\xi_p = 1$ , those of  $S$ , ZT,  $(ZT)_{Mott}$ , VC1, and  $T_s$  present the same results:  $-1.322 \times 10^{-4} \frac{V}{K}$ , 0.715, 3.290,  $1.105 \times 10^{-4} \frac{V}{K}$ , and  $1.657 \times 10^{-4} \frac{V}{K}$ , respectively, and (iii) for  $\xi_p \approx 1.8138$ ,  $(ZT)_{Mott} = 1$ .

For  $x=0$ ,

In the degenerate Ga-  $X(x)$  – alloy, for  $N = 2 \times N_{CDP}(r_{Ga}) = 1.9185205 \times 10^{19} \text{ cm}^{-3}$ , one gets:

|                            |        |                  |        |                  |         |
|----------------------------|--------|------------------|--------|------------------|---------|
| T(K)                       | 168.52 | <b>172.18917</b> | 175.88 | <b>234.30852</b> | 234.54  |
| $\xi_p$                    | 1.880  | <b>1.8138</b>    | 1.750  | <b>1</b>         | 0.998   |
| $S(10^{-4} \frac{V}{K})$   | -1.562 | <b>-1.563</b>    | -1.562 | <b>-1.322</b>    | -1.320  |
| ZT                         | 0.999  | <b>1</b>         | 0.998  | <b>0.715</b>     | 0.713   |
| $(ZT)_{Mott}$              | 0.931  | <b>1</b>         | 1.074  | <b>3.290</b>     | 3.305   |
| $VC1(10^{-4} \frac{V}{K})$ | -0.061 | <b>0</b>         | 0.063  | <b>1.105</b>     | 1.109   |
| $VC2(10^{-2} \frac{V}{K})$ | -0.103 | <b>0</b>         | 0.110  | <b>2.589</b>     | 2.601   |
| $T_s(10^{-4} \frac{V}{K})$ | -0.092 | <b>0</b>         | 0.094  | <b>1.657</b>     | 1.663   |
| Pt ( $10^{-2}V$ )          | -2.632 | <b>-2.691</b>    | -2.747 | <b>-3.0969</b>   | -3.0961 |

In the degenerate Mg-  $X(x)$  – alloy, for  $N = 2 \times N_{CDP}(r_{Mg}) = 2.2664086 \times 10^{19} \text{ cm}^{-3}$ , one gets

|                            |        |                  |        |                  |         |
|----------------------------|--------|------------------|--------|------------------|---------|
| T(K)                       | 188.32 | <b>192.42153</b> | 196.55 | <b>261.83996</b> | 262.1   |
| $\xi_p$                    | 1.880  | <b>1.8138</b>    | 1.750  | <b>1</b>         | 0.998   |
| $S(10^{-4} \frac{V}{K})$   | -1.562 | <b>-1.563</b>    | -1.562 | <b>-1.322</b>    | -1.320  |
| ZT                         | 0.999  | <b>1</b>         | 0.999  | <b>0.715</b>     | 0.713   |
| $(ZT)_{Mott}$              | 0.931  | <b>1</b>         | 1.074  | <b>3.290</b>     | 3.305   |
| $VC1(10^{-4} \frac{V}{K})$ | -0.061 | <b>0</b>         | 0.063  | <b>1.105</b>     | 1.109   |
| $VC2(10^{-2} \frac{V}{K})$ | -0.115 | <b>0</b>         | 0.123  | <b>2.893</b>     | 2.906   |
| $T_s(10^{-4} \frac{V}{K})$ | -0.092 | <b>0</b>         | 0.094  | <b>1.657</b>     | 1.663   |
| Pt ( $10^{-2}V$ )          | -2.941 | <b>-3.007</b>    | -3.070 | <b>-3.4607</b>   | -3.4599 |

In the degenerate In-  $X(x)$  – alloy, for  $N = 2 \times N_{CDP}(r_{In}) = 2.5136974 \times 10^{19} \text{ cm}^{-3}$ , one gets:

|                            |        |                   |        |                  |         |
|----------------------------|--------|-------------------|--------|------------------|---------|
| T(K)                       | 201.78 | <b>206.175403</b> | 210.59 | <b>280.55571</b> | 280.83  |
| $\xi_p$                    | 1.880  | <b>1.8138</b>     | 1.750  | <b>1</b>         | 0.998   |
| $S(10^{-4} \frac{V}{K})$   | -1.562 | <b>-1.563</b>     | -1.562 | <b>-1.322</b>    | -1.320  |
| ZT                         | 0.999  | <b>1</b>          | 0.999  | <b>0.715</b>     | 0.713   |
| $(ZT)_{Mott}$              | 0.931  | <b>1</b>          | 1.074  | <b>3.290</b>     | 3.305   |
| $VC1(10^{-4} \frac{V}{K})$ | -0.061 | <b>0</b>          | 0.063  | <b>1.105</b>     | 1.109   |
| $VC2(10^{-2} \frac{V}{K})$ | -0.124 | <b>0</b>          | 0.132  | <b>3.100</b>     | 3.114   |
| $T_s(10^{-4} \frac{V}{K})$ | -0.092 | <b>0</b>          | 0.094  | <b>1.657</b>     | 1.663   |
| Pt ( $10^{-2}V$ )          | -3.152 | <b>-3.222</b>     | -3.289 | <b>-3.7081</b>   | -3.7072 |

In the degenerate Cd-  $X(x)$  – alloy, for  $N = 2 \times N_{CDP}(r_{Cd}) = 2.842425 \times 10^{19} \text{ cm}^{-3}$ , one gets:

|                            |        |                   |        |                 |         |
|----------------------------|--------|-------------------|--------|-----------------|---------|
| T(K)                       | 219.02 | <b>223.779792</b> | 228.58 | <b>304.5111</b> | 304.82  |
| $\xi_p$                    | 1.880  | <b>1.8138</b>     | 1.750  | <b>1</b>        | 0.998   |
| $S(10^{-4} \frac{V}{K})$   | -1.562 | <b>-1.563</b>     | -1.562 | <b>-1.322</b>   | -1.320  |
| ZT                         | 0.999  | <b>1</b>          | 0.999  | <b>0.715</b>    | 0.713   |
| $(ZT)_{Mott}$              | 0.931  | <b>1</b>          | 1.074  | <b>3.290</b>    | 3.305   |
| $VC1(10^{-4} \frac{V}{K})$ | -0.061 | <b>0</b>          | 0.063  | <b>1.105</b>    | 1.109   |
| $VC2(10^{-2} \frac{V}{K})$ | -0.134 | <b>0</b>          | 0.143  | <b>3.365</b>    | 3.380   |
| $T_s(10^{-4} \frac{V}{K})$ | -0.092 | <b>0</b>          | 0.094  | <b>1.657</b>    | 1.663   |
| Pt ( $10^{-2}V$ )          | -3.421 | <b>-3.498</b>     | -3.570 | <b>-4.0247</b>  | -4.0237 |

For x=0.5,

In the degenerate Ga-  $X(x)$  – alloy, for  $N = 2 \times N_{CDP} (r_{Ga}) = 1.1942777 \times 10^{19} \text{ cm}^{-3}$ , one gets:

|                             |        |                   |         |                  |         |
|-----------------------------|--------|-------------------|---------|------------------|---------|
| T(K)                        | 136.51 | <b>139.483412</b> | 142.484 | <b>189.80377</b> | 189.998 |
| $\xi_p$                     | 1.880  | <b>1.8138</b>     | 1.750   | <b>1</b>         | 0.998   |
| $S (10^{-4} \frac{V}{K})$   | -1.562 | <b>-1.563</b>     | -1.562  | <b>-1.322</b>    | -1.320  |
| ZT                          | 0.999  | <b>1</b>          | 0.998   | <b>0.715</b>     | 0.713   |
| $(ZT)_{Mott}$               | 0.931  | <b>1</b>          | 1.074   | <b>3.290</b>     | 3.306   |
| $VC1 (10^{-4} \frac{V}{K})$ | -0.061 | <b>0</b>          | 0.063   | <b>1.105</b>     | 1.109   |
| $VC2 (10^{-2} \frac{V}{K})$ | -0.084 | <b>0</b>          | 0.090   | <b>2.097</b>     | 2.107   |
| $T_s (10^{-4} \frac{V}{K})$ | -0.092 | <b>0</b>          | 0.094   | <b>1.657</b>     | 1.663   |
| Pt ( $10^{-2} V$ )          | -2.132 | <b>-2.180</b>     | -2.226  | <b>-2.5086</b>   | -2.5080 |

In the degenerate Mg-  $X(x)$  – alloy, for  $N = 2 \times N_{CDP} (r_{Mg}) = 1.4108379 \times 10^{19} \text{ cm}^{-3}$ , one gets:

|                             |         |                  |         |                  |         |
|-----------------------------|---------|------------------|---------|------------------|---------|
| T(K)                        | 152.549 | <b>155.87283</b> | 159.226 | <b>212.10587</b> | 212.323 |
| $\xi_p$                     | 1.880   | <b>1.8138</b>    | 1.750   | <b>1</b>         | 0.997   |
| $S (10^{-4} \frac{V}{K})$   | -1.562  | <b>-1.563</b>    | -1.562  | <b>-1.322</b>    | -1.320  |
| ZT                          | 0.999   | <b>1</b>         | 0.999   | <b>0.715</b>     | 0.713   |
| $(ZT)_{Mott}$               | 0.931   | <b>1</b>         | 1.074   | <b>3.290</b>     | 3.306   |
| $VC1 (10^{-4} \frac{V}{K})$ | -0.061  | <b>0</b>         | 0.063   | <b>1.105</b>     | 1.109   |
| $VC2 (10^{-2} \frac{V}{K})$ | -0.093  | <b>0</b>         | 0.100   | <b>2.344</b>     | 2.355   |
| $T_s (10^{-4} \frac{V}{K})$ | -0.092  | <b>0</b>         | 0.094   | <b>1.657</b>     | 1.663   |
| Pt ( $10^{-2} V$ )          | -2.383  | <b>-2.436</b>    | -2.487  | <b>-2.8034</b>   | -2.8027 |

In the degenerate In-  $X(x)$  – alloy, for  $N = 2 \times N_{CDP} (r_{In}) = 1.5647749 \times 10^{19} \text{ cm}^{-3}$ , one gets:

|                             |         |                   |         |                  |         |
|-----------------------------|---------|-------------------|---------|------------------|---------|
| T(K)                        | 163.453 | <b>167.014273</b> | 170.607 | <b>227.26672</b> | 227.499 |
| $\xi_p$                     | 1.880   | <b>1.8138</b>     | 1.750   | <b>1</b>         | 0.998   |
| $S (10^{-4} \frac{V}{K})$   | -1.562  | <b>-1.563</b>     | -1.562  | <b>-1.322</b>    | -1.320  |
| ZT                          | 0.999   | <b>1</b>          | 0.999   | <b>0.715</b>     | 0.713   |
| $(ZT)_{Mott}$               | 0.931   | <b>1</b>          | 1.074   | <b>3.290</b>     | 3.306   |
| $VC1 (10^{-4} \frac{V}{K})$ | -0.061  | <b>0</b>          | 0.063   | <b>1.105</b>     | 1.109   |
| $VC2 (10^{-2} \frac{V}{K})$ | -0.100  | <b>0</b>          | 0.107   | <b>2.511</b>     | 2.523   |
| $T_s (10^{-4} \frac{V}{K})$ | -0.092  | <b>0</b>          | 0.094   | <b>1.657</b>     | 1.663   |
| Pt ( $10^{-2} V$ )          | -2.553  | <b>-2.610</b>     | -2.665  | <b>-3.0038</b>   | -3.0030 |

In the degenerate Cd-  $X(x)$  – alloy, for  $N = 2 \times N_{CDP} (r_{Cd}) = 1.7694076 \times 10^{19} \text{ cm}^{-3}$ , one gets:

|                             |        |                  |         |                  |         |
|-----------------------------|--------|------------------|---------|------------------|---------|
| T(K)                        | 177.41 | <b>181.27487</b> | 185.175 | <b>246.67201</b> | 246.925 |
| $\xi_p$                     | 1.880  | <b>1.8138</b>    | 1.750   | <b>1</b>         | 0.998   |
| $S (10^{-4} \frac{V}{K})$   | -1.562 | <b>-1.563</b>    | -1.562  | <b>-1.322</b>    | -1.320  |
| ZT                          | 0.999  | <b>1</b>         | 0.999   | <b>0.715</b>     | 0.713   |
| $(ZT)_{Mott}$               | 0.931  | <b>1</b>         | 1.074   | <b>3.290</b>     | 3.306   |
| $VC1 (10^{-4} \frac{V}{K})$ | -0.061 | <b>0</b>         | 0.063   | <b>1.105</b>     | 1.109   |
| $VC2 (10^{-2} \frac{V}{K})$ | -0.109 | <b>0</b>         | 0.116   | <b>2.725</b>     | 2.738   |
| $T_s (10^{-4} \frac{V}{K})$ | -0.092 | <b>0</b>         | 0.094   | <b>1.657</b>     | 1.663   |
| Pt ( $10^{-2} V$ )          | -2.771 | <b>-2.833</b>    | -2.892  | <b>-3.2603</b>   | -3.2594 |

For x=1,

In the degenerate Ga-  $X(x)$  – alloy, for  $N = 2 \times N_{CDP} (r_{Ga}) = 7.2192156 \times 10^{18} \text{ cm}^{-3}$ , one gets:

|      |         |                   |         |                   |        |
|------|---------|-------------------|---------|-------------------|--------|
| T(K) | 109.792 | <b>112.184162</b> | 114.597 | <b>152.655974</b> | 152.81 |
|------|---------|-------------------|---------|-------------------|--------|

|  |        |               |        |                |         |
|--|--------|---------------|--------|----------------|---------|
| $\xi_p$                                  | 1.880  | <b>1.8138</b> | 1.750  | <b>1</b>       | 0.998   |
| $S \left( 10^{-4} \frac{V}{K} \right)$   | -1.562 | <b>-1.563</b> | -1.562 | <b>-1.322</b>  | -1.320  |
| ZT                                       | 0.999  | <b>1</b>      | 0.998  | <b>0.715</b>   | 0.713   |
| $(ZT)_{Mott}$                            | 0.931  | <b>1</b>      | 1.074  | <b>3.290</b>   | 3.305   |
| $VC1 \left( 10^{-4} \frac{V}{K} \right)$ | -0.061 | <b>0</b>      | 0.063  | <b>1.105</b>   | 1.109   |
| $VC2 \left( 10^{-2} \frac{V}{K} \right)$ | -0.067 | <b>0</b>      | 0.072  | 1.687          | 1.695   |
| $T_s \left( 10^{-4} \frac{V}{K} \right)$ | -0.092 | <b>0</b>      | 0.094  | <b>1.657</b>   | 1.663   |
| Pt ( $10^{-2} V$ )                       | -1.715 | <b>-1.753</b> | -1.790 | <b>-2.0176</b> | -2.0171 |

In the degenerate Mg-X(x)-alloy, for  $N = 2 \times N_{CDP}(r_{Mg}) = 8.5282866 \times 10^{18} \text{ cm}^{-3}$ , one gets:

|  |        |                   |        |                  |         |
|--|--------|-------------------|--------|------------------|---------|
| T(K)                                     | 122.7  | <b>125.365892</b> | 128.06 | <b>170.59318</b> | 170.76  |
| $\xi_p$                                  | 1.880  | <b>1.8138</b>     | 1.750  | <b>1</b>         | 0.998   |
| $S \left( 10^{-4} \frac{V}{K} \right)$   | -1.562 | <b>-1.563</b>     | -1.562 | <b>-1.322</b>    | -1.320  |
| ZT                                       | 0.999  | <b>1</b>          | 0.998  | <b>0.715</b>     | 0.713   |
| $(ZT)_{Mott}$                            | 0.931  | <b>1</b>          | 1.074  | <b>3.290</b>     | 3.305   |
| $VC1 \left( 10^{-4} \frac{V}{K} \right)$ | -0.061 | <b>0</b>          | 0.063  | <b>1.105</b>     | 1.109   |
| $VC2 \left( 10^{-2} \frac{V}{K} \right)$ | -0.075 | <b>0</b>          | 0.080  | 1.885            | 1.893   |
| $T_s \left( 10^{-4} \frac{V}{K} \right)$ | -0.092 | <b>0</b>          | 0.094  | <b>1.657</b>     | 1.663   |
| Pt ( $10^{-2} V$ )                       | -1.916 | <b>-1.959</b>     | -2.000 | <b>-2.2547</b>   | -2.2542 |

In the degenerate In-X(x)-alloy, for  $N = 2 \times N_{CDP}(r_{In}) = 9.458811 \times 10^{18} \text{ cm}^{-3}$ , one gets:

|  |        |                  |        |                 |         |
|--|--------|------------------|--------|-----------------|---------|
| T(K)                                     | 131.47 | <b>134.32677</b> | 137.21 | <b>182.7868</b> | 182.97  |
| $\xi_p$                                  | 1.880  | <b>1.8138</b>    | 1.750  | <b>1</b>        | 0.998   |
| $S \left( 10^{-4} \frac{V}{K} \right)$   | -1.562 | <b>-1.563</b>    | -1.562 | <b>-1.322</b>   | -1.320  |
| ZT                                       | 0.999  | <b>1</b>         | 0.998  | <b>0.715</b>    | 0.713   |
| $(ZT)_{Mott}$                            | 0.931  | <b>1</b>         | 1.074  | <b>3.290</b>    | 3.305   |
| $VC1 \left( 10^{-4} \frac{V}{K} \right)$ | -0.061 | <b>0</b>         | 0.063  | <b>1.105</b>    | 1.109   |
| $VC2 \left( 10^{-2} \frac{V}{K} \right)$ | -0.080 | <b>0</b>         | 0.086  | 2.020           | 2.029   |
| $T_s \left( 10^{-4} \frac{V}{K} \right)$ | -0.092 | <b>0</b>         | 0.094  | <b>1.657</b>    | 1.663   |
| Pt ( $10^{-2} V$ )                       | -2.053 | <b>-2.099</b>    | -2.143 | <b>-2.4159</b>  | -2.4153 |

In the degenerate Cd-X(x)-alloy, for  $N = 2 \times N_{CDP}(r_{Cd}) = 1.0695783 \times 10^{19} \text{ cm}^{-3}$ , one gets:

|  |        |                  |        |                  |         |
|--|--------|------------------|--------|------------------|---------|
| T(K)                                     | 142.69 | <b>145.79633</b> | 148.93 | <b>198.39414</b> | 198.59  |
| $\xi_p$                                  | 1.880  | <b>1.8138</b>    | 1.750  | <b>1</b>         | 0.998   |
| $S \left( 10^{-4} \frac{V}{K} \right)$   | -1.562 | <b>-1.563</b>    | -1.562 | <b>-1.322</b>    | -1.320  |
| ZT                                       | 0.999  | <b>1</b>         | 0.999  | <b>0.715</b>     | 0.713   |
| $(ZT)_{Mott}$                            | 0.931  | <b>1</b>         | 1.074  | <b>3.290</b>     | 3.305   |
| $VC1 \left( 10^{-4} \frac{V}{K} \right)$ | -0.061 | <b>0</b>         | 0.063  | <b>1.105</b>     | 1.109   |
| $VC2 \left( 10^{-2} \frac{V}{K} \right)$ | -0.087 | <b>0</b>         | 0.094  | 2.192            | 2.202   |
| $T_s \left( 10^{-4} \frac{V}{K} \right)$ | -0.092 | <b>0</b>         | 0.094  | <b>1.657</b>     | 1.663   |
| Pt ( $10^{-2} V$ )                       | -2.229 | <b>-2.279</b>    | -2.326 | <b>-2.6222</b>   | -2.6215 |

**Table 6n:** Here, for a given T and with decreasing N, the reduced Fermi-energy  $\xi_n$  decreases, and other thermoelectric coefficients are in variations, as indicated by the arrows as: (increase:  $\nearrow$ , decrease:  $\searrow$ ). One notes here that with increasing T: (i) for  $\xi_n \approx 1.8138$ , while the numerical results of S present a same minimum ( $S_{\min} \approx -1.563 \times 10^{-4} \frac{V}{K}$ ), those of ZT show a same maximum ( $ZT_{\max} = 1$ ), (ii) for  $\xi_n = 1$ , those of S, ZT, ( $ZT$ )<sub>Mott</sub>, VC1, and  $T_s$  present the same results:

$-1.322 \times 10^{-4} \frac{V}{K}$ , 0.715, 3.290,  $-1.105 \times 10^{-4} \frac{V}{K}$ , and  $1.657 \times 10^{-4} \frac{V}{K}$ , respectively, and (iii) for  $\xi_n \approx 1.8138$ ,  $(ZT)_{Mott} = 1$ .

For x=0

In the degenerate P- X(x) – alloy, for T= 44.769183 K, one gets:

|                             |        |           |        |            |        |
|-----------------------------|--------|-----------|--------|------------|--------|
| $N(10^{17} \text{cm}^{-3})$ | 3.4274 | 3.3719916 | 3.319  | 2.74813904 | 2.7466 |
| $\xi_n$                     | 1.880  | 1.8138    | 1.750  | 1          | 0.998  |
| $S(10^{-4} \frac{V}{K})$    | -1.562 | -1.563    | -1.562 | -1.322     | -1.320 |
| ZT                          | 0.999  | 1         | 0.998  | 0.715      | 0.713  |
| $(ZT)_{Mott}$               | 0.931  | 1         | 1.074  | 3.290      | 3.305  |
| $VC1(10^{-4} \frac{V}{K})$  | -0.061 | 0         | 0.063  | 1.105      | 1.109  |
| $VC2(10^{-4} \frac{V}{K})$  | -2.746 | 0         | 2.817  | 49.467     | 49.641 |
| $T_s(10^{-4} \frac{V}{K})$  | -0.092 | 0         | 0.094  | 1.657      | 1.663  |
| Pt ( $10^{-3} V$ )          | -6.993 | -6.997    | -6.993 | -5.917     | -5.910 |

In the degenerate As- X(x) – alloy, for T= 46.979655 K, one gets:

|                             |        |           |        |           |        |
|-----------------------------|--------|-----------|--------|-----------|--------|
| $N(10^{17} \text{cm}^{-3})$ | 3.6843 | 3.6247868 | 3.568  | 2.9541646 | 2.9525 |
| $\xi_n$                     | 1.880  | 1.8138    | 1.750  | 1         | 0.998  |
| $S(10^{-4} \frac{V}{K})$    | -1.562 | -1.563    | -1.562 | -1.322    | -1.320 |
| ZT                          | 0.999  | 1         | 0.998  | 0.715     | 0.713  |
| $(ZT)_{Mott}$               | 0.931  | 1         | 1.074  | 3.290     | 3.305  |
| $VC1(10^{-4} \frac{V}{K})$  | -0.061 | 0         | 0.063  | 1.105     | 1.109  |
| $VC2(10^{-4} \frac{V}{K})$  | -2.879 | 0         | 2.947  | 51.910    | 52.093 |
| $T_s(10^{-4} \frac{V}{K})$  | -0.092 | 0         | 0.094  | 1.657     | 1.663  |
| Pt ( $10^{-3} V$ )          | -7.338 | -7.343    | -7.338 | -6.209    | -6.202 |

In the degenerate Sb- X(x) – alloy, for T= 70.128324 K, one gets:

|                             |         |           |         |            |        |
|-----------------------------|---------|-----------|---------|------------|--------|
| $N(10^{17} \text{cm}^{-3})$ | 6.72    | 6.6108594 | 6.507   | 5.38778352 | 5.3846 |
| $\xi_n$                     | 1.880   | 1.8138    | 1.750   | 1          | 0.998  |
| $S(10^{-4} \frac{V}{K})$    | -1.562  | -1.563    | -1.562  | -1.322     | -1.320 |
| ZT                          | 0.999   | 1         | 0.999   | 0.715      | 0.713  |
| $(ZT)_{Mott}$               | 0.931   | 1         | 1.074   | 3.290      | 3.306  |
| $VC1(10^{-4} \frac{V}{K})$  | -0.062  | 0         | 0.063   | 1.105      | 1.109  |
| $VC2(10^{-4} \frac{V}{K})$  | -4.321  | 0         | 4.411   | 77.488     | 77.774 |
| $T_s(10^{-4} \frac{V}{K})$  | -0.092  | 0         | 0.094   | 1.657      | 1.663  |
| Pt ( $10^{-3} V$ )          | -10.954 | -10.961   | -10.954 | -9.269     | -9.257 |

In the degenerate Sn- X(x) – alloy, for T=79.154538, one gets:

|                             |        |           |        |           |        |
|-----------------------------|--------|-----------|--------|-----------|--------|
| $N(10^{17} \text{cm}^{-3})$ | 8.058  | 7.9274126 | 7.803  | 6.4607611 | 6.457  |
| $\xi_n$                     | 1.880  | 1.8138    | 1.750  | 1         | 0.998  |
| $S(10^{-4} \frac{V}{K})$    | -1.562 | -1.563    | -1.562 | -1.322    | -1.320 |
| ZT                          | 0.999  | 1         | 0.999  | 0.715     | 0.713  |
| $(ZT)_{Mott}$               | 0.931  | 1         | 1.074  | 3.290     | 3.305  |
| $VC1(10^{-4} \frac{V}{K})$  | -0.061 | 0         | 0.063  | 1.105     | 1.109  |
| $VC2(10^{-4} \frac{V}{K})$  | -4.866 | 0         | 4.974  | 87.461    | 87.780 |
| $T_s(10^{-4} \frac{V}{K})$  | -0.092 | 0         | 0.094  | 1.657     | 1.663  |

Pt ( $10^{-3}V$ ) -12.364 ↘ -12.372 ↗ -12.364 ↗ **-10.462** ↗ -10.449

For x=0.5,

In the degenerate P- X(x) – alloy, for T= **52.538752 K**, one gets:

|  |        |                  |        |                 |         |
|--|--------|------------------|--------|-----------------|---------|
| $N(10^{19} \text{cm}^{-3})$              | 6.487  | <b>6.3822952</b> | 6.2823 | <b>5.201506</b> | 5.1985  |
| $\xi_m$                                  | 1.880  | <b>1.8138</b>    | 1.750  | <b>1</b>        | 0.998   |
| $S(10^{-4} \frac{\text{V}}{\text{K}})$   | -1.562 | <b>-1.563</b>    | -1.562 | <b>-1.322</b>   | -1.320  |
| ZT                                       | 0.999  | <b>1</b>         | 0.999  | <b>0.715</b>    | 0.713   |
| $(ZT)_{Mott}$                            | 0.931  | <b>1</b>         | 1.074  | <b>3.290</b>    | 3.305   |
| $VC1(10^{-4} \frac{\text{V}}{\text{K}})$ | -0.061 | <b>0</b>         | 0.063  | <b>1.105</b>    | 1.109   |
| $VC2(10^{-4} \frac{\text{V}}{\text{K}})$ | -3.217 | <b>0</b>         | 3.296  | <b>58.052</b>   | 58.262  |
| $T_s(10^{-4} \frac{\text{V}}{\text{K}})$ | -0.092 | <b>0</b>         | 0.094  | <b>1.657</b>    | 1.663   |
| Pt ( $10^{-3}V$ )                        | -8.206 | <b>-8.212</b>    | -8.206 | <b>-6.9441</b>  | -6.9353 |

In the degenerate As- X(x) – alloy, for T= **55.132846 K**, one gets:

|  |        |                  |        |                  |         |
|--|--------|------------------|--------|------------------|---------|
| $N(10^{19} \text{cm}^{-3})$              | 6.973  | <b>6.8607702</b> | 6.753  | <b>5.5914583</b> | 5.5882  |
| $\xi_m$                                  | 1.879  | <b>1.8138</b>    | 1.750  | <b>1</b>         | 0.998   |
| $S(10^{-4} \frac{\text{V}}{\text{K}})$   | -1.562 | <b>-1.563</b>    | -1.562 | <b>-1.322</b>    | -1.320  |
| ZT                                       | 0.999  | <b>1</b>         | 0.999  | <b>0.715</b>     | 0.713   |
| $(ZT)_{Mott}$                            | 0.931  | <b>1</b>         | 1.074  | <b>3.290</b>     | 3.305   |
| $VC1(10^{-4} \frac{\text{V}}{\text{K}})$ | -0.061 | <b>0</b>         | 0.063  | <b>1.105</b>     | 1.109   |
| $VC2(10^{-4} \frac{\text{V}}{\text{K}})$ | -3.367 | <b>0</b>         | 3.468  | <b>60.919</b>    | 61.141  |
| $T_s(10^{-4} \frac{\text{V}}{\text{K}})$ | -0.092 | <b>0</b>         | 0.094  | <b>1.657</b>     | 1.663   |
| Pt ( $10^{-3}V$ )                        | -8.612 | <b>-8.617</b>    | -8.612 | <b>-7.2869</b>   | -7.2777 |

In the degenerate Sb- X(x) – alloy, for T= **82.298904 K**, one gets:

|  |         |                  |         |                   |          |
|--|---------|------------------|---------|-------------------|----------|
| $N(10^{18} \text{cm}^{-3})$              | 1.2718  | <b>1.2512622</b> | 1.2316  | <b>1.01976604</b> | 1.01916  |
| $\xi_m$                                  | 1.880   | <b>1.8138</b>    | 1.750   | <b>1</b>          | 0.998    |
| $S(10^{-4} \frac{\text{V}}{\text{K}})$   | -1.562  | <b>-1.563</b>    | -1.562  | <b>-1.322</b>     | -1.320   |
| ZT                                       | 0.999   | <b>1</b>         | 0.999   | <b>0.715</b>      | 0.713    |
| $(ZT)_{Mott}$                            | 0.931   | <b>1</b>         | 1.074   | <b>3.290</b>      | 3.306    |
| $VC1(10^{-4} \frac{\text{V}}{\text{K}})$ | -0.061  | <b>0</b>         | 0.063   | <b>1.105</b>      | 1.109    |
| $VC2(10^{-4} \frac{\text{V}}{\text{K}})$ | -5.042  | <b>0</b>         | 5.178   | <b>90.936</b>     | 91.274   |
| $T_s(10^{-4} \frac{\text{V}}{\text{K}})$ | -0.092  | <b>0</b>         | 0.094   | <b>1.657</b>      | 1.663    |
| Pt ( $10^{-3}V$ )                        | -12.855 | <b>-12.863</b>   | -12.855 | <b>-10.8775</b>   | -10.8634 |

In the degenerate Sn- X(x) – alloy, for T= **92.891593 K** one gets:

|  |         |                  |         |                  |         |
|--|---------|------------------|---------|------------------|---------|
| $N(10^{18} \text{cm}^{-3})$              | 1.5251  | <b>1.5004512</b> | 1.4769  | <b>1.2228525</b> | 1.22215 |
| $\xi_m$                                  | 1.880   | <b>1.8138</b>    | 1.750   | <b>1</b>         | 0.998   |
| $S(10^{-4} \frac{\text{V}}{\text{K}})$   | -1.562  | <b>-1.563</b>    | -1.562  | <b>-1.322</b>    | -1.320  |
| ZT                                       | 0.999   | <b>1</b>         | 0.999   | <b>0.715</b>     | 0.713   |
| $(ZT)_{Mott}$                            | 0.931   | <b>1</b>         | 1.074   | <b>3.290</b>     | 3.305   |
| $VC1(10^{-4} \frac{\text{V}}{\text{K}})$ | -0.061  | <b>0</b>         | 0.063   | <b>1.105</b>     | 1.109   |
| $VC2(10^{-4} \frac{\text{V}}{\text{K}})$ | -5.696  | <b>0</b>         | 5.838   | <b>102.640</b>   | 103.009 |
| $T_s(10^{-4} \frac{\text{V}}{\text{K}})$ | -0.092  | <b>0</b>         | 0.094   | <b>1.657</b>     | 1.663   |
| Pt ( $10^{-3}V$ )                        | -14.510 | <b>-14.519</b>   | -14.510 | <b>-12.277</b>   | -12.262 |

For  $x=1$ ,

In the degenerate P-  $\text{X}(\text{x})$  – alloy, for  $T=58.616225 \text{ K}$ , one gets:

|   |        |           |         |            |          |
|---|--------|-----------|---------|------------|----------|
| $N(10^{18} \text{cm}^{-3})$                     | 1.0467 | 1.0297905 | 1.01362 | 0.83926887 | 0.838772 |
| $\xi_n$   | 1.880  | 1.8138    | 1.750   | 1          | 0.998    |
| $S(10^{-4} \frac{\text{V}}{\text{K}})$          | -1.562 | -1.563    | -1.562  | -1.322     | -1.320   |
| ZT  | 0.999  | 1         | 0.999   | 0.715      | 0.713    |
| $(\text{ZT})_{\text{Mott}}$                     | 0.931  | 1         | 1.074   | 3.290      | 3.306    |
| $\text{VC1}(10^{-4} \frac{\text{V}}{\text{K}})$ | -0.061 | 0         | 0.063   | 1.105      | 1.109    |
| $\text{VC2}(10^{-4} \frac{\text{V}}{\text{K}})$ | -3.593 | 0         | 3.685   | 64.768     | 65.008   |
| $T_s(10^{-4} \frac{\text{V}}{\text{K}})$        | -0.092 | 0         | 0.094   | 1.657      | 1.663    |
| $Pt(10^{-3}\text{V})$                           | -9.156 | -9.162    | -9.156  | -7.7473    | -7.7374  |

In the degenerate As-  $\text{X}(\text{x})$  – alloy, for  $T=61.510393 \text{ K}$ , one gets:

|   |        |          |        |           |         |
|---|--------|----------|--------|-----------|---------|
| $N(10^{18} \text{cm}^{-3})$                     | 1.1251 | 1.106993 | 1.0896 | 0.9021881 | 0.90168 |
| $\xi_n$   | 1.879  | 1.8138   | 1.750  | 1         | 0.998   |
| $S(10^{-4} \frac{\text{V}}{\text{K}})$          | -1.562 | -1.563   | -1.562 | -1.322    | -1.320  |
| ZT  | 0.999  | 1        | 0.999  | 0.715     | 0.713   |
| $(\text{ZT})_{\text{Mott}}$                     | 0.931  | 1        | 1.074  | 3.290     | 3.305   |
| $\text{VC1}(10^{-4} \frac{\text{V}}{\text{K}})$ | -0.061 | 0        | 0.063  | 1.105     | 1.109   |
| $\text{VC2}(10^{-4} \frac{\text{V}}{\text{K}})$ | -3.756 | 0        | 3.870  | 67.965    | 68.205  |
| $T_s(10^{-4} \frac{\text{V}}{\text{K}})$        | -0.091 | 0        | 0.094  | 1.657     | 1.663   |
| $Pt(10^{-3}\text{V})$                           | -9.608 | -9.614   | -9.608 | -8.1298   | -8.1199 |

In the degenerate Sb-  $\text{X}(\text{x})$  – alloy, for  $T=91.818907 \text{ K}$ , one gets:

|   |         |           |         |            |          |
|---|---------|-----------|---------|------------|----------|
| $N(10^{18} \text{cm}^{-3})$                     | 2.052   | 2.0189256 | 1.9873  | 1.64540394 | 1.64443  |
| $\xi_n$   | 1.880   | 1.8138    | 1.750   | 1          | 0.998    |
| $S(10^{-4} \frac{\text{V}}{\text{K}})$          | -1.562  | -1.563    | -1.562  | -1.322     | -1.320   |
| ZT  | 0.999   | 1         | 0.999   | 0.715      | 0.713    |
| $(\text{ZT})_{\text{Mott}}$                     | 0.931   | 1         | 1.074   | 3.290      | 3.306    |
| $\text{VC1}(10^{-4} \frac{\text{V}}{\text{K}})$ | -0.061  | 0         | 0.063   | 1.105      | 1.109    |
| $\text{VC2}(10^{-4} \frac{\text{V}}{\text{K}})$ | -5.615  | 0         | 5.758   | 101.455    | 101.831  |
| $T_s(10^{-4} \frac{\text{V}}{\text{K}})$        | -0.092  | 0         | 0.094   | 1.657      | 1.663    |
| $Pt(10^{-3}\text{V})$                           | -14.342 | -14.351   | -14.342 | -12.1357   | -12.1201 |

In the degenerate Sn-  $\text{X}(\text{x})$  – alloy, for  $T=103.636916 \text{ K}$ , one gets:

|   |         |           |         |           |          |
|---|---------|-----------|---------|-----------|----------|
| $N(10^{18} \text{cm}^{-3})$                     | 2.4607  | 2.4209948 | 2.383   | 1.9730863 | 1.97195  |
| $\xi_n$   | 1.880   | 1.8138    | 1.750   | 1         | 0.998    |
| $S(10^{-4} \frac{\text{V}}{\text{K}})$          | -1.562  | -1.563    | -1.562  | -1.322    | -1.320   |
| ZT  | 0.999   | 1         | 0.999   | 0.715     | 0.713    |
| $(\text{ZT})_{\text{Mott}}$                     | 0.931   | 1         | 1.074   | 3.290     | 3.305    |
| $\text{VC1}(10^{-4} \frac{\text{V}}{\text{K}})$ | -0.061  | 0         | 0.063   | 1.105     | 1.109    |
| $\text{VC2}(10^{-4} \frac{\text{V}}{\text{K}})$ | -6.344  | 0         | 6.512   | 114.513   | 114.926  |
| $T_s(10^{-4} \frac{\text{V}}{\text{K}})$        | -0.092  | 0         | 0.094   | 1.657     | 1.663    |
| $Pt(10^{-3}\text{V})$                           | -16.188 | -16.198   | -16.188 | -13.6977  | -13.6806 |

**Table 6p:** Here, for a given  $T$  and with decreasing  $N$ , the reduced Fermi-energy  $\xi_p$  decreases, and other thermoelectric coefficients are in variations, as indicated by the arrows as: (increase:  $\nearrow$ , decrease:  $\searrow$ ). One notes here that with increasing  $T$ : (i) for  $\xi_p \approx 1.8138$ , while the numerical results of  $S$  present a same minimum ( $S_{\min} \approx -1.563 \times 10^{-4} \frac{\text{V}}{\text{K}}$ ), those of ZT

show a same maximum  $(ZT)_{\max} = 1$ , (ii) for  $\xi_p = 1$ , those of S, ZT,  $(ZT)_{\text{Mott}}$ , VC1, and  $T_s$  present the same results:  $-1.322 \times 10^{-4} \frac{\text{V}}{\text{K}}$ , 0.715, 3.290,  $-1.105 \times 10^{-4} \frac{\text{V}}{\text{K}}$ , and  $1.657 \times 10^{-4} \frac{\text{V}}{\text{K}}$ , respectively, and (iii) for  $\xi_p \approx 1.8138$ ,  $(ZT)_{\text{Mott}} = 1$ .

For x=0,

In the degenerate Ga- X(x) – alloy, for T=172.18917 K, one gets:

|  |               |                  |        |                   |         |
|--|---------------|------------------|--------|-------------------|---------|
| $N(10^{19} \text{cm}^{-3})$              | 1.950         | <b>1.9185205</b> | 1.8885 | <b>1.56357483</b> | 1.5627  |
| $\xi_p$                                  | 1.880         | <b>1.8138</b>    | 1.750  | <b>1</b>          | 0.998   |
| $S(10^{-4} \frac{\text{V}}{\text{K}})$   | -1.562        | <b>-1.563</b>    | -1.562 | <b>-1.322</b>     | -1.320  |
| ZT                                       | 0.999         | <b>1</b>         | 0.999  | <b>0.715</b>      | 0.713   |
| $(ZT)_{\text{Mott}}$                     | 0.931         | <b>1</b>         | 1.074  | <b>3.290</b>      | 3.305   |
| $VC1(10^{-4} \frac{\text{V}}{\text{K}})$ | -0.061        | <b>0</b>         | 0.063  | <b>1.105</b>      | 1.109   |
| $VC2(10^{-2} \text{V})$                  | -0.105        | <b>0</b>         | 0.108  | <b>1.902</b>      | 1.909   |
| $T_s(10^{-4} \frac{\text{V}}{\text{K}})$ | <b>-0.092</b> | <b>0</b>         | 0.094  | <b>1.657</b>      | 1.663   |
| Pt ( $10^{-2} \text{V}$ )                | -2.690        | <b>-2.691</b>    | -2.690 | <b>-2.2758</b>    | -2.2731 |

In the degenerate Mg- X(x) – alloy, for T= 192.42153 K, one gets:

|  |               |                  |        |                  |         |
|--|---------------|------------------|--------|------------------|---------|
| $N(10^{19} \text{cm}^{-3})$              | 2.3036        | <b>2.2664086</b> | 2.2308 | <b>1.8471001</b> | 1.84601 |
| $\xi_p$                                  | 1.880         | <b>1.8138</b>    | 1.750  | <b>1</b>         | 0.998   |
| $S(10^{-4} \frac{\text{V}}{\text{K}})$   | -1.562        | <b>-1.563</b>    | -1.562 | <b>-1.322</b>    | -1.320  |
| ZT                                       | 0.999         | <b>1</b>         | 0.999  | <b>0.715</b>     | 0.713   |
| $(ZT)_{\text{Mott}}$                     | 0.931         | <b>1</b>         | 1.074  | <b>3.290</b>     | 3.306   |
| $VC1(10^{-4} \frac{\text{V}}{\text{K}})$ | -0.061        | <b>0</b>         | 0.063  | <b>1.105</b>     | 1.109   |
| $VC2(10^{-2} \text{V})$                  | -0.118        | <b>0</b>         | 0.121  | <b>2.126</b>     | 2.134   |
| $T_s(10^{-4} \frac{\text{V}}{\text{K}})$ | <b>-0.092</b> | <b>0</b>         | 0.094  | <b>1.657</b>     | 1.663   |
| Pt ( $10^{-2} \text{V}$ )                | -3.006        | <b>-3.007</b>    | -3.006 | <b>-2.5432</b>   | -2.5400 |

In the degenerate In- X(x) – alloy, for T=206.175403 K, one gets:

|  |               |                  |        |                   |         |
|--|---------------|------------------|--------|-------------------|---------|
| $N(10^{19} \text{cm}^{-3})$              | 2.555         | <b>2.5136974</b> | 2.2308 | <b>2.04863793</b> | 2.04743 |
| $\xi_p$                                  | 1.880         | <b>1.8138</b>    | 1.750  | <b>1</b>          | 0.998   |
| $S(10^{-4} \frac{\text{V}}{\text{K}})$   | -1.562        | <b>-1.563</b>    | -1.562 | <b>-1.322</b>     | -1.320  |
| ZT                                       | 0.999         | <b>1</b>         | 0.999  | <b>0.715</b>      | 0.713   |
| $(ZT)_{\text{Mott}}$                     | 0.931         | <b>1</b>         | 1.074  | <b>3.290</b>      | 3.306   |
| $VC1(10^{-4} \frac{\text{V}}{\text{K}})$ | -0.061        | <b>0</b>         | 0.063  | <b>1.105</b>      | 1.109   |
| $VC2(10^{-2} \text{V})$                  | -0.126        | <b>0</b>         | 0.121  | <b>2.278</b>      | 2.286   |
| $T_s(10^{-4} \frac{\text{V}}{\text{K}})$ | <b>-0.092</b> | <b>0</b>         | 0.094  | <b>1.657</b>      | 1.663   |
| Pt ( $10^{-2} \text{V}$ )                | -3.220        | <b>-3.222</b>    | -3.006 | <b>-2.7250</b>    | -2.7215 |

In the degenerate Cd- X(x) – alloy, for T=223.779792 K, one gets:

|  |               |                 |         |                  |         |
|--|---------------|-----------------|---------|------------------|---------|
| $N(10^{19} \text{cm}^{-3})$              | 2.889         | <b>2.842425</b> | 2.79776 | <b>2.3165476</b> | 2.3152  |
| $\xi_p$                                  | 1.880         | <b>1.8138</b>   | 1.750   | <b>1</b>         | 0.998   |
| $S(10^{-4} \frac{\text{V}}{\text{K}})$   | -1.562        | <b>-1.563</b>   | -1.562  | <b>-1.322</b>    | -1.320  |
| ZT                                       | 0.999         | <b>1</b>        | 0.999   | <b>0.715</b>     | 0.713   |
| $(ZT)_{\text{Mott}}$                     | 0.931         | <b>1</b>        | 1.074   | <b>3.290</b>     | 3.305   |
| $VC1(10^{-4} \frac{\text{V}}{\text{K}})$ | -0.061        | <b>0</b>        | 0.063   | <b>1.105</b>     | 1.109   |
| $VC2(10^{-2} \text{V})$                  | -0.137        | <b>0</b>        | 0.141   | <b>2.473</b>     | 2.482   |
| $T_s(10^{-4} \frac{\text{V}}{\text{K}})$ | <b>-0.092</b> | <b>0</b>        | 0.094   | <b>1.657</b>     | 1.663   |
| Pt ( $10^{-2} \text{V}$ )                | -3.495        | <b>-3.498</b>   | -3.495  | <b>-2.9577</b>   | -2.9540 |

For x=0.5,

In the degenerate Ga- X(x) – alloy, for T=139.483412 K, one gets:

|  |               |                  |        |                   |         |
|--|---------------|------------------|--------|-------------------|---------|
| $N(10^{19} \text{cm}^{-3})$              | 1.2139        | <b>1.1942777</b> | 1.1756 | <b>0.97332424</b> | 0.97275 |
| $\xi_p$                                  | 1.880         | <b>1.8138</b>    | 1.750  | <b>1</b>          | 0.998   |
| $S(10^{-4} \frac{\text{V}}{\text{K}})$   | -1.562        | <b>-1.563</b>    | -1.562 | <b>-1.322</b>     | -1.320  |
| ZT                                       | 0.999         | <b>1</b>         | 0.999  | <b>0.715</b>      | 0.713   |
| $(ZT)_{\text{Mott}}$                     | 0.931         | <b>1</b>         | 1.074  | <b>3.290</b>      | 3.306   |
| $VC1(10^{-4} \frac{\text{V}}{\text{K}})$ | -0.061        | <b>0</b>         | 0.063  | <b>1.105</b>      | 1.109   |
| $VC2(10^{-2} \text{V})$                  | -0.085        | <b>0</b>         | 0.087  | <b>1.541</b>      | 1.547   |
| $T_s(10^{-4} \frac{\text{V}}{\text{K}})$ | <b>-0.092</b> | <b>0</b>         | 0.094  | <b>1.657</b>      | 1.663   |
| $Pt(10^{-2} \text{V})$                   | -2.179        | <b>-2.180</b>    | -2.179 | <b>-1.8435</b>    | -1.8412 |

In the degenerate Mg- X(x) – alloy, for T=155.87283 K, one gets:

|  |               |                  |        |                  |         |
|--|---------------|------------------|--------|------------------|---------|
| $N(10^{19} \text{cm}^{-3})$              | 1.434         | <b>1.4108379</b> | 1.3887 | <b>1.1498186</b> | 1.14915 |
| $\xi_p$                                  | 1.880         | <b>1.8138</b>    | 1.750  | <b>1</b>         | 0.998   |
| $S(10^{-4} \frac{\text{V}}{\text{K}})$   | -1.562        | <b>-1.563</b>    | -1.562 | <b>-1.322</b>    | -1.320  |
| ZT                                       | 0.999         | <b>1</b>         | 0.999  | <b>0.715</b>     | 0.713   |
| $(ZT)_{\text{Mott}}$                     | 0.931         | <b>1</b>         | 1.074  | <b>3.290</b>     | 3.305   |
| $VC1(10^{-4} \frac{\text{V}}{\text{K}})$ | -0.061        | <b>0</b>         | 0.063  | <b>1.105</b>     | 1.109   |
| $VC2(10^{-2} \text{V})$                  | -0.095        | <b>0</b>         | 0.098  | <b>1.722</b>     | 1.728   |
| $T_s(10^{-4} \frac{\text{V}}{\text{K}})$ | <b>-0.092</b> | <b>0</b>         | 0.094  | <b>1.657</b>     | 1.663   |
| $Pt(10^{-2} \text{V})$                   | -2.435        | <b>-2.436</b>    | -2.435 | <b>-2.0602</b>   | -2.0576 |

In the degenerate In- X(x) – alloy, for T=167.014273 K, one gets:

|  |               |                  |        |                   |         |
|--|---------------|------------------|--------|-------------------|---------|
| $N(10^{19} \text{cm}^{-3})$              | 1.59049       | <b>1.5647749</b> | 1.5402 | <b>1.27527567</b> | 1.27452 |
| $\xi_p$                                  | 1.880         | <b>1.8138</b>    | 1.750  | <b>1</b>          | 0.998   |
| $S(10^{-4} \frac{\text{V}}{\text{K}})$   | -1.562        | <b>-1.563</b>    | -1.562 | <b>-1.322</b>     | -1.320  |
| ZT                                       | 0.999         | <b>1</b>         | 0.999  | <b>0.715</b>      | 0.713   |
| $(ZT)_{\text{Mott}}$                     | 0.931         | <b>1</b>         | 1.074  | <b>3.290</b>      | 3.306   |
| $VC1(10^{-4} \frac{\text{V}}{\text{K}})$ | -0.061        | <b>0</b>         | 0.063  | <b>1.105</b>      | 1.109   |
| $VC2(10^{-2} \text{V})$                  | -0.102        | <b>0</b>         | 0.105  | <b>1.845</b>      | 1.852   |
| $T_s(10^{-4} \frac{\text{V}}{\text{K}})$ | <b>-0.092</b> | <b>0</b>         | 0.094  | <b>1.657</b>      | 1.663   |
| $Pt(10^{-2} \text{V})$                   | -2.609        | <b>-2.610</b>    | -2.609 | <b>-2.2074</b>    | -2.2046 |

In the degenerate Cd- X(x) – alloy, for T=181.27487 K, one gets:

|  |               |                  |         |                   |         |
|--|---------------|------------------|---------|-------------------|---------|
| $N(10^{19} \text{cm}^{-3})$              | 1.79848       | <b>1.7694076</b> | 1.74161 | <b>1.44204927</b> | 1.44112 |
| $\xi_p$                                  | 1.880         | <b>1.8138</b>    | 1.750   | <b>1</b>          | 0.998   |
| $S(10^{-4} \frac{\text{V}}{\text{K}})$   | -1.562        | <b>-1.563</b>    | -1.562  | <b>-1.322</b>     | -1.320  |
| ZT                                       | 0.999         | <b>1</b>         | 0.999   | <b>0.715</b>      | 0.713   |
| $(ZT)_{\text{Mott}}$                     | 0.931         | <b>1</b>         | 1.074   | <b>3.290</b>      | 3.306   |
| $VC1(10^{-4} \frac{\text{V}}{\text{K}})$ | -0.061        | <b>0</b>         | 0.063   | <b>1.105</b>      | 1.109   |
| $VC2(10^{-2} \text{V})$                  | -0.111        | <b>0</b>         | 0.114   | <b>2.003</b>      | 2.010   |
| $T_s(10^{-4} \frac{\text{V}}{\text{K}})$ | <b>-0.092</b> | <b>0</b>         | 0.094   | <b>1.657</b>      | 1.663   |
| $Pt(10^{-2} \text{V})$                   | -2.831        | <b>-2.833</b>    | -2.831  | <b>-2.3959</b>    | -2.3928 |

For x=1,

In the degenerate Ga- X(x) – alloy, for T=112.184162 K, one gets:

|  |        |                  |        |                  |        |
|--|--------|------------------|--------|------------------|--------|
| $N(10^{18} \text{cm}^{-3})$            | 7.3378 | <b>7.2192156</b> | 7.1062 | <b>5.8835877</b> | 1.8801 |
| $\xi_p$                                | 1.880  | <b>1.8138</b>    | 1.750  | <b>1</b>         | 0.998  |
| $S(10^{-4} \frac{\text{V}}{\text{K}})$ | -1.562 | <b>-1.563</b>    | -1.562 | <b>-1.322</b>    | -1.320 |

|                            |               |        |        |              |         |
|----------------------------|---------------|--------|--------|--------------|---------|
| ZT                         | 0.999         | 1      | 0.999  | <b>0.715</b> | 0.713   |
| $(ZT)_{Mott}$              | 0.931         | 1      | 1.074  | <b>3.290</b> | 3.306   |
| $VC1(10^{-4} \frac{V}{K})$ | -0.061        | 0      | 0.063  | <b>1.105</b> | 1.109   |
| $VC2(10^{-2}V)$            | -0.069        | 0      | 0.070  | 1.239        | 1.244   |
| $T_s(10^{-4} \frac{V}{K})$ | <b>-0.092</b> | 0      | 0.094  | <b>1.657</b> | 1.663   |
| Pt ( $10^{-2}V$ )          | -1.752        | -1.753 | -1.752 | -1.4827      | -1.4808 |

In the degenerate Mg- X(x) – alloy, for T=125.365892 K, one gets:

|                               |               |                  |        |                  |         |
|-------------------------------|---------------|------------------|--------|------------------|---------|
| N( $10^{18} \text{cm}^{-3}$ ) | 8.6684        | <b>8.5282866</b> | 8.3943 | <b>6.9504673</b> | 6.9464  |
| $\xi_p$                       | 1.880         | <b>1.8138</b>    | 1.750  | <b>1</b>         | 0.998   |
| $S(10^{-4} \frac{V}{K})$      | -1.562        | <b>-1.563</b>    | -1.562 | <b>-1.322</b>    | -1.320  |
| ZT                            | 0.999         | 1                | 0.999  | <b>0.715</b>     | 0.713   |
| $(ZT)_{Mott}$                 | 0.931         | 1                | 1.074  | <b>3.290</b>     | 3.305   |
| $VC1(10^{-4} \frac{V}{K})$    | -0.061        | 0                | 0.063  | <b>1.105</b>     | 1.109   |
| $VC2(10^{-2}V)$               | -0.077        | 0                | 0.079  | 1.385            | 1.390   |
| $T_s(10^{-4} \frac{V}{K})$    | <b>-0.092</b> | 0                | 0.094  | <b>1.657</b>     | 1.663   |
| Pt ( $10^{-2}V$ )             | -1.958        | -1.959           | -1.958 | -1.6570          | -1.6549 |

In the degenerate In- X(x) – alloy, for T=134.32677 K, one gets:

|                               |               |                 |        |                  |         |
|-------------------------------|---------------|-----------------|--------|------------------|---------|
| N( $10^{18} \text{cm}^{-3}$ ) | 9.614         | <b>9.458811</b> | 9.3102 | <b>7.7088353</b> | 7.70426 |
| $\xi_p$                       | 1.880         | <b>1.8138</b>   | 1.750  | <b>1</b>         | 0.998   |
| $S(10^{-4} \frac{V}{K})$      | -1.562        | <b>-1.563</b>   | -1.562 | <b>-1.322</b>    | -1.320  |
| ZT                            | 0.999         | 1               | 0.999  | <b>0.715</b>     | 0.713   |
| $(ZT)_{Mott}$                 | 0.931         | 1               | 1.074  | <b>3.290</b>     | 3.306   |
| $VC1(10^{-4} \frac{V}{K})$    | -0.061        | 0               | 0.063  | <b>1.105</b>     | 1.109   |
| $VC2(10^{-2}V)$               | -0.082        | 0               | 0.084  | 1.484            | 1.489   |
| $T_s(10^{-4} \frac{V}{K})$    | <b>-0.092</b> | 0               | 0.094  | <b>1.657</b>     | 1.663   |
| Pt ( $10^{-2}V$ )             | -2.098        | -2.099          | -2.098 | -1.7754          | -1.7731 |

In the degenerate Cd- X(x) – alloy, for T=145.79633 K, one gets:

|                               |               |                  |        |                   |         |
|-------------------------------|---------------|------------------|--------|-------------------|---------|
| N( $10^{19} \text{cm}^{-3}$ ) | 1.08715       | <b>1.0695783</b> | 1.0528 | <b>0.87169547</b> | 0.87118 |
| $\xi_p$                       | 1.880         | <b>1.8138</b>    | 1.750  | <b>1</b>          | 0.998   |
| $S(10^{-4} \frac{V}{K})$      | -1.562        | <b>-1.563</b>    | -1.562 | <b>-1.322</b>     | -1.320  |
| ZT                            | 0.999         | 1                | 0.999  | <b>0.715</b>      | 0.713   |
| $(ZT)_{Mott}$                 | 0.931         | 1                | 1.074  | <b>3.290</b>      | 3.306   |
| $VC1(10^{-4} \frac{V}{K})$    | -0.061        | 0                | 0.063  | <b>1.105</b>      | 1.109   |
| $VC2(10^{-2}V)$               | -0.089        | 0                | 0.091  | 1.611             | 1.617   |
| $T_s(10^{-4} \frac{V}{K})$    | <b>-0.092</b> | 0                | 0.094  | <b>1.657</b>      | 1.663   |
| Pt ( $10^{-2}V$ )             | -2.277        | -2.279           | -2.277 | -1.9270           | -1.9245 |