World Journal of Engineering Research and Technology

www.wjert.org

Impact Factor: 7.029 Coden USA: WJERA4

# OPTICAL, ELECTRICAL AND THERMOELECTRIC LAWS IN n(p)-TYPE DEGENERATE "COMPENSATED" InAs(1-x) Sb(x)-CRYSTALLINE ALLOY, ENHACED BY: OPTICO-ELECTRICAL -AND-ELECTRO-OPTICAL PHENOMENA, AND OUR STATIC DIELECTRIC CONSTANT LAW, ACCURATE FERMI ENERGY AND CONDUCTIVITY MODELS. (VI)

**Prof. Dr. Huynh Van Cong*, Michel Cayrol, Vincent L'Henaff, Prof. Dr. Serge Dumont**

Université de Perpignan Via Domitia, Laboratoire de Mathématiques et Physique (LAMPS), EA 4217, Département de Physique, 52, Avenue Paul Alduy, F-66 860 Perpignan, France.

**Article Received on 19/10/2025** **Article Revised on 08/11/2025** **Article Published on 01/12/2025**

***Corresponding Author**
**Prof. Dr. Huynh Van Cong**
Université de Perpignan Via Domitia, Laboratoire de Mathématiques et Physique (LAMPS), EA 4217, Département de Physique, 52, Avenue Paul Alduy, F-66 860 Perpignan, France.

https://doi.org/10.5281/zenodo.17750020

**How to cite this Article:** Prof. Dr. Huynh Van Cong*, Michel Cayrol, Vincent L'Henaff, and Prof. Dr. Serge Dumont. (2025). Optical, Electrical and Thermoelectric Laws in n(p)-Type Degenerate "Compensated" inas(1-x) sb(x)-crystalline Alloy, Enhaced by: Optico-Electrical -and-Electro-Optical Phenomena, and our Static Dielectric Constant Law, Accurate Fermi Energy and Conductivity Models. (vi). World Journal of Engineering Research and Technology, 11(11), 74–114.



## ABSTRACT

In degenerate n^+ (p^+)-p(n)- X(x)≡InAs(1-x)Sb(x)- crystalline alloy, $0 \leq x \leq 1$, various optical, electrical and thermoelectric laws, relations, and coefficients, enhanced by: the optico-electrical phenomenon (O-EP) and the electro-optical phenomenon (E-OP), and our static dielectric constant law given in Equations (1a, 1b), accurate Fermi energy expression in Eq. (11), and conductivity model in Eq. (18), are now investigated, by basing on the same physical model and mathematical treatment method, as those used in our recent works.[1-5] One notes that, for x=0, this crystalline alloy is reduced to the n(p)-type degenerate **InAs -crystal**. Some concluding remarks are given as follows. -By basing on our optical [electrical] conductivity models, $\sigma_{O[E]}$, given in Eq. (18), all the optical, electrical, thermoelectric coefficients have been determined, as those given in Equations (19a-19d, 20a-20d, 21-31). -In particular, for the physical conditions, as those given in Eq. (15), one remarks that the optical conductivity, $\sigma_O$, obtained from the O-EP, has a same form with that of the electrical conductivity, given from the E-OP, $\sigma_E$, as those determined in Eq. (20a), but $\sigma_O > \sigma_E$ since $m_r(x) < m_{c(v)}(x)$, $m_{c(v)}$ and $m_r$, being the unperturbed reduced effective electron (hole) mass in conduction (valence)

bands and the relative carrier mass, respectively. -Finally, the numerical results of such optical, electrical and thermoelectric coefficients, calculated by using Equations (18, 19a-19d, 20a-20d, 21-31), are reported in Tables 3-11, suggesting the new ones.

**KEYWORDS**: Optical-and-electrical conductivity, Seebeck coefficient, Figure of merit), First Van-Cong coefficient, Second Van-Cong coefficient, Thomson coefficient, Peltier coefficient.

## INTRODUCTION

In the $\mathbf{n^+(p^+) - X(x) \equiv InAs(1-x)Sb(x)}$ -crystalline alloy, $0 \le x \le 1$, x being the concentration, the optical, electrical and thermoelectric coefficients, enhanced by : (i) the optico-electrical phenomenon (O-EP) and the electro-optical phenomenon (E-OP), (ii) our static dielectric constant law, $\varepsilon(r_{d(a)}, x)$, $r_{d(a)}$ being the donor (acceptor) d(a)-radius, given in Equations (1a, 1b), (iii) our accurate reduced Fermi energy, $\xi_{n(p)}$, given in Eq. (11), accurate with a precision of the order of $2.11 \times 10^{-4}$ [9], affecting all the expressions of optical, electrical and thermoelectric coefficients, and (iv) our optical-and-electrical conductivity models, given in Eq. (18, 20a), are now investigated by basing on our physical model and Fermi-Dirac distribution function, as those given in our recent works.[1-5] It should be noted here that for x=0, the present obtained numerical results are reduced to those given in the n(p)-type degenerate **InAs-**crystal.[1, 6-16]

Then, some important remarks can be reported as follows.

**(1)** As observed in Equations (3, 5, 6a, 6b), the critical impurity density $N_{CDn(CDp)}$, defined by the generalized Mott criterium in the metal-insulator transition (**MIT**), is just the density of electrons (holes), localized in the exponential conduction (valence)-band tail (**EBT**), N_CDn(CDp)^EBT, being obtained with a precision of the order of $\mathbf{2.91 \times 10^{-7}}$, as given in our recent work.[3] Therefore, the effective electron (hole)-density can be defined as: N^*≡N-N_CDn(CDp) ≃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)** For given $[N, r_{d(a)}, x, T]$, the coefficients: $\sigma_{O[E]}(E)$, $\kappa_{O[E]}(E)$, $\varepsilon_{2\ O[E]}(E)$, and $\propto_{O[E]}(E)$, are determined in Equations (18, 19b-19d), as functions of the photon energy E, and then their numerical results are reported in Tables 3-8, being new ones.

**(4)** Finally, for particular physical conditions, as those given in Eq. (15), one observes that the optical conductivity $\sigma_O$ has a same form with that of the electrical conductivity, $\sigma_E$, as those given in Eq. (20a), but $\sigma_O > \sigma_E$ since $m_r(x) < m_{c(v)}(x)$, $m_{c(v)}$ and $m_r$, being the unperturbed reduced effective electron (hole) mass in conduction (valence) bands and the relative carrier mass, respectively. Then, by basing on those $\sigma_{O[E]}$ -expressions, the thermoelectric laws, relations, and coefficients are determined in Equations (21-31), and their numerical results are reported in Tables 9 and 10, being new ones.

In the following, various Sections are presented in order to investigate the optical, electrical and thermoelectric coefficients, given in the degenerate $n^+(p^+) - \mathbf{X}(\mathbf{x})$- crystalline alloy.

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

First of all, in the degenerate $n^+(p^+) - \mathbf{X}(\mathbf{x})$- crystalline alloy, at T=0 K[1-5], we denote : the donor (acceptor) d(a)-radius by $r_{d(a)}$, the corresponding intrinsic one by: $\mathbf{r_{do(ao)}}=\mathbf{r_{As(In)}}$, respectively, the effective averaged numbers of equivalent conduction (valence)-bands by: $g_{c(v)}$, the unperturbed reduced effective electron (hole) mass in conduction (valence) bands by $m_{c(v)}(x)/m_o$, $m_o$ being the free electron mass, the relative carrier mass by: $m_r(x) \equiv \frac{m_c(x)\times m_v(x)}{m_c(x)+m_v(x)} < m_{c(v)}(x)$ for given x , the unperturbed static dielectric constant by: $\varepsilon_o(x)$, and the intrinsic band gap by: $E_{go}(x)$, as those given in **Table 1, reported in Appendix 1**.

Here, the effective carrier mass $m^*_{n(p)}(x)$ is equal to $m_{c(v)}(x)$. Therefore, we can define the effective donor (acceptor)-ionization energy in absolute values as $E_{do(ao)}(x) = \frac{13600\times[m_{c(v)}(x)/m_o]}{[\varepsilon_o(x)]^2}$ meV , and then, the isothermal bulk modulus, by : $B_{do(ao)}(x) \equiv \frac{E_{do(ao)}(x)}{\left(\frac{4\pi}{3}\right)\times\left(r_{do(ao)}\right)^3}$.

**Our Static Dielectric Constant Law** $[m^*_{n(p)}(x) \equiv m_{c(v)}(x)]$

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

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

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 $E_{gn(gp)}(r_{d(a)}, x)$, 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 : $\pm [\Delta\alpha(r_{d(a)}, x)]_{n(p)}$,

$E_{gn(gp)}(r_{d(a)}, x) - E_{go}(x) = E_{d(a)}(r_{d(a)}, x) - E_{do(ao)}(x) = E_{do(ao)}(x) \times \left[\left(\frac{\varepsilon_o(x)}{\varepsilon(r_{d(a)})}\right)^2 - 1\right] = +[\Delta\alpha(r_{d(a)}, x)]_{n(p)}$, for $r_{d(a)} \geq r_{do(ao)}$, and for $r_{d(a)} \leq r_{do(ao)}$, $E_{gn(gp)}(r_{d(a)}, x) - E_{go}(x) = E_{d(a)}(r_{d(a)}, x) - E_{do(ao)}(x) = E_{do(ao)}(x) \times \left[\left(\frac{\varepsilon_o(x)}{\varepsilon(r_{d(a)})}\right)^2 - 1\right] = -[\Delta\alpha(r_{d(a)}, x)]_{n(p)}$.

There fore, 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 $\varepsilon(r_{d(a)}, x) = \frac{\varepsilon_o(x)}{\sqrt{1+\left[\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 - 1\right] \times \ln\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3}} \leq \varepsilon_o(x)$, being a **new** $\boldsymbol{\varepsilon(r_{d(a)}, x)}$**-law**,

$E_{gn(gp)}(r_{d(a)}, x) - E_{go}(x) = E_{d(a)}(r_{d(a)}, x) - E_{do(ao)}(x) = E_{do(ao)}(x) \times \left[\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 - 1\right] \times \ln\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 \geq 0$, (1 a) 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 $\varepsilon(r_{d(a)}, x) = \frac{\varepsilon_o(x)}{\sqrt{1-\left[\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 - 1\right] \times \ln\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3}} \geq \varepsilon_o(x)$, 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 $\boldsymbol{\varepsilon(r_{d(a)}, x)}$ -law**, $E_{gn(gp)}(r_{d(a)}, x) - E_{go}(x) = E_{d(a)}(r_{d(a)}, x) - E_{do(ao)}(x) = -E_{do(ao)}(x) \times \left[\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 - 1\right] \times \ln\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 \leq 0$, (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 optical, electrical and thermoelectric properties strongly depend on this **new $\boldsymbol{\varepsilon(r_{d(a)}, x)}$-law.**

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

$$a_{Bn(Bp)}(r_{d(a)}, x) \equiv \frac{\varepsilon(r_{d(a)}, x) \times \hbar^2}{m^*_{n(p)}(x) \times m_o \times q^2} = 0.53 \times 10^{-8}\ \text{cm} \times \frac{\varepsilon(r_{d(a)}, x)}{m^*_{n(p)}(x)} \quad (2)$$

**Generalized Mott Criterium in the MIT** $[m^*_{n(p)}(x) \equiv m_{c(v)}(x)]$

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[3]

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

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

This excellent one can be explained from the definition of the reduced effective Wigner-Seitz (**WS**) radius $r_{sn(sp),M}$, in the Mott's criterium, being characteristic of interactions, by

$r_{sn(sp),M}(N = N_{CDn(CDp)}(r_{d(a)}, x), r_{d(a)}, x) \equiv \left(\frac{3}{4\pi N_{CDn(CDp)}(r_{d(a)}, x)}\right)^{\frac{1}{3}} \times \frac{1}{a_{Bn(Bp)}(r_{d(a)}, x)} =$ **2.4813963**, (4)

for any $(r_{d(a)}, x)$-values. Then, from Eq. (4), one also has :

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

(5)

**explaining thus the existence of the Mott's criterium**.

Furthermore, by using $M_{n(p)} = 0.25$, according to the empirical Heisenberg parameter $\boldsymbol{\mathcal{H}_{n(p)}} = \mathbf{0.47137}$, as those given in our previous work[3], we have also showed that $N_{CDn(CDp)}$ is just **the density of electrons (holes) localized in the exponential conduction (valence)-band tail $N^{EBT}_{CDn(CDp)}$**, with a precision of the order of $\mathbf{2.91 \times 10^{-7}}$, respectively.[3] So, $N_{CDn(NDp)}(r_{d(a)}, x) \cong N^{EBT}_{CDn(CDp)}(r_{d(a)}, x)$. (6a)

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

There fore, the effective density of electrons (holes) given in parabolic conduction (valence) bands, $N^*$, can be defined, as that given in compensated materials

$N^*(N, r_{d(a)}, x) \equiv N - N_{CDn(NDp)}(r_{d(a)}, x) \cong N - N^{EBT}_{CDn(CDp)}(r_{d(a)}, x)$. (6b)

In summary, as observed in our previous paper[3], 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 $N^{EBT}_{CDn(CDp)}(r_{d(a)}, x)$ increase, affecting strongly all the optical, electrical, and thermoelectric coefficients, as those observed in following Sections.

## PHYSICAL MODEL

In the degenerate $n^+(p^+) - \mathbf{X}(\mathbf{x})$ -crystalline alloy, 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

$$\gamma \times r_{sn(sp)}(N^*, r_{d(a)}, x) \equiv \frac{k^{-1}_{Fn(Fp)}}{a_{Bn(Bp)}} < 1 \quad , \quad r_{sn(sp)}(N^*, r_{d(a)}, x) \equiv \left(\frac{3g_{c(v)}}{4\pi N^*}\right)^{1/3} \times \frac{1}{a_{Bn(Bp)}(r_{d(a)}, x)} \quad ,$$

being proportional to $N^{*-1/3}$. Here, $\gamma = (4/9\pi)^{1/3}$, $k_{Fn(Fp)}(N^*) \equiv \left(\frac{3\pi^2 N^*}{g_{c(v)}}\right)^{\frac{1}{3}}$ is the Fermi wave.

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

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

(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)- pproximation**, the ratio $R_{snTF(spTF)}(N^*)$ is reduced to $R_{snTF(spTF)}(N^*) \equiv \frac{k_{snTF(spTF)}}{k_{Fn(Fp)}} = \frac{k_{Fn(Fp)}^{-1}}{k_{snTF(spTF)}^{-1}} = \sqrt{\frac{4\gamma r_{sn(sp)}}{\pi}} \ll 1$, (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

$$R_{sn(sp)WS}(N^*) \equiv \frac{k_{sn(sp)WS}}{k_{Fn}} = 0.5 \times \left(\frac{3}{2\pi} - \gamma \frac{d\left[r_{sn(sp)}^2 \times E_{CE}(N^*)\right]}{dr_{sn(sp)}}\right) \quad (9a)$$

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

$$E_{CE}(N^*) = \frac{-0.87553}{0.0908 + r_{sn(sp)}} + \frac{\frac{0.87553}{0.0908 + r_{sn(sp)}} + \left(\frac{2[1-\ln(2)]}{\pi^2}\right) \times \ln(r_{sn(sp)}) - 0.093288}{1 + 0.03847728 \times r_{sn(sp)}^{1.67378876}}.$$

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

$$\frac{k_{Fn(Fp)}^{-1}}{a_{Bn(Bp)}} < \frac{\eta_{n(p)}}{E_{Fno(Fpo)}} \equiv \frac{1}{A_{n(p)}} < \frac{k_{Fn(Fp)}^{-1}}{k_{sn(sp)}^{-1}} \equiv R_{sn(sp)} < 1 \;, \qquad \eta_{n(p)}(N^*) \equiv \frac{\sqrt{2\pi \times (\frac{N^*}{g_{c(v)}})}}{\varepsilon(r_{d(a)})} \times q^2 k_{sn(sp)}^{-1/2} \;, \quad (9b)$$

which gives: $A_{n(p)}(N^*) = \frac{E_{Fno(Fpo)}(N^*)}{\eta_{n(p)}(N^*)}$, $E_{Fno(Fpo)}(N^*, r_{d(a)}, x) \equiv \frac{\hbar^2 \times k_{Fn(Fp)}^2(N^*)}{2 \times m_{n(p)}^*(x) \times m_o}$.

## BAND GAP NARROWING (BGN)

First, the BGN is found to be given by

$$\Delta E_{gn(gp)}(N^*, r_{d(a)}, x) \simeq$$

$$a_1 + \frac{\varepsilon_o(x)}{\varepsilon(r_{d(a)}, x)} \times N_r^{\frac{1}{3}} + a_2 \times \frac{\varepsilon_o(x)}{\varepsilon(r_{d(a)}, x)} \times N_r^{\frac{1}{3}} \times \left(2.503 \times \left[-E_{CE}(r_{sn(sp)})\right] \times r_{sn(sp)}\right) + a_3 \times \left[\frac{\varepsilon_o(x)}{\varepsilon(r_{d(a)}, x)}\right]^{\frac{5}{4}} \times \sqrt{\frac{m_{v(c)}}{m_{n(p)}^*(x)}} \times N_r^{\frac{1}{4}} + 2a_4 \times \left[\frac{\varepsilon_o(x)}{\varepsilon(r_{d(a)}, x)}\right]^{\frac{1}{2}} \times N_r^{\frac{1}{2}} + 2a_5 \times \left[\frac{\varepsilon_o(x)}{\varepsilon(r_{d(a)}, x)}\right]^{\frac{3}{2}} \times N_r^{\frac{1}{6}}, \; N_r =$$

$\frac{N^*}{9.999\times10^{17}cm^{-3}}$,
(10a)

Here, for $\Delta E_{gn;N}(N^*, r_d, x)$, one has: $a_1 = 3.8 \times 10^{-3}(eV)$, $a_2 = 6.5 \times 10^{-4}(eV)$, $a_3 = 2.8 \times 10^{-3}(eV)$, $a_4 = 5.597 \times 10^{-3}(eV)$, and $a_5 = 8.1 \times 10^{-4}(eV)$, and for $\Delta E_{gp;N}(N^*, r_a, x)$, one has: $a_1 = 3.15 \times 10^{-3}(eV)$, $a_2 = 5.41 \times 10^{-4}(eV)$, $a_3 = 2.32 \times 10^{-3}(eV)$, $a_4 = 4.12 \times 10^{-3}(eV)$, and $a_5 = 9.8 \times 10^{-5}(eV)$.

Therefore, at T=0 K and $N^* = 0$, and for any x and $r_{d(a)}$, one gets: $\Delta E_{gn(gp)} = 0$, according to the metal-insulator transition (MIT).
Secondly, one has:
$\Delta E_{gn(gp)}(T, x) = 10^{-4}T^2 \times \left[\frac{7.205\times x}{T+94} + \frac{5.405\times(1-x)}{T+204}\right](eV)$. (10b)

## 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 degenerate $p^+ - \mathbf{X}(\mathbf{x})$-crystalline alloy, in order to obtain the same one, as given in the degenerate $n^+ - \mathbf{X}(\mathbf{x})$ - 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[9], obtained with a precision of the order of $2.11 \times 10^{-4}$, is found to be given by

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

where u is the reduced electron density, $u(N^*, r_{d(a)}, x, T) \equiv \frac{N^*}{N_{c(v)}(T,x)}$, $N_{c(v)}(T, x) = 2g_{c(v)} \times \left(\frac{m^*_{n(p)}(x)\times m_o\times k_B T}{2\pi\hbar^2}\right)^{\frac{3}{2}}$ $(cm^{-3})$, $F(u) = au^{\frac{2}{3}}\left(1 + bu^{-\frac{4}{3}} + cu^{-\frac{8}{3}}\right)^{-\frac{2}{3}}$, $a = [3\sqrt{\pi}/4]^{2/3}$, $b = \frac{1}{8}\left(\frac{\pi}{a}\right)^2$, $c = \frac{62.3739855}{1920}\left(\frac{\pi}{a}\right)^4$, 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 $\mathbf{u \longrightarrow 0}$, **the limiting non-degenerate condition**, and in the very degenerate case ($u \gg 1$),

one gets: $E_{Fn(Fp)}(u \gg 1) = k_B T \times F(u) = k_B T \times a u^{\frac{2}{3}} \left(1 + b u^{-\frac{4}{3}} + c u^{-\frac{8}{3}}\right)^{-\frac{2}{3}} \simeq \frac{\hbar^2 \times k_{Fn(Fp)}^2(N^*)}{2 \times m_{n(p)}^*(x) \times m_o}$ as $\mathbf{u \longrightarrow \infty}$, **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, as $T \to 0\,K$, since $u^{-1} \to 0$, Eq. (11) is reduced to: $E_{Fno(Fpo)}(N^*) \equiv \frac{\hbar^2 \times k_{Fn(Fp)}^2(N^*)}{2 \times m_{n(p)}^*(x) \times m_o}$, proportional to $(N^*)^{2/3}$, noting that, for a given $N^*$, $E_{Fno(Fpo)}\left(m_{n(p)}^*(x) = m_r(x)\right) > E_{Fno(Fpo)}\left(m_{n(p)}^*(x) = m_{c(v)}(x)\right)$ since $m_r(x) < m_{c(v)}(x)$ for given x. Further, at T=0 K and $N^* = 0$, being the physical conditions, given for the metal-insulator transition (MIT).

In the following, it should be noted that all the optical and electrical-and-thermoelectric properties strongly depend on such the accurate expression of $\xi_{n(p)}\left(N^*, r_{d(a)}, x, T\right)$.[9]

**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 works[1, 6] 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, $-\frac{\partial f}{\partial E} = \delta\left(E - E_{Fno(Fpo)}\right)$, $\delta\left(E - E_{Fno(Fpo)}\right)$ being the Dirac delta ($\delta$)-function. Therefore, $G_p\left(E_{Fno(Fpo)}\right) = 1$.

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

$G_p\left(E_{Fn(Fp)}\right) \equiv 1 + E_{Fn(Fp)}^{-p} \times \int_{-\infty}^{\infty} \frac{e^{\gamma}}{(1+e^{\gamma})^2} \times \left(k_B T \gamma + E_{Fn(Fp)}\right)^p d\gamma = 1 + \sum_{\mu=1,2,\ldots}^{p} C_p^{\beta} \times (k_B T)^{\beta} \times E_{Fn(Fp)}^{-\beta} \times I_{\beta}$, where $C_p^{\beta} \equiv p(p-1)\ldots(p-\beta+1)/\beta!$ and the integral $I_{\beta}$ is given by:

$I_{\beta} = \int_{-\infty}^{\infty} \frac{\gamma^{\beta} \times e^{\gamma}}{(1+e^{\gamma})^2} d\gamma = \int_{-\infty}^{\infty} \frac{\gamma^{\beta}}{\left(e^{\gamma/2}+e^{-\gamma/2}\right)^2} d\gamma$, vanishing for old values of $\beta$. Then, for even values of $\beta = 2n$, with n=1, 2, …, 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:

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

(12)

where $y \equiv \frac{\pi}{\xi_{n(p)}(N^*, r_{d(a)}, x, T)} = \frac{\pi k_B T}{E_{Fn(Fp)}(N^*, r_{d(a)}, x, T)}$, noting that $G_{p=1}(y \equiv \frac{\pi k_B T}{E_{Fn(Fp)}} = \frac{\pi}{\xi_{n(p)}}) = 1$ , and as T→ 0 K, $G_{p>1}(y \to 0) \to 1$.

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

## OPTICAL-AND-ELECTRICAL PROPERTIES

### Optico-Electrical Phenomenon (O-EP) and Electro-Optical Phenomenon (E-OP)

In the degenerate $n^+(p^+) - \mathbf{X}(\mathbf{x})$-crystalline alloy, one has

(i) in the **E-OP**, the reduced band gap is defined by

$E_{gn2(gp2)} \equiv E_{gn(gp)} - \Delta E_{gn(gp)}(N^*, r_{d(a)}, x) - \Delta E_{gn(gp)}(T, x)$ (13)

Where the intrinsic band gap $E_{gn(gp)}$ is defined in Equations (1a, 1b), $\Delta E_{gn(gp)}(N^*, r_{d(a)}, x)$ and $\Delta E_{gn(gp)}(T, x)$ are respectively determined in Equations (10a, 10b), and

(ii) in the (**O-EP**), the photon energy is defined by: $E \equiv \hbar\omega$, and the optical band gap, as: $E_{gn1(gp1)} \equiv E_{gn2(gp2)} + E_{Fn(Fp)}$.

Therefore, for $E \geq E_{gn1(gp1)}(E_{gn2(gp2)})$, the effective photon energy $E^*$ is found to be given by:

$E^* \equiv E - E_{gn1(gp1)}(E_{gn2(gp2)}) \geq 0$.

(14)

From above Equations, one notes that: $E^* \equiv [E - E_{gn1(gp1)}] = E_{Fn(Fp)}$, given in the O-EP, if $E = [E_{gn1(gp1)} + E_{Fn(Fp)}] \equiv E_{gn(gp)O}$ and $m^*_{n(p)}(x) = m_r(x)$, and $E^* \equiv E - E_{gn2(gp2)} = E_{Fn(Fp)}$ , given in the E-OP, if $E = [E_{gn2(gp2)} + E_{Fn(Fp)}] \equiv E_{gn(gp)E}$ and $m^*_{n(p)}(x) =$

$m_{c(v)}(x)$, noting that $E_{Fn(Fp)}(m_r(x)) > E_{Fn(Fp)}(m_{c(v)}(x))$, since $m_r(x) < m_{c(v)}(x)$, for a given x. (15)

Eq. (15) thus shows that, in both O-EP and E-OP, the Fermi energy-level penetrations into conduction (valence)-bands, observed in the $n^+(p^+)-$ type degenerate $n^+(p^+)-\mathbf{X(x)}$-crystalline alloy, $E_{Fn(Fp)}$, are well defined.

**Optical Coefficients**

The optical properties for any medium, defined in the O-EP and E-OP, respectively, according to: $[m^*_{n(p)} \equiv m_r(x)[m_{c(v)}(x)]]$, can be described by the complex refraction: $\mathbb{N}_{O[E]} \equiv n_{O[E]} - i\kappa_{O[E]}$, $n_{O[E]}$ and $\kappa_{O[E]}$ being the refraction index and the extinction coefficient, the complex dielectric function: $\mathcal{E}_{O[E]} = \varepsilon_{1\,O[E]} - i\varepsilon_{2\,O[E]}$, where $i^2 = -1$, and $\mathcal{E}_{O[E]} = \mathbb{N}_{O[E]}{}^2$. Further, if denoting the normal-incidence reflectance and the optical absorption by $R_{O[E]}$ and $\propto_{O[E]}$, and the effective joint parabolic conduction (parabolic valence)-band density of states by $JDOS_{n(p)\,O[E]}(E, N^*, r_{d(a)}, x, T) \equiv \frac{1}{2\pi^2} \times \left(\frac{2m^*_{n(p)}(x)}{\hbar^2}\right)^{3/2} \times \sqrt{E_{Fno(Fpo)}(N^*)} \times \left[\frac{E-E_{gn1(gp1)}(E_{gn2(gp2)})}{E-[E_{gn1(gp1)}(E_{gn2(gp2)})+E_{Fn(Fp)}-E_{Fno(Fpo)}]}\right]^2$,

and $F_{O[E]}(E) \equiv \frac{\hbar q^2 \times |v(E)|^2}{n_{O[E]}(E) \times cE \times \varepsilon(r_{d(a)},x) \times \varepsilon_{free\ space}}$, one gets [2]:

$\propto_{O[E]}(E) = JDOS_{n(p)\,O[E]}(E) \times F_{O[E]}(E) = \frac{E \times \varepsilon_{2\,O[E]}(E)}{\hbar c\, n_{O[E]}(E)} = \frac{2E \times \kappa_{O[E]}(E)}{\hbar c} = \frac{4\pi\sigma_{O[E]}(E)}{c n_{O[E]}(E) \times \varepsilon(r_{d(a)},x) \times \varepsilon_{free\ space}}$, $\varepsilon_{1\,O[E]}(E) \equiv n_{O[E]}{}^2 - \kappa_{O[E]}{}^2$, $\varepsilon_{2\,O[E]}(E) \equiv 2\kappa_{O[E]} n_{O[E]}$, and $R_{O[E]}(E) \equiv \frac{[n_{O[E]}-1]^2 + \kappa_{O[E]}{}^2}{[n_{O[E]}+1]^2 + \kappa_{O[E]}{}^2}$. (16a)

One notes here that, at the MIT-conditions : $N^* = 0$, both $E_{gn1(gp1)}(E_{gn2(gp2)}) = E_{gn(gp)}$, according to

$\left[\frac{E-E_{gn1(gp1)}(E_{gn2(gp2)})}{E-[E_{gn1(gp1)}(E_{gn2(gp2)})+E_{Fn(Fp)}-E_{Fno(Fpo)}]}\right]^2 = \frac{0}{0}$ for $E=E_{gn(gp)}$,

$\left[\frac{E-E_{gn1(gp1)}(E_{gn2(gp2)})}{E-[E_{gn1(gp1)}(E_{gn2(gp2)})+E_{Fn(Fp)}-E_{Fno(Fpo)}]}\right]^2 = 1$ for $E \gtrsim E_{gn(gp)}$, so that, in such the MIT,

$JDOS_{n(p)\,O[E]}(E, N^*, r_{d(a)}, x, T) \equiv \frac{1}{2\pi^2} \times \left(\frac{2m^*_{n(p)}(x)}{\hbar^2}\right)^{\frac{3}{2}} \times \sqrt{E_{Fno(Fpo)}(N^* = 0)} = 0$, for $E \gtrsim$ ,

which is largely verified since $N_{CDn(NDp)}(r_{d(a)}, x\ ) \cong N^{EBT}_{CDn(CDp)}(r_{d(a)}, x)$ or

$E_{gn2(gp2)}(N_{CDn(NDp)}, T = 0K) \cong E_{gn2(gp2)}(N^{EBT}_{CDn(CDp)}, T = 0K) \cong E_{gn(gp)}$, as those given in Equations (6a, 6b). In other words, the critical photon energy can be defined by: $E \cong E_{gn(gp)}$.

Then, Eq. (6a) states that $N_{CDn(CDp)}$, given in parabolic conduction (parabolic valence)-band density of states, is just the density of electrons (holes) localized in the exponential conduction (valence)-band tail, $N^{EBT}_{CDn(CDp)}$, with a precision of the order of $\mathbf{2.91 \times 10^{-7}}$, respectively.[3] Therefore, for $E \cong E_{gn(gp)}$, the exponential conduction (valence)-band tail states can be approximated with a same precision to:

$$JDOS^{EBT}_{n(p)O[E]}(E, N^*, r_{d(a)}, x, T) \equiv \frac{1}{2\pi^2} \times \left(\frac{2m^*_{n(p)}(x)}{\hbar^2}\right)^{\frac{3}{2}} \times \sqrt{E_{Fno(Fpo)}(N^* = N_{CDn(NDp)})}.$$

(16b)

Here, $\varepsilon_{free\ space} = 8.854187817 \times 10^{-12}\left(\frac{C^2}{N \times m^2}\right)$ is the permittivity of the free space, -q is the charge of the electron, $\left|v_{\mathbf{O[E]}}(E)\right|$ is the matrix elements of the velocity operator between valence (conduction)-and-conduction (valence) bands, and our approximate expression for the refraction index $n_{\mathbf{O[E]}}$ is found to be defined by

$$n_{O[E]}(E, N^*, r_{d(a)}, x, T) = n_\infty(r_{d(a)}, x) + \sum_{i=1}^{4} \frac{X_i(E_{gn1(gp1)}) \times E + Y_i(E_{gn1(gp1)})}{E^2 - B_i E + C_i} \quad (17)$$

going to a constant as $E \to \infty$, since $n(E \to \infty, r_{d(a)}, x) \to n_\infty(r_{d(a)}, x) = \sqrt{\varepsilon(r_{d(a)}, x)} \times \frac{\omega_T}{\omega_L}$, given in the well-known Lyddane-Sachs-Teller relation, in which $\omega_T \simeq 5.1 \times 10^{13}\ s^{-1}$ and $\omega_L \simeq 8.9755 \times 10^{13}\ s^{-1}$ are the transverse (longitudinal) optical phonon frequencies, giving rise to: $n_\infty(r_{d(a)}, x) \simeq \sqrt{\varepsilon(r_{d(a)}, x)} \times 0.568$.

Here, the other parameters are determined by: $X_i(E_{gn1(gp1)}) = \frac{A_i}{Q_i} \times \left[-\frac{B_i^2}{2} + E_{gn1(gp1)} B_i - E^2_{gn1(gp1)} + C_i\right]$, $Y_i(E_{gn1(gp1)}) = \frac{A_i}{Q_i} \times \left[\frac{B_i \times (E^2_{gn1(gp1)} + C_i)}{2} - 2E_{gn1(gp1)} C_i\right]$, $Q_i = \frac{\sqrt{4C_i - B_i^2}}{2}$, where, for i=(1, 2, 3, and 4),

$A_i = 4.7314 \times 10^{-4}$, $0.2313655, 0.1117995, 0.0116323$, $B_i = 5.871, 6.154, 9.679$, $13.232$, and $C_i = 8.619, 9.784, 23.803, 44.119$.

Now, the optical [electrical] conductivity $\sigma_{O[E]}$ can be defined and expressed in terms of the kinetic energy of the electron (hole), $E_k \equiv \frac{\hbar^2 \times k^2}{2\times m^*_{n(p)}(x)\times m_o}$, k being the wave number, as

$\sigma_{O[E]}(k) \equiv \frac{q^2\times k}{\pi\times\hbar} \times \frac{k}{k_{sn(sp)}} \times [k\times a_{Bn(Bp)}] \times \left(\frac{E_k}{\eta_{n(p)}}\right)^{\frac{1}{2}} \left(\frac{1}{\Omega\times cm}\right)$, which is thus proportional to ${E_k}^2$,

where $\frac{q^2}{\pi\times\hbar} = 7.7480735 \times 10^{-5}\ \text{ohm}^{-1}$.

Then, we obtain: $\langle E^2\rangle_{FDDF} \equiv G_2\left(y = \frac{\pi k_B T}{E_{Fn(Fp)}}\right) \times E^2_{Fn(Fp)}$ , and $G_2(y) = \left(1 + \frac{y^2}{3}\right) \equiv G_2(N, r_{d(a)}, x, T)$, with $y \equiv \frac{\pi}{\xi_{n(p)}}$, $\xi_{n(p)} = \xi_{n(p)}(N^*, r_{d(a)}, x, T)$ for a presentation simplicity.

Therefore, from above equations (16, 17), if denoting the function $H(N, r_{d(a)}, x, T)$ by:

$H(N^*, r_{d(a)}, x, T) =$

$\left[\frac{k_{Fn(Fp)}(N^*)}{R_{sn(sp)}(N^*)} \times [k_{Fn(Fp)}(N^*) \times a_{Bn(Bp)}(r_{d(a)}, x)] \times \sqrt{A_{n(p)}(N^*) = \frac{E_{Fno(Fpo)}(N^*)}{\eta_{n(p)}(N^*)}}\right] \times G_2(N^*, r_{d(a)}, x, T)$, where $R_{sn(sp)}(N^*) \equiv \frac{k_{sn(sp)}}{k_{Fn(Fp)}}$, being proportional to $E^2_{Fno(Fpo)}$.

Then, our optical [electrical] conductivity models, defined in the O-EP and E-OP, respectively, for a simply representation, can thus be assumed to be as:

$\sigma_O(E, N^*, r_{d(a)}, x, T) =$

$\frac{q^2}{\pi\times\hbar} \times H(N^*, r_{d(a)}, x, T) \times \left[\frac{E - E_{gn1(gp1)}}{E - [E_{gn1(gp1)} + E_{Fn(Fp)} - E_{Fno(Fpo)}]}\right]^2 \left(\frac{1}{\Omega\times cm}\right)$, and

$\sigma_E(E, N, r_{d(a)}, x, T) =$

$$\frac{q^2}{\pi\times\hbar} \times H(N^*, r_{d(a)}, x, T) \times \left[\frac{E - E_{gn2(gp2)}}{E - [(E_{gn2(gp2)} + E_{Fn(Fp)} - E_{Fno(Fpo)}]}\right]^2 \left(\frac{1}{\Omega\times cm}\right). \qquad (18)$$

It should be noted here that

(i) $\sigma_{O[E]}(E = E_{gn1(gp1)}[E_{gn2(gp2)}]) = 0$ , and $\sigma_{O[E]}(E \to \infty) \to \text{Constant}$ for given $(N, r_{d(a)}, x, T)$ −physical conditions, and

(ii) as T→ 0 K and $N^* = 0$ [or $E_{Fno(Fpo)}(N^*) = 0$], according to: $H(N^*, r_{d(a)}, x, T) = 0$, and for a given E, $[E - E_{gn1(gp1)}] = [E - E_{gn(gp)}]$ =Constant, then from Equations (16-18), $n_{O[E]}$ (E)= Constant, $\sigma_{O[E]}(E) = 0$, $\kappa_{O-EP[E-OP]}(E) = 0$, $\varepsilon_{1\,O[E]}(E) = (n_\infty)^2 = \text{Constant}$, $\varepsilon_2(E) = 0$, and $\propto_{O[E]}(E) = 0$.

This result (18) should be new, in comparison with that, obtained from an improved Forouhi-Bloomer parameterization, as given in our previous work.[2]

Using Equations (16-18), one obtains all the analytically results as

$$\frac{|v(E)|^2}{E} = \frac{8\pi^2\hbar}{(2m_r)^{\frac{3}{2}}\times\sqrt{\eta_{n(p)}}} \times \left[\frac{k_{Fn(Fp)}(N^*)}{R_{sn(sp)}(N^*)} \times \left[k_{Fn(Fp)}(N^*) \times a_{Bn(Bp)}\left(r_{d(a)}, x\right)\right]\right] \times G_2\left(N^*, r_{d(a)}, x, T\right), \quad 19a)$$

$$\kappa_O(E) = \frac{2q^2}{n(E)\times\varepsilon(r_{d(a)},x)\times\varepsilon_{free\ space}\times E} \times H\left(N^*, r_{d(a)}, x, T\right) \times \left[\frac{E-E_{gn1(gp1)}}{E-[E_{gn1(gp1)}+E_{Fn(Fp)}-E_{Fno(Fpo)}]}\right]^2 \quad \text{and} \quad \kappa_E(E) = \frac{2q^2}{n(E)\times\varepsilon(r_{d(a)},x)\times\varepsilon_{free\ space}\times E} \times H\left(N^*, r_{d(a)}, x, T\right) \times \left[\frac{E-E_{gn2(gp2)}}{E-[(E_{gn2(gp2)}+E_{Fn(Fp)}-E_{Fno(Fpo)}]}\right]^2, \quad 19b)$$

Which gives: $\kappa_{O[E]}\left(E = E_{gn1(gp1)}[E_{gn2(gp2)}]\right) = 0$, and $\kappa_{O[E]}(E \to \infty) \to 0$, as those given in Ref. [2],

$$\varepsilon_{2\,O}(E) = \frac{4q^2}{\varepsilon(r_{d(a)},x)\times\varepsilon_{free\ space}\times E} \times H\left(N^*, r_{d(a)}, x, T\right) \times \left[\frac{E-E_{gn1(gp1)}}{E-[E_{gn1(gp1)}+E_{Fn(Fp)}-E_{Fno(Fpo)}]}\right]^2 \quad \text{and}$$

$$\varepsilon_{2\,E}(E) = \frac{4q^2}{\varepsilon(r_{d(a)},x)\times\varepsilon_{free\ space}\times E} \times H\left(N^*, r_{d(a)}, x, T\right) \times \left[\frac{E-E_{gn2(gp2)}}{E-[(E_{gn2(gp2)}+E_{Fn(Fp)}-E_{Fno(Fpo)}]}\right]^2, \quad (19c)$$

Which gives: $\varepsilon_{2O-EP[2E-OP]}\left(E = E_{gn1(gp1)}[E_{gn2(gp2)}]\right) = 0$, and $\varepsilon_{2O-EP[2E-OP]}(E \to \infty) \to 0$, as those given in Ref. [2],

$$\propto_O(E) = \frac{4q^2}{\hbar c n(E)\times\varepsilon(r_{d(a)},x)\times\varepsilon_{free\ space}} \times H\left(N^*, r_{d(a)}, x, T\right) \times \left[\frac{E-E_{gn1(gp1)}}{E-[E_{gn1(gp1)}+E_{Fn(Fp)}-E_{Fno(Fpo)}]}\right]^2 \left(\frac{1}{cm}\right) \quad \text{and}$$

$$\propto_E(E) = \frac{4q^2}{\hbar c n(E)\times\varepsilon(r_{d(a)},x)\times\varepsilon_{free\ space}} \times H\left(N^*, r_{d(a)}, x, T\right) \times \left[\frac{E-E_{gn2(gp2)}}{E-[(E_{gn2(gp2)}+E_{Fn(Fp)}-E_{Fno(Fpo)}]}\right]^2 \left(\frac{1}{cm}\right), \quad (19d)$$

which gives: $\propto_{O[E]}\left(E = E_{gn1(gp1)}[E_{gn2(gp2)}]\right) = 0$, and $\propto_{O[E]}(E \to \infty) \to \text{Constant}$, as those given in [2].

Furthermore, from Equations (16, 17, 19b), we can also determine $\varepsilon_{1\,O[E]}(E)$ and $R_{O[E]}(E)$. Now, from Equations (18, 19b, 19c, 19d), using Eq. (15) as $E \equiv E_{gn(gp)O[E]}$, one obtains respectively, as

$\sigma_O(N^*, r_{d(a)}, x, T) = \frac{q^2}{\pi\times\hbar} \times H(N^*, r_{d(a)}, x, T) \times \left(\frac{E_{Fn(Fp)}}{E_{Fno(Fpo)}}\right)^2 \left(\frac{1}{\Omega\times cm}\right)$, having the same form with that of $\sigma_E(N, r_{d(a)}, x, T)$ [1], as $\sigma_E(N^*, r_{d(a)}, x, T) = \frac{q^2}{\pi\times\hbar} \times H(N^*, r_{d(a)}, x, T) \times \left(\frac{E_{Fn(Fp)}}{E_{Fno(Fpo)}}\right)^2 \left(\frac{1}{\Omega\times cm}\right)$, (20a)

Noting here that for given $(N^*, r_{d(a)}, x, T)$ -physical conditions we obtain: $\sigma_O > \sigma_E$ since $m_r(x) < m_{c(v)}(x)$,

$\kappa_O(N^*, r_{d(a)}, x, T) = \frac{2q^2}{n(E)\times\varepsilon(r_{d(a)},x)\times\varepsilon_{free\ space}\times(E_{gn1(gp1)}+E_{Fn(Fp)})} \times H(N^*, r_{d(a)}, x, T) \times \left(\frac{E_{Fn(Fp)}}{E_{Fno(Fpo)}}\right)^2$ and

$\kappa_E(N^*, r_{d(a)}, x, T) = \frac{2q^2}{n(E)\times\varepsilon(r_{d(a)},x)\times\varepsilon_{free\ space}\times(E_{gn2(gp2)}+E_{Fn(Fp)})} \times H(N^*, r_{d(a)}, x, T) \times \left(\frac{E_{Fn(Fp)}}{E_{Fno(Fpo)}}\right)^2$, (20b)

$\varepsilon_{2\,O}(N^*, r_{d(a)}, x, T) = \frac{4q^2}{\varepsilon(r_{d(a)},x)\times\varepsilon_{free\ space}\times(E_{gn1(gp1)}+E_{Fn(Fp)})} \times H(N^*, r_{d(a)}, x, T) \times \left(\frac{E_{Fn(Fp)}}{E_{Fno(Fpo)}}\right)^2$

and

$\varepsilon_{2\,E}(N^*, r_{d(a)}, x, T) = \frac{4q^2}{\varepsilon(r_{d(a)},x)\times\varepsilon_{free\ space}\times(E_{gn2(gp2)}+E_{Fn(Fp)})} \times H(N^*, r_{d(a)}, x, T) \times \left(\frac{E_{Fn(Fp)}}{E_{Fno(Fpo)}}\right)^2$, (20c)

$\propto_O(N^*, r_{d(a)}, x, T) = \frac{4q^2}{\hbar c n(E)\times\varepsilon(r_{d(a)},x)\times\varepsilon_{free\ space}} \times H(N^*, r_{d(a)}, x, T) \times \left(\frac{E_{Fn(Fp)}}{E_{Fno(Fpo)}}\right)^2 \left(\frac{1}{cm}\right)$ and

$\propto_E(N^*, r_{d(a)}, x, T) = \frac{4q^2}{\hbar c n(E)\times\varepsilon(r_{d(a)},x)\times\varepsilon_{free\ space}} \times H(N^*, r_{d(a)}, x, T) \times \left(\frac{E_{Fn(Fp)}}{E_{Fno(Fpo)}}\right)^2 \left(\frac{1}{cm}\right)$. (20d)

Further, from Equations (16, 17, 20b), we can also determine $\varepsilon_{1\,O[E]}(E)$ and $R_{O[E]}(E)$.

Then, the numerical results of various O[E]-coefficients, $X_{O[E]}(E, N^*, r_{d(a)}, x, T)$, as functions of E, obtained from Equations (18, 19b-19d, 20a-20d) for given $(N^*, r_{d(a)}, x, T)$-physical conditions and $E \geq (\text{or } \leq) E_{gn1(gp1)}(E_{gn2(gp2)})$, giving raise to the metal-insulator transition (MIT) and the non-MIT (N-MIT), are reported and discussed as follows.

First of all, one notes that from Equations (3, 6a, 6b) the MIT occurs as T=0 K and $N^*(N, r_{d(a)}, x) \equiv N - N_{CDn(NDp)}(r_{d(a)}, x) \cong N - N^{EBT}_{CDn(CDp)}(r_{d(a)}, x) = 0$, according, for $E \geq E_{gn(gp)}$, to: $E_{Fno(Fpo)}(N^* = 0) \equiv \frac{\hbar^2 \times k^2_{Fn(Fp)}(N^*)}{2 \times m^*_{n(p)}(x) \times m_o} = 0$, and $\kappa^{MIT}_{O[E]}(E, N^* = 0) = 0$, $\varepsilon^{MIT}_{2\,O[E]}(E, N^* = 0) = 0$, $\sigma^{MIT}_{O[E]}(E, N^* = 0) = 0$ and $\propto^{MIT}_{O[E]}(E, N^* = 0)$=0, since, for example, $\sigma_{E[O]}(E, N^* = 0)$ is proportional to $E^2_{Fno(Fpo)}$, or to $(N^* = 0)^{\frac{4}{3}} = 0$. But, for such the same physical conditions: T=0 K, $N^* = 0$ and $E \geq E_{gn(gp)}$, we obtain other numerical results such as: $n^{N-MIT}_{O[E]}(N^* = 0, E) \neq 0$, $\varepsilon^{N-MIT}_{1\,O[E]}(N^* = 0, E) \neq 0$ and $R^{N-MIT}_{O[E]}(N^* = 0, E) \neq 0$, for $E \geq E_{gn(gp)}$, according to the non-MIT (N-MIT), as showed in **Tables 3, 4n and 4p, reported in Appendix 1**. These Tables also state that, at T=0 K and $N^* = 0$, and for $E \geq E_{gn(gp)}$, there is an **[O-EP]-[E-OP] transition at a given E**, characterized by: $n^{N-MIT}_{O} = n^{N-MIT}_{E}$, $\varepsilon^{N-MIT}_{1\,O} = \varepsilon^{N-MIT}_{1\,E}$ and $R^{N-MIT}_{O} = R^{N-MIT}_{E}$, since, in this case, $E_{gn1(gp1)} = E_{gn2(gp2)} = E_{gn(gp)}$.

Then, by using Eq. (16b), from Equations (18, 19b, 19c, 19d), for $E \cong E_{gn(gp)}$, one can determine the exponential conduction (valence)-band tail states, due to those coefficients: $\sigma^{EBT}_{O[E]}(E \cong E_{gn(gp)}, N^* = N_{CDn(NDp)})$, $\kappa^{EBT}_{O[E]}(E \cong E_{gn(gp)}, N^* = N_{CDn(NDp)})$, $\varepsilon^{EBT}_{2O[2E]}(E \cong E_{gn(gp)}, N^* = N_{CDn(NDp)})$ and $\propto^{EBT}_{O[E]}(E \cong E_{gn(gp)}, N^* = N_{CDn(NDp)})$, and then their numerical results are given in **Table 5, reported in Appendix 1.**

Further, the numerical results of $n_{O[E]}(E)$, $\kappa_{O[E]}(E)$, $\varepsilon_{2O[2E]}(E)$ and $\varepsilon_{1\,O[E]}(E)$, are obtained by using Equations (17, 19b, 19c and 16), expressed as functions of N for (E=3.2 eV and T=20 K)-conditions, and as functions of T for (E=3.2 eV and $N = 10^{20}\,cm^{-3}$)-conditions, as those given in **Tables 6n, 6p, 7n and 7p, being reported in Appendix 1**, respectively.

Finally, for T=20K and $N = 10^{20}\,cm^{-3}$, and for given x and $r_d$, the numerical results of $\sigma_{O[E]}(E)$, $\varepsilon_{2O[2E]}(E)$ and $\propto_{O[E]}(E)$, are obtained by using Equations (18, 19c, 19d), and given in

**Tables 8n and 8p, being reported in Appendix 1.**

In the following, we will determine the electrical-and-thermoelectric laws, by basing on our $\sigma_{O[E]}$-models, given in Eq. (20a).

## OPTICAL [ELECTRICAL]-AND-THERMOELECTRIC PROPERTIES $[m^*_{n(p)} \equiv m_r(x)[m_{c(v)}(x)]]$

Here, if denoting, for majority electrons (holes), the thermal conductivity by $\sigma_{Th.\ O[E]}(N^*, r_{d(a)}, x, T)$ in $\frac{W}{cm\times K}$, and the Lorenz number L by: $L = \frac{\pi^2}{3} \times \left(\frac{k_B}{q}\right)^2 = 2.4429637 \left(\frac{W\times ohm}{K^2}\right) = 2.4429637 \times 10^{-8}\ (V^2 \times K^{-2})$, then the well-known Wiedemann-Frank law states that the ratio, $\frac{\sigma_{Th.O[E]}}{\sigma_{O[E]]}}$, due to the O-EP [E-OP], is proportional to the temperature T(K), as: $\frac{\sigma_{Th\ .O[E]}(N^*, r_{d(a)}, x, T)}{\sigma_{O[E]}(N^*, r_{d(a)}, x, T)} = L \times T.$ 21)

Further, the resistivity is found to be given by: $\rho_{O[E]}(N^*, r_{d(a)}, x, T) \equiv 1/\sigma_{O[E]}(N^*, r_{d(a)}, x, T)$, noting again that $N^* \equiv N - N_{CDn(NDp)}(r_{d(a)}, x)$.

In Eq. (20a), one notes that at T= 0 K, $\sigma_{O[E]}(N^*, r_{d(a)}, x, T)$ is proportional to $E^2_{Fno(Fpo)}$, or to $(N^*)^{\frac{4}{3}}$. Thus , from Eq. (21), one has: $\sigma_{O[E]}(N^* = 0, r_{d(a)}, x, T = 0K) = 0$ and also $\sigma_{Th.\ O[E]}(N^* = 0, r_{d(a)}, x, T = 0K) = 0$ at $N^* = 0$, at which the MIT occurs.

### Optical [Electrical] Coefficients

The relaxation time $\tau_{O[E]}$ is related to $\sigma_{O[E]}$ by [1]

$\tau_{O[E]}(N^*, r_{d(a)}, x, T) \equiv \sigma_{O[E]}(N^*, r_{d(a)}, x, T) \times \frac{m^*_{n(p)}(x)\times m_o}{q^2\times(N^*/g_{c(v)})}$ . Therefore, the mobility $\mu_{O[E]}$ is given by:

$$\mu_{O[E]]}(N^*, r_{d(a)}, x, T) = \frac{q\times\tau_{O[E]}(N^*, r_{d(a)}, x, T)}{m^*_{n(p)}(x)\times m_o} = \frac{\sigma_{O[E]}(N^*, r_{d(a)}, x, T)}{q\times(N^*/g_{c(v)})} \left(\frac{cm^2}{V\times s}\right) \quad (22)$$

Here, at T= 0K, $\mu_{O[E]}(N^*, r_{d(a)}, x, T)$ is thus proportional to $(N^*)^{1/3}$, since $\sigma_{O[E]}(N^*, r_{d(a)}, x, T = 0K)$ is proportional to $(N^*)^{4/3}$. Thus, $\tau_{O[E]}(N^* = 0, r_{d(a)}, x, T = 0K) = 0$ and $\mu_{O[E]}(N^* = 0, r_{d(a)}, x, T = 0K) = 0$ at $N^* = 0$, at which the MIT occurs.

Then, the Hall factor is defined by

$r_{HO[HE]}(N^*, r_{d(a)}, x, T) \equiv \frac{\langle \tau_{O[E]}{}^2 \rangle_{FDDF}}{[\langle \tau_{O[E]} \rangle_{FDDF}]^2} = \frac{G_4(y)}{[G_2(y)]^2}$, $y \equiv \frac{\pi}{\xi_{n(p)}(N^*, r_{d(a)}, x, T)} = \frac{\pi k_B T}{E_{Fn(Fp)}(N^*, r_{d(a)}, x, T)}$, and

therefore, the Hall mobility yields:

$\mu_{HO[HE]}(N^*, r_{d(a)}, x, T) \equiv \mu_{O[E]}(N^*, r_{d(a)}, x, T) \times r_{HO[HE]}(N^*, r_{d(a)}, x, T)\ (\frac{cm^2}{V \times s})$ (23) noting that, at T=0K, since $r_{HE[HO]}(N^*, r_{d(a)}, x, T) = 1$, one therefore gets: $\mu_{HO[HE]}(N^*, r_{d(a)}, x, T) \equiv \mu_{O[E]}(N^*, r_{d(a)}, x, T)$.

**Our generalized Einstein relation**

Our generalized Einstein relation is found to be defined as [1]

$\frac{D_{O[E]}(N^*, r_{d(a)}, x, T)}{\mu_{O[E]}(N^*, r_{d(a)}, x, T)} \equiv \frac{N^*}{q} \times \frac{dE_{Fn(Fp)}}{dN^*} \equiv \frac{k_B \times T}{q} \times \left(u \frac{d\xi_{n(p)}(u)}{du}\right) = \sqrt{\frac{3 \times L}{\pi^2}} \times T \times \left(u \frac{d\xi_{n(p)}(u)}{du}\right)$, $\frac{k_B}{q} = \sqrt{\frac{3 \times L}{\pi^2}}$, (24)

Where $D_{E[O]}(N^*, r_{d(a)}, x, T)$ is the diffusion coefficient, $\xi_{n(p)}(u)$ is defined in Eq. (11), and the mobility $\mu_{O[E]}(N^*, r_{d(a)}, x, T)$ is determined in Eq. (22). 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: $\frac{D_{O[E]}(N^*, r_{d(a)}, x, T)}{\mu_{O[E]}(N^*, r_{d(a)}, x, T)} = \frac{k_B \times T}{q} \times u \frac{V'(u) \times W(u) - V(u) \times W'(u)}{W^2(u)}$ where $W'(u) = ABu^{B-1}$ and $V'(u) = u^{-1} + 2^{-\frac{3}{2}} e^{-du}(1 - du) + \frac{2}{3} A u^{B-1} F(u) \left[ \left(1 + \frac{3B}{2}\right) + \frac{4}{3} \times \frac{bu^{-\frac{4}{3}} + 2cu^{-\frac{8}{3}}}{1 + bu^{-\frac{4}{3}} + cu^{-\frac{8}{3}}} \right]$. One remarks that: (i) as $u \to 0$, one has: $W^2 \simeq 1$ and $u[V' \times W - V \times W'] \simeq 1$, and therefore: $\frac{D_{O[E]}(u)}{\mu_{O[E]}} \simeq \frac{k_B \times T}{q}$, and (ii) as $u \to \infty$, one has: $W^2 \approx A^2 u^{2B}$ and $u[V' \times W - V \times W'] \approx \frac{2}{3} a u^{2/3} A^2 u^{2B}$, and therefore, in this **highly degenerate case** and at T=0K, the **above generalized Einstein relation** is reduced to the **usual Einstein one**: $\frac{D_{O[E]}(N^*, r_{d(a)}, x, T=0K)}{\mu_{O[E]}(N^*, r_{d(a)}, x, T=0K)} \approx \frac{2}{3} E_{Fno(Fpo)}(N^*)/q$. In other words, **Eq. (24) verifies the correct limiting conditions**.

Furthermore, in the present degenerate case ($u \gg 1$), Eq. (24) gives:

$$\frac{D_{O[E]}(N^*, r_{d(a)}, x, T=0K)}{\mu_{O[E]}(N^*, r_{d(a)}, x, T=0K)} \simeq \frac{2}{3} \times \frac{E_{Fno(Fpo)}(u)}{q} \times \left[ 1 + \frac{4}{3} \times \frac{\left(bu^{-\frac{4}{3}} + 2cu^{-\frac{8}{3}}\right)}{\left(1 + bu^{-\frac{4}{3}} + cu^{-\frac{8}{3}}\right)} \right],$$

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

Then, in **Tables 9n and 9p, reported in Appendix1**, the numerical results of $\sigma_{O[E]}$, $\mu_{O[E]}$ and $D_{O[E]}$ for given

x and T=(4.2 K and 77 K), are obtained by using Equations (20a, 22 and 24), suggesting that, for a given N, they decrease [decrease], with increasing $r_{d(a)}$.

**Thermoelectric Coefficients**

Here, as noted above, $E_{Fn(Fp)}(m_r(x)) > E_{Fn(Fp)}\left(m_{c(v)}(x)\right)$ or $\xi_{n(p)}(m_r(x)) > \xi_{n(p)}\left(m_{c(v)}(x)\right)$ for a given T, since $m_r(x) < m_{c(v)}(x)$ for given x, corresponding to: $\sigma_O(m_r(x)) > \sigma_E\left(m_{c(v)}(x)\right)$.

Then, from Eq. (20a), obtained for $\sigma_{O[E]}(N^*, r_{d(a)}, x, T)$, the well-known Mott definition for the thermoelectric power or for the Seebeck coefficient, $S_{E[O]}$, is found to be given by:

$$S_{O[E]}(N^*, r_{d(a)}, x, T) \equiv \frac{-\pi^2}{3} \times \frac{k_B}{q>0} \times k_B T \times \frac{\partial \ln\sigma_{O[E]}}{\partial E}\Big]_{E=E_{Fn(Fp)}} = \frac{-\pi^2}{3} \times \frac{k_B}{q} \times \frac{\partial \ln\sigma_{O[E]}(\xi_{n(p)})}{\partial \xi_{n(p)}}.$$

Then, using Eq. (11), for the degenerate case, $\xi_{n(p)} \geq 0$ , one gets, by putting $Y_{Sb\ O[E]}(N^*, r_{d(a)}, x, T) \equiv \left[1 - \frac{y^2}{3\times G_2\left(y=\frac{\pi}{\xi_{n(p)}}\right)}\right]$, $S_{O[E]}(N^*, r_{d(a)}, x, T) \equiv \frac{-\pi^2}{3} \times \frac{k_B}{q} \times \frac{2Y_{Sb\ O[E]}(N^*, r_{d(a)}, x, T)}{\xi_{n(p)}} = -\sqrt{\frac{3\times L}{\pi^2}} \times \frac{2\times\xi_{n(p)}}{\left(1+\frac{3\times\xi_{n(p)}{}^2}{\pi^2}\right)} = -2\sqrt{L} \times \frac{\sqrt{ZT_{O[E]Mott}}}{1+ZT_{O[E]Mott}}\left(\frac{V}{K}\right) < 0$, $ZT_{O[E]Mott} = \frac{\pi^2}{3\times\xi_{n(p)}^2}$, (25)

According to

$$\frac{\partial S_{O[E]}}{\partial \xi_{n(p)}} = \sqrt{\frac{3\times L}{\pi^2}} \times 2 \times \frac{\frac{3\times\xi_{n(p)}{}^2}{\pi^2} - 1}{\left(1+\frac{3\times\xi_{n(p)}{}^2}{\pi^2}\right)^2} = \sqrt{\frac{3\times L}{\pi^2}} \times 2 \times \frac{ZT_{O[E]Mott}\times[1-ZT_{O[E]Mott}]}{[1+ZT_{O[E]Mott}]^2}.$$

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

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

$$ZT_{O[E]}\left(N^*, r_{d(a)}, x, T\right) \equiv \frac{S^2 \times \sigma_{O[E]} \times T}{\kappa} = \frac{S^2}{L} = \frac{4 \times ZT_{O[E]Mott}}{\left[1 + ZT_{O[E]Mott}\right]^2}. \quad (26)$$

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

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

$$VC1_{O[E]}\left(N^*, r_{d(a)}, x, T\right) \equiv -N^* \times \frac{d\, S_{O[E]}}{dN^*}\left(\frac{V}{K}\right) = N^* \times \frac{\partial\, S_{O[E]}}{\partial \xi_{n(p)}} \times -\frac{\partial \xi_{n(p)}}{\partial N^*}, \quad (27)$$

being equal to 0 for $\xi_{n(p)} = \sqrt{\frac{\pi^2}{3}}$,

and the second Van-Cong coefficient as

$$VC2_{O[E]}\left(N^*, r_{d(a)}, x, T\right) \equiv T \times VC1_{O[E]}\ (V), \quad (28)$$

the Thomson coefficient, Ts , by

$$Ts_{O[E]}\left(N^*, r_{d(a)}, x, T\right) \equiv T \times \frac{d\, S_{O[E]}}{dT}\left(\frac{V}{K}\right) = T \times \frac{\partial\, S_{O[E]}}{\partial \xi_{n(p)}} \times \frac{\partial \xi_{n(p)}}{\partial T}, \quad (29)$$

being equal to 0 for $\xi_{n(p)} = \sqrt{\frac{\pi^2}{3}}$ , and the Peltier coefficient, $Pt_{E[O]}$ , as:

$$Pt_{O[E]}\left(N^*, r_{d(a)}, x, T\right) \equiv T \times S_{O[E]}\ (V). \quad (30)$$

Then, in **Tables 10n and 10p, reported in Appendix 1**, the numerical results of various thermoelectric coefficients such as: $\sigma_{Th.O[E]}$, $S_{O[E]}$, $VC1_{O[E]}$, $VC2_{O[E]}$, $Ts_{O[E]}$, $Pt_{O[E]}$ and $ZT_{O[E]}$, for given x, $r_{d(a)}$, T=(3K and 80K) and N, are obtained by using Equations (21, 25, 27, 28, 29, 30 and 26), respectively.

In summary, in the O-EP [E-OP] and for given physical conditions: x, $r_{d(a)}$, N (or T), the same values of $\xi_{n(p)}$ decrease, according to the increasing T (or to the decreasing N), since $VC1_{O[E]}\left(N, r_{d(a)}, x, T\right)$ and $Ts_{O[E]}\left(N, r_{d(a)}, x, T\right)$ are expressed in terms of $\frac{-d\, S_{O[E]}}{dN^*}$ and $\frac{d\, S_{O[E]}}{dT}$, one has: $[VC1_{O[E]}, Ts_{O[E]}] < 0$ for $\xi_{n(p)} > \sqrt{\frac{\pi^2}{3}}$, $[VC1_{O[E]}, Ts_{O[E]}] = 0$ for $\xi_{n(p)} = \sqrt{\frac{\pi^2}{3}}$, and

$[VC1_{O[E]}, Ts_{O[E]}] > 0$ for $\xi_{n(p)} < \sqrt{\frac{\pi^2}{3}}$, stating that for $\boldsymbol{\xi_{n(p)}} = \sqrt{\frac{\boldsymbol{\pi^2}}{\mathbf{3}}} \simeq \mathbf{1.8138}$: $S_{O[E]}$, determined in Eq. (25), thus presents **a same minimum** $S_{O[E]\,min.} = -\sqrt{L} \simeq -1.563 \times 10^{-4}\left(\frac{V}{K}\right)$, and $ZT_{O[E]}$, determined in Eq. (26), therefore presents **a same maximum:** $ZT_{O[E]\,max.} = 1$, and $(ZT)_{Mott} = 1$. Furthermore, for $\boldsymbol{\xi_{n(p)}} = \mathbf{1}$, the numerical results of $S_{O[E]}$, $ZT_{O[E]}$, $ZT_{O[E]Mott}$, $VC1_{E[O]}$, and $Ts_{O[E]}$, 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, as those observed in [4, 5], and those given in **Table 11, reported in Appendix 1.**

It seems that these same obtained results could represent **a new law for the thermoelectric properties, obtained in the degenerate case ($\xi_{n(p)} \geq 0$)**.

Furthermore, it is interesting to remark that the $VC2_{O[E]}$-coefficient is related to our generalized Einstein relation (24) by

$$\frac{k_B}{q} \times VC2_{O[E]}\left(N^*, r_{d(a)}, x, T\right) \equiv -\frac{\partial S_{O[E]}}{\partial \xi_{n(p)}} \times \frac{D_{O[E]}(N^*, r_{d(a)}, x, T)}{\mu_{O[E]}(N^*, r_{d(a)}, x, T)}\left(\frac{V^2}{K}\right), \quad \frac{k_B}{q} = \sqrt{\frac{3 \times L}{\pi^2}}, \quad (31)$$

According, in this work, with the use of our Eq. (25), to:

$$VC2_{O[E]}\left(N, r_{d(a)}, x, T\right) \equiv -\frac{D_{O[E]}(N^*, r_{d(a)}, x, T)}{\mu_{O[E]}(N^*, r_{d(a)}, x, T)} \times 2 \times \frac{ZT_{O[E]Mott} \times [1 - ZT_{O[E]Mott}]}{[1 + ZT_{O[E]Mott}]^2} \ (V).$$

Of course, our relation (31) is reduced to: $\frac{D_{O[E]}}{\mu_{O[E]}}$, $VC1_{O[E]}$ and $VC2_{O[E]}$, being determined respectively by Equations (24, 27, 28). This may be a new result.

## CONCLUDING REMARKS

In the $\mathbf{n^+(p^+) - X(x)}$-crystalline alloy, $0 \leq x \leq 1$, x being the concentration, the optical, electrical and thermoelectric coefficients, enhanced by : **(i)** the optico-electrical phenomenon (O-EP) and the electro-optical phenomenon (E-OP), **(ii)** our static dielectric constant law, $\varepsilon(r_{d(a)}, x)$, $r_{d(a)}$ being the donor (acceptor) d(a)-radius, given in Equations (1a, 1b), **(iii)** our accurate reduced Fermi energy, $\xi_{n(p)}$, given in Eq. (11), accurate with a precision of the order of $2.11 \times 10^{-4}$.[9], affecting all the expressions of optical, electrical and thermoelectric coefficients, and **(iv)** our optical-and-electrical conductivity models, given in Eq. (18, 20a), are now investigated by basing on our physical model and Fermi-Dirac distribution function, as those given in our recent works.[1-5]

Some important concluding remarks can be given and discussed as follows.

**(I)**-First of all, one notes that from Equations (3, 6a, 6b) the MIT occurs as T=0 K and $N^*(N, r_{d(a)}, x) \equiv N - N_{CDn(NDp)}(r_{d(a)}, x\ ) \cong N - N^{EBT}_{CDn(CDp)}\left(r_{d(a)}, x\right) = 0$ , according, for $E \geq E_{gn(gp)}$ , to : $E_{Fno(Fpo)}(N^* = 0) \equiv \frac{\hbar^2 \times k^2_{Fn(Fp)}(N^*)}{2 \times m^*_{n(p)}(x) \times m_o} = 0$, and $\kappa^{MIT}_{O[E]}(E, N^* = 0) = 0$ , $\varepsilon^{MIT}_{2\ O[E]}(E, N^* = 0) = 0$, $\sigma^{MIT}_{O[E]}(E, N^* = 0) = 0$ and $\propto^{MIT}_{O[E]}(E, N^* = 0)$=0, since, for example, $\sigma_{E[O]}(E, N^* = 0)$ is proportional to $E^2_{Fno(Fpo)}$, or to $(N^* = 0)^{\frac{4}{3}} = 0$. But, for such the same physical conditions: T=0 K, $N^* = 0$ and $E \geq E_{gn(gp)}$, we obtain other numerical results such as: $n^{N-MIT}_{O[E]}(N^* = 0, E) \neq 0$ , $\varepsilon^{N-MIT}_{1\ O[E]}(N^* = 0, E) \neq 0$ and $R^{N-MIT}_{O[E]}(N^* = 0, E) \neq 0$ , for $E \geq E_{gn(gp)}$, according to the non-MIT (N-MIT), as showed in Tables 3, 4n and 4p, reported in Appendix 1. These Tables also state that, at T=0 K and $N^* = 0$, and for $E \geq E_{gn(gp)}$, there is an [O-EP]-[E-OP] transition at a given E, as: $n^{N-MIT}_{O} = n^{N-MIT}_{E}$, $\varepsilon^{N-MIT}_{1\ O} = \varepsilon^{N-MIT}_{1\ E}$ and $R^{N-MIT}_{O} = R^{N-MIT}_{E}$, since, in this case, $E_{gn1(gp1)} = E_{gn2(gp2)} = E_{gn(gp)}$.

Then, by using Eq. (16b), from Equations (18, 19b, 19c, 19d), for $E \cong E_{gn(gp)}$, one can determine the exponential conduction (valence)-band tail states, due to those coefficients: $\sigma^{EBT}_{O[E]}\left(E \cong E_{gn(gp)}, N^* = N_{CDn(NDp)}\right)$ , $\kappa^{EBT}_{O[E]}\left(E \cong E_{gn(gp)}, N^* = N_{CDn(NDp)}\right)$ , $\varepsilon^{EBT}_{2O[2E]}\left(E \cong E_{gn(gp)}, N^* = N_{CDn(NDp)}\right)$ and $\propto^{EBT}_{O[E]}\left(E \cong E_{gn(gp)}, N^* = N_{CDn(NDp)}\right)$ , and then their numerical results are given in Table 5, reported in Appendix 1.

**(II)**-Further, the numerical results of $n_{O[E]}(E)$, $\kappa_{O[E]}(E)$, $\varepsilon_{2O[2E]}(E)$ and $\varepsilon_{1\ O[E]}(E)$, are obtained by using Equations (17, 19b, 19c and 16), expressed as functions of N for (E=3.2 eV and T=20 K)-conditions, and as functions of T for (E=3.2 eV and $N = 10^{20} cm^{-3}$)-conditions, as those given in Tables 6n, 6p, 7n and 7p, being reported in Appendix 1, respectively.

Finally, for T=20K and $N = 10^{20} cm^{-3}$, and for given x and $r_d$, the numerical results of $\sigma_{O[E]}(E)$, $\varepsilon_{2O[2E]}(E)$ and $\propto_{O[E]}(E)$ , are obtained by using Equations (18, 19c, 19d), and given in Tables 8n and 8p, being reported in Appendix 1.

**(III)**-In Tables 9n and 9p, reported in Appendix1, the numerical results of $\sigma_{O[E]}$, $\mu_{O[E]}$ and $D_{O[E]}$ for given x and T=(4.2 K and 77 K), are obtained by using Equations (20a, 22 and 24), suggesting that, for a given N, they decrease [decrease], with increasing

$r_{d(a)}$. Further, in Tables 10n and 10p, reported in Appendix 1, the numerical results of various thermoelectric coefficients such as: $\sigma_{Th.O[E]}$, $S_{O[E]}$, $VC1_{O[E]}$, $VC2_{O[E]}$, $Ts_{O[E]}$, $Pt_{O[E]}$ and $ZT_{O[E]}$, for given x, $r_{d(a)}$, T=(3K and 80K) and N, are obtained by using Equations (21, 25, 27, 28, 29, 30 and 26), respectively.

**(IV)-**Finally, from Equations (20a, 21-30), for any given x, $r_{d(a)}$ and N (or T), with increasing T (or decreasing N), one obtains: (i) for $\xi_{n(p)} = \sqrt{\frac{\pi^2}{3}} \simeq 1.8138$, while the numerical results of $S_{O[E]}$ present a same minimum $S_{O[E]\,min.}\left(\simeq -1.563 \times 10^{-4}\frac{V}{K}\right)$, those of $ZT_{O[E]}$ show a same maximum $ZT_{ET[OT]\,max.} = 1$, (ii) for $\xi_{n(p)} = 1$, the numerical results of $S_{O[E]}$, $ZT_{O[E]}$, $ZT_{O[E]\,Mott}$, $VC1_{O[E]]}$, and $Ts_{O[E]}$, 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 $\xi_{n(p)} = \sqrt{\frac{\pi^2}{3}} \simeq 1.8138$, $ZT_{O[E]\,Mott} = 1$, as those given in Table 11, reported in Appendix 1.

**REFERENCES**

1. Van Cong, H. Optical, Electrical and Thermoelectric Laws in n(p)-Type Degenerate "Compensated" InP(1-x)As(x)-Crystalline Alloy, Enhanced by: Optico-Electrical Phenomenon and Electro-Optical Phenomenon, and our Static Dielectric Constant Law, Accurate Fermi Energy and Conductivity Models (I). WJERT, 2025; 11(11): 16-58.
2. Van Cong, H. et al. Optical Coefficients in the n(p)-Type Degenerate InP(1-x) As(x) Crystalline Alloy, Due to the New Static Dielectric Constant-Law and the Generalized Mott Criterium in the Metal-Insulator Transition (20). WJERT, 2024; 10(12): 378-399.
3. Van Cong, H. Critical Impurity Density in Metal-Insulator Transition, obtained in Various n(p)-Type Degenerate Crystalline Alloys, being just That of Carriers Localized in Exponential Band Tails. (II). WJERT, 2024; 10(4): 65-96.
4. Van Cong H. Same maximum figure of merit ZT(=1), due to the effect of impurity size, obtained in the n(p)-type degenerate Ge -crystal ($\xi_{n(p)} \geq 1$), at same reduced Fermi energy $\xi_{n(p)} = \sqrt{\frac{\pi^2}{3}} \simeq 1.8138$, same minimum Seebeck coefficient $(S)_{min.}\left(\simeq -1.563 \times 10^{-4}\frac{V}{K}\right)$, same maximum $(ZT)_{max.} = 1$, and same $(ZT)_{Mott}\left(= \frac{\pi^2}{3\xi^2_{n(p)}} = 1\right)$, SCIREA Journal of Physics. 2023; 8(4): 407-430.

5. Van Cong, H. Same Maximal Figure of Merit ZT(=1), Due to the Effect of Impurity Size, Obtained in the n(p)-Type Degenerate GaAs-Crystal ($\xi_{n(p)} \geq 1$), at Same Reduced Fermi Energy $\xi_{n(p)}(= 1.8138)$ and Same Minimum Seebeck Coefficient $S\left(= -1.563 \times 10^{-4}\frac{V}{K}\right)$, at which Same $(ZT)_{Mott}\left(= \frac{\pi^2}{3\xi_{n(p)}^2} = 1\right)$. SCIREA Journal of Physics, 2023; 8(2): 133-157.
6. Van Cong, H. Effects of donor size and heavy doping on optical, electrical and thermoelectric properties of various degenerate donor-silicon systems at low temperatures. American Journal of Modern Physics, 2018; 7(4): 136-165.
7. Kim, H. S. et al. Characterization of Lorenz number with Seebeck coefficient measurement. APL Materials, 2015; 3(4): 041506.
8. Hyun, B. D. et al. Electrical-and-Thermoelectric Properties of $90\%Bi_2Te_3 - 5\%Sb_2Te_3 - 5\%Sb_2Se_3$ Single Crystals Doped with $SbI_3$. Scripta Materialia, 1998; 40(1): 49-56.
9. Van Cong, H. and Debiais, G. A simple accurate expression of the reduced Fermi energy for any reduced carrier density. J. Appl. Phys., 1993; 73: 1545-1546.
10. Van Cong, H. et al. Size effect on different impurity levels in semiconductors. Solid State Communications, 1984; 49: 697-699.
11. Van Cong, H. Diffusion coefficient in degenerate semiconductors. Phys. Stat. Sol. (b), 1984; 101: K27.
12. Van Cong, H. and Doan Khanh, B. Simple accurate general expression of the Fermi-Dirac integral $F_j(a)$ and for j> -1. Solid-State Electron., 1992; 35(7): 949-951.
13. Van Cong, H. New series representation of Fermi-Dirac integral $F_j(-\infty < a < \infty)$ for arbitrary j> -1, and its effect on $F_j(a \geq 0_+)$ for integer j≥ 0. Solid-State Electron., 1991; 34(5): 489-492.
14. Van Cong, H. and G. Mesnard. Thermoelectric effects of heavily doped semiconductors at low temperatures. Phys. Stat. Sol. (b), 1972; 50(1): 53-58.
15. Van Cong, H. Fermi energy and band-tail parameters in heavily doped semiconductors. Journal of Physics and Chemistry of Solids, 1975; 36(11): 1237-1240.
16. Van Cong, H. Quantum efficiency and radiative lifetime in degerate n-type GaAs. Journal of Physics and Chemistry of Solids, 1981; 36(11): 95-99.

## APPENDIX 1

**Table 1:** In the $X(x) \equiv InAs_{1-x}Sb_x$-crystalline alloy, the different values of energy-band-structure parameters, for a given x, are given in the following [3].

In the $\mathbf{X(x)}$-**crystalline alloy**, in which $r_{do(ao)} = r_{\mathbf{As(In)}}$ =0.118 nm (0.144 nm), we have [3]: $g_{c(v)}(x) = 1 \times x + 1 \times (1-x) = 1$, $m_{c(v)}(x)/m_o = 0.1\ (0.4) \times x + 0.09\ (0.3) \times (1-x)$, $\varepsilon_o(x) = 16.8 \times x + 14.55 \times (1-x)$, $E_{go}(x) = 0.23 \times x + 0.43 \times (1-x)$.

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

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

**Table 3.** For T=0K and N=$N_{CDn(CDp)}(r_{d(a)}, x)$, the numerical results of $n_{O[E]}^{N-MIT}$, $\varepsilon_{1\,O[E]}^{N-MIT}$ and $R_{O[E]}^{N-MIT}$ are obtained, using Equations (17, 16), suggesting that they decrease (↘) with increasing (↗) $r_{d(a)}$ and $E_{gn(gp)}$, and further they are found to be the same, for given $r_{d(a)}$ and $E_{gn(gp)}$, since $E_{gn1(gp1)} = E_{gn2(gp2)} = E_{gn(gp)}$.

| Donor | | P | **As** | Sb | Sn |
|---|---|---|---|---|---|
| $r_d$ (nm) [4] | ↗ | 0.110 | **0.118** | 0.136 | 0.140 |
| At **x=0**, | | | | | |
| $E_{gn}$(meV) | ↗ | 429.8 [429.8] | 430.0 [430.0] | 431.3 [431.3] | 432.0 [432.0] |
| $n_{O[E]}^{N-MIT}$ | ↘ | 4.225 [4.225] | 4.203 [4.203] | 4.094 [4.094] | 4.047 [4.047] |
| $\varepsilon_{1\,O[E]}^{N-MIT}$ | ↘ | 17.85 [17.85] | 17.66 [17.66] | 16.76 [16.76] | 16.38 [16.38] |
| $R_{O[E]}^{N-MIT}$ | ↘ | 0.381 [0.381] | 0.379 [0.379] | 0.369 [0.369] | 0.364 [0.364] |
| At **x=0.5**, | | | | | |
| $E_{gn}$(meV) | ↗ | 329.8 [329.8] | 330.0 [330.0] | 331.2 [331.2] | 331.8 [331.8] |
| $n_{O[E]}^{N-MIT}$ | ↘ | 4.371 [4.371] | 4.347 [4.347] | 4.235 [4.235] | 4.186 [4.186] |
| $\varepsilon_{1\,O[E]}^{N-MIT}$ | ↘ | 19.10 [19.10] | 18.90 [18.90] | 17.93 [17.93] | 17.52 [17.52] |
| $R_{O[E]}^{N-MIT}$ | ↘ | 0.394 [0.394] | 0.392 [0.392] | 0.382 [0.382] | 0.377 [0.377] |
| At **x=1**, | | | | | |
| $E_{gn}$(meV) | ↗ | 229.8 [229.8] | 230.0 [230.0] | 231.09 [231.09] | 231.66 [231.66] |
| $n_{O[E]}^{N-MIT}$ | ↘ | 4.513 [4.513] | 4.489 [4.489] | 4.373 [4.373] | 4.322 [4.322] |
| $\varepsilon_{1\,O[E]}^{N-MIT}$ | ↘ | 20.37 [20.37] | 20.15 [20.15] | 19.12 [19.12] | 18.68 [18.68] |
| $R_{O[E]}^{N-MIT}$ | ↘ | 0.406 [0.406] | 0.404 [0.404] | 0.394 [0.394] | 0.390 [0.390] |
| **Acceptor** | | Ga | Mg | **In** | Cd |
| $r_a$ (nm) | ↗ | 0.126 | 0.140 | **0.144** | 0.148 |
| At **x=0**, | | | | | |
| $E_{gp}$(meV) | ↗ | 427.45 [427.45] | 429.87 [429.87 ] | 430.0 [430.0] | 430.1 [430.1] |
| $n_{O[E]}^{N-MIT}$ | ↘ | 4.283 [4.283] | 4.207 [4.207] | 4.203 [4.203] | 4.199 [4.199] |
| $\varepsilon_{1\,O[E]}^{N-MIT}$ | ↘ | 18.34 [18.34] | 17.70 [17.70] | 17.66 [17.66] | 17.63 [17.63] |
| $R_{O[E]}^{N-MIT}$ | ↘ | 0.386 [0.386] | 0.379 [0.379] | 0.3789 [0.3789] | 0.3786 [0.3786] |
| At **x=0.5**, | | | | | |
| $E_{gp}$(meV) | ↗ | 327.4 [327.4] | 329.9 [329.9] | 330.0 [330.0] | 330.1 [330.1] |
| $n_{O[E]}^{N-MIT}$ | ↘ | 4.430 [4.430] | 4.351 [4.351] | 4.347 [4.347] | 4.343 [4.343] |

| | | | | | |
|---|---|---|---|---|---|
| $\varepsilon_{1\,O[E]}^{N-MIT}$ | ↘ | 19.63 [19.63] | 18.93 [18.93] | 18.90 [18.90] | 18.86 [18.86] |
| $\varepsilon_{1\,O[E]}^{N-MIT}$ | ↘ | 0.399 [0.399] | 0.392 [0.392] | 0.3919 [0.3919] | 0.3915 [0.3915] |
| At **x=1**, | | | | | |
| $E_{gp}$(meV) | ↗ | 227.4 [227.4] | 229.9 [229.9] | 230.0 [230.0] | 230.1 [230.1] |
| $n_{O[E]}^{N-MIT}$ | ↘ | 4.575 [4.575] | 4.493 [4.493] | 4.489 [4.489] | 4.485 [4.485] |
| $\varepsilon_{1\,O[E]}^{N-MIT}$ | ↘ | 20.93 [20.93] | 20.19 [20.19] | 20.15 [20.15] | 20.11 [20.11] |
| $\varepsilon_{1\,O[E]}^{N-MIT}$ | ↘ | 0.411 [0.411] | 0.4044 [0.4044 ] | 0.404 [0.404] | 0.4037 [0.4037] |

**Table 4n.** For T=0K and $N=N_{CDn}(r_d, x)$, and for given x and $r_d$, the numerical results of $n_{O[E]}^{N-MIT}$, $\varepsilon_{1\,O[E]}^{N-MIT}$ and $R_{O[E]}^{N-MIT}$ are obtained, using Equations (17, 16), suggesting that, for a given E, they are found to be the same, since $E_{gn1} = E_{gn2} = E_{gn}$.

| E in eV | $n_{O[E]}^{N-MIT}$ | $\varepsilon_{1\,O[E]}^{N-MIT}$ | $R_{O[E]}^{N-MIT}$ |
|---|---|---|---|
| At x=0, and in the As-X(x)-system, in which $E_{gn}(r_{As}, x=0) = 0.43$ eV, | | | |
| **0.43** | **4.203 [4.203]** | **17.66 [17.66]** | **0.379 [0.379]** |
| 2 | 6.111 [6.111] | 37.34 [37.34] | 0.516 [0.516] |
| 2.5 | 7.498 [7.498] | 56.22 [56.22] | 0.585 [0.585] |
| 3 | 6.290 [6.290] | 39.56 [39.56] | 0.526 [0.526] |
| 3.5 | 3.725 [3.725] | 13.87 [13.87] | 0.332 [0.332] |
| 4 | 4.022 [4.022] | 16.18 [16.18] | 0.362[0.362] |
| 4.5 | 4.666 [4.666] | 21.77 [21.77] | 0.419 [0.419] |
| 5 | 1.561 [1.561] | 2.437 [2.437] | 0.048 [0.048] |
| 5.5 | -0.287 [-0.287] | 0.082 [0.082] | 3.254 [3.254] |
| 6 | 0.103 [0.103] | 0.011 [0.011] | 0.661 [0.661] |
| … | | | |
| **$10^{22}$** | **2.167 [2.167]** | **4.694 [4.694]** | **0.136 [0.136]** |
| At x=0.5, and in the As-X(x)-system, in which $E_{gn}(r_{As}, x=0.5) = 0.33$ eV, | | | |
| **0.330** | **4.347 [4.347]** | **18.90 [18.90]** | **0.392 [0.392]** |
| 2 | 6.440 [6.440] | 41.47 [41.47] | 0.534 [0.535] |
| 2.5 | 7.903 [7.903] | 62.46 [62.46] | 0.601 [0.601] |
| 3 | 6.535 [6.535] | 42.71 [42.71] | 0.539 [0.539] |
| 3.5 | 3.773 [3.773] | 14.24 [14.24] | 0.337 [0.337] |
| 4 | 4.092 [4.092] | 16.75 [16.75] | 0.369 [0.369] |
| 4.5 | 4.770 [4.770] | 22.75 [22.75] | 0.427 [0.427] |
| 5 | 1.525 [1.525] | 2.325 [2.325] | 0.043 [0.043] |
| 5.5 | -0.385 [-0.385] | 0.148 [0.148] | 5.062 [5.062] |
| 6 | 0.036 [0.036] | 0.001 [0.001] | 0.867 [0.867] |
| … | | | |
| **$10^{22}$** | **2.249 [2.249]** | **5.057 [5.057]** | **0.148 [0.148]** |
| At x=1, and in the As-X(x)-system, in which $E_{gn}(r_{As}, x=1) = 0.23$ eV, | | | |
| **0.230** | **4.489 [4.489]** | **20.15 [20.15]** | **0.404 [0.404]** |
| 2 | 6.773 [6.773] | 45.88 [45.88] | 0.552 [0.552] |
| 2.5 | 8.315 [8.315] | 69.13 [69.13] | 0.617 [0.617] |
| 3 | 6.779 [6.779] | 45.95 [45.95] | 0.552 [0.552] |
| 3.5 | 3.814 [3.814] | 14.55 [14.55] | 0.342 [0.342] |
| 4 | 4.156 [4.156] | 17.27 [17.27] | 0.375 [0.375] |
| 4.5 | 4.868 [4.868] | 23.70 [23.70] | 0.434 [0.434] |
| 5 | 1.481 [1.481] | 2.192 [2.192] | 0.037 [0.037] |
| 5.5 | -0.491 [-0.491] | 0.241 [0.241] | 8.596 [8.596] |
| 6 | -0.040 [-0.040] | 0.002 [0.002] | 1.172 [1.172] |
| … | | | |
| **$10^{22}$** | **2.328 [2.328]** | **5.420 [5.420]** | **0.159 [0.159]** |

| E in eV | $n_{O[E]}^{MIT}$ | $\varepsilon_{1\,O[E]}^{MIT}$ | $R_{O[E]}^{MIT}$ |
|---|---|---|---|
| At x=0, and in the Sb-X(x)-system, in which $E_{gn}(r_{Sb}, x=0) = 0.4313$ eV, | | | |
| **0.4313** | **4.094 [4.094]** | **16.76 [16.76]** | **0.369 [0.369]** |
| 2 | 6.000 [6.000] | 36.00 [36.00] | 0.510 [0.510] |
| 2.5 | 7.386 [7.386] | 54.55 [54.55] | 0.580 [0.580] |

| | | | |
|---|---|---|---|
| 3 | 6.180 [6.180] | 38.19 [38.19] | 0.520 [0.520] |
| 3.5 | 3.618 [3.618] | 13.09 [13.09] | 0.321 [0.321] |
| 4 | 3.915 [3.915] | 15.32 [15.32] | 0.352 [0.352] |
| 4.5 | 4.558 [4.558] | 20.78 [20.78] | 0.410 [0.410] |
| 5 | 1.455 [1.455] | 2.116 [2.116] | 0.034 [0.034] |
| 5.5 | -0.392 [-0.392] | 0.154 [0.154] | 5.243 [5.243] |
| 6 | -0.002 [-0.002] | 0.000007 [0.000007] | 1.011 [1.011] |
| … | | | |
| **$10^{22}$** | **2.059 [2.059]** | **4.239 [4.239]** | **0.120 [0.120]** |
| At x=0.5, and in the Sb-X(x)-system, in which $E_{gn}(r_{Sb}, x = 0.5) = 0.3312$ eV, | | | |
| **$0.3312$** | **4.235 [4.235]** | **17.93 [17.93]** | **0.382 [0.382]** |
| 2 | 6.325 [6.325] | 40.00 [40.00] | 0.528 [0.528] |
| 2.5 | 7.787 [7.787] | 60.64 [60.64] | 0.597 [0.597] |
| 3 | 6.421 [6.421] | 41.23 [41.23] | 0.534 [0.534] |
| 3.5 | 3.662 [3.662] | 13.41 [13.41] | 0.326 [0.326] |
| 4 | 3.981 [3.981] | 15.85 [15.85] | 0.358 [0.358] |
| 4.5 | 4.658[4.658] | 21.69 [21.69] | 0.418 [0.418] |
| 5 | 1.415 [1.415] | 2.001 [2.001] | 0.029 [0.029] |
| 5.5 | -0.494 [-0.494] | 0.244 [0.244] | 8.726 [8.726] |
| 6 | -0.074 [-0.074] | 0.005 [0.005] | 1.347 [1.347] |
| … | | | |
| **$10^{22}$** | **2.137[2.137]** | **34.567 [4.567]** | **0.131 [0.131]** |
| At x=1, and in the Sb-X(x)-system, in which $E_{gn}(r_{Sb}, x = 1) = 0.2311$ eV, | | | |
| **$0.2311$** | **4.373 [4.373]** | **19.12 [19.12]** | **0.394 [0.394]** |
| 2 | 6.655 [6.655] | 44.29 [44.29] | 0.546 [0.546] |
| 2.5 | 8.195 [8.195] | 67.16 [67.16] | 0.612 [0.612] |
| 3 | 6.661 [6.661] | 44.37 [44.37] | 0.546 [0.546] |
| 3.5 | 3.699 [3.699] | 13.68 [13.68] | 0.330 [0.330] |
| 4 | 4.040 [4.040] | 16.33 [16.33] | 0.364 [0.364] |
| 4.5 | 4.752 [4.752] | 22.58 [22.58] | 0.425 [0.425] |
| 5 | 1.366 [1.366] | 1.867 [1.867] | 0.024 [0.024] |
| 5.5 | -0.605 [-0.605] | 0.366 [0.366] | 16.51 [16.51] |
| 6 | -0.154 [-0.154] | 0.023 [0.023] | 1.858 [1.858] |
| … | | | |
| **$10^{22}$** | **2.212 [2.212]** | **4.895 [4.895]** | **0.142 [0.142]** |

**Table 4p.** For T=0K and N=$N_{CDp}(r_a, x)$, and for given x and $r_d$, the numerical results of $n^{N-MIT}_{O[E]}$, $\varepsilon^{N-MIT}_{1\,O[E]}$ and $R^{N-MIT}_{O[E]}$ are obtained, using Equations (17, 16), suggesting that, for a given E, they are found to be the same, since $E_{gp1} = E_{gp2} = E_{gp}$.

| E in eV | $n^{N-MIT}_{O[E]}$ | $\varepsilon^{N-MIT}_{1\,O[E]}$ | $R^{N-MIT}_{O[E]}$ |
|---|---|---|---|
| At x=0, and in the Mg-X(x)-system, in which $E_{gp}(r_{Mg}, x = 0) = 0.4299$ eV, | | | |
| **$0.4299$** | **4.207 [4.207]** | **17.70 [17.70]** | **0.3794 [0.379]** |
| 2 | 6.115 [6.115] | 37.39 [37.39] | 0.517 [0.5172] |
| 2.5 | 7.502 [7.502] | 56.28 [56.28] | 0.585 [0.585] |
| 3 | 6.294 [6.294] | 39.61 [39.61] | 0.527 [0.527] |
| 3.5 | 3.728 [3.728] | 13.90 [13.90] | 0.333 [0.333] |
| 4 | 4.026 [4.026] | 16.21 [16.21] | 0.362 [0.362] |
| 4.5 | 4.670 [4.670] | 21.81 [21.81] | 0.419 [0.419] |
| 5 | 1.564 [1.564] | 2.448 [2.448] | 0.048 [0.048] |
| 5.5 | -0.283 [-0.283] | 0.080 [0.080] | 3.205 [3.205] |
| 6 | 0.106 [0.106] | 0.011 [0.011] | 0.652 [0.652] |
| … | | | |
| **$10^{22}$** | **2.170 [2.170]** | **4.710 [4.710]** | **0.136 [0.136]** |
| At x=0.5, and in the Mg-X(x)-system, in which $E_{gp}(r_{Mg}, x = 0.5) = 0.3299$ eV, | | | |
| **$0.3299$** | **4.351 [4.351]** | **18.93 [18.93]** | **0.392 [0.392]** |
| 2 | 6.444 [6.444] | 24.23 [24.23] | 0.439 [0.439] |
| 2.5 | 7.907 [7.907] | 35.49 [35.49] | 0.508 [0.508] |
| 3 | 6.539 [6.539] | 42.76 [42.76] | 0.540 [0.540] |
| 3.5 | 3.777 [3.777] | 14.27 [14.27] | 0.338 [0.338] |

| | | | |
|---|---|---|---|
| 4 | 4.096 [4.096] | 16.78 [16.78] | 0.369 [0.369] |
| 4.5 | 4.774 [4.774] | 22.79 [22.79] | 0.427 [0.427] |
| 5 | 1.529 [1.529] | 2.337 [2.337] | 0.044 [0.044] |
| 5.5 | -0.381 [-0.381] | 0.145 [0.145] | 4.977 [4.977] |
| 6 | 0.039 [0.039] | 0.001 [0.001] | 0.854 [0.854] |
| … | | | |
| **$10^{22}$** | **2.253 [2.253]** | **5.074 [5.074]** | **0.148 [0.148]** |
| At x=1, and in the Mg-X(x)-system, in which $E_{gp}(r_{Mg}, x = 1) = 0.2299$ eV, | | | |
| **$0.2299$** | **4.493 [4.493]** | **20.19 [20.19]** | **0.404 [0.404]** |
| 2.5 | 8.319 [8.319] | 69.21 [69.21] | 0.617 [0.617] |
| 3 | 6.783 [6.783] | 46.01 [46.01] | 0.552 [0.552] |
| 3.5 | 3.818 [3.818] | 14.58 [14.58] | 0.342 [0.342] |
| 4 | 4.160 [4.160] | 17.30 [17.30] | 0.375 [0.375] |
| 4.5 | 4.872 [4.872] | 23.74 [23.74] | 0.435 [0.435] |
| 5 | 1.484 [1.484] | 2.204 [2.204] | 0.038 [0.038] |
| 5.5 | -0.487 [-0.487] | 0.238 [0.238] | 8.428 [8.428] |
| 6 | -0.036 [-0.036] | 0.001 [0.001] | 1.154 [1.154] |
| … | | | |
| **$10^{22}$** | **2.332 [2.332]** | **5.439 [5.439]** | **0.160 [0.160]** |
| E in eV | $n_{O-EP[E-OP]}$ | $\varepsilon_{1O-EP[E-OP]}$ | $R_{O-EP[E-OP]}$ |
| At x=0, and in the In-X(x)-system, in which $E_{gp}(r_{In}, x = 0) = 0.43$ eV, | | | |
| **$0.4300$** | **4.203 [4.203]** | **17.66 [17.66]** | **0.379 [0.379]** |
| 2 | 6.111 [6.111] | 37.34 [37.34] | 0.516 [0.516] |
| 2.5 | 7.498 [7.498] | 56.22 [56.22] | 0.585 [0.585] |
| 3 | 6.290 [6.290] | 39.56 [39.56] | 0.526 [0.526] |
| 3.5 | 3.725 [3.725] | 13.87 [13.87] | 0.332 [0.332] |
| 4 | 4.022 [4.022] | 16.18 [16.18] | 0.362 [0.362] |
| 4.5 | 4.666 [4.666] | 21.77 [21.77] | 0.419 [0.419] |
| 5 | 1.561 [1.561] | 2.437 [2.437] | 0.048 [0.048] |
| 5.5 | -0.287 [-0.287] | 0.082 [0.082] | 3.254 [3.254] |
| 6 | 0.103 [0.103] | 0.011 [0.011] | 0.661 [0.661] |
| … | | | |
| **$10^{22}$** | **2.167 [2.167]** | **4.694 [4.694]** | **0.136 [0.136]** |
| At x=0.5, and in the In-X(x)-system, in which $E_{gp}(r_{In}, x = 0.5) = 0.33$ eV, | | | |
| **$0.330$** | **4.347 [4.347]** | **18.90 [18.90]** | **0.392 [0.392]** |
| 2 | 6.440 [6.440] | 41.47 [41.47] | 0.535 [0.535] |
| 2.5 | 7.903 [7.903] | 62.46 [62.46] | 0.601 [0.601] |
| 3 | 6.535 [6.535] | 42.71 [42.71] | 0.539 [0.539] |
| 3.5 | 3.773 [3.773] | 14.24 [14.24] | 0.337 [0.337] |
| 4 | 4.092 [4.092] | 16.75 [16.75] | 0.369 [0.369] |
| 4.5 | 4.770 [4.770] | 22.75 [22.75] | 0.427 [0.427] |
| 5 | 1.525 [1.525] | 2.325 [2.325] | 0.043 [0.043] |
| 5.5 | -0.385 [-0.385] | 0.148 [0.148] | 5.062 [5.062] |
| 6 | 0.036 [0.036] | 0.001 [0.001] | 0.867 [0.867] |
| … | | | |
| **$10^{22}$** | **2.249 [2.249]** | **5.057 [5.057]** | **0.148 [0.148]** |
| At x=1, and in the In-X(x)-system, in which $E_{gno}(r_{In}, x = 1) = 0.23$ eV, | | | |
| **$0.230$** | **4.489 [4.489]** | **20.15 [20.15]** | **0.404 [0.404]** |
| 2 | 6.773 [6.773] | 45.88 [45.88] | 0.552 [0.552] |
| 2.5 | 8.315 [8.315] | 69.13 [69.13] | 0.617 [0.617] |
| 3 | 6.779 [6.779] | 45.95 [45.95] | 0.552 [0.552] |
| 3.5 | 3.814 [3.814] | 14.55 [14.55] | 0.342 [0.342] |
| 4 | 4.156 [4.156] | 17.27 [17.27] | 0.375 [0.375] |
| 4.5 | 4.868 [4.868] | 23.70 [23.70] | 0.434 [0.434] |
| 5 | 1.481 [1.481] | 2.192 [2.192] | 0.037 [0.037] |
| 5.5 | -0.491 [-0.491] | 0.241 [0.241] | 8.596 [8.596] |
| 6 | -0.040 [-0.040] | 0.001 [0.001] | 1.172 [1.172] |
| … | | | |
| **$10^{22}$** | **2.328 [2.328]** | **5.420 [5.420]** | **0.159 [0.159]** |

**Table 5.** For T=0K, $E \cong E_{gn(gp)}$ and $N^* = N_{CDn(NDp)}$, and from Eq. (16b), the numerical results of $\sigma^{EBT}_{O[E]}$, $\kappa^{EBT}_{O[E]}$, $\varepsilon^{EBT}_{2O[2E]}$ and $\propto^{EBT}_{O[E]}$ are obtained, using Equations (18, 19b, 19c, 19d), suggesting that they increase (↗) with increasing (↗) $r_{d(a)}$.

| Donor | P | **As** | Sb | Sn |
|---|---|---|---|---|
| $r_d$ (nm) [4] ↗ | 0.110 | **0.118** | 0.136 | 0.140 |
| At **x=0**, | | | | |
| $\sigma^{EBT}_{O[E]}\left(\frac{10^2}{\Omega\times cm}\right)$ ↗ | 1.349 [0.961] | 1.377 [0.981] | 1.525 [1.086] | 1.596 [1.137] |
| $\kappa^{EBT}_{O[E]}\times 10^3$ ↗ | 2.326 [1.655] | 2.434 [1.732] | 3.053 [2.172] | 3.378 [2.403] |
| $\varepsilon^{EBT}_{2O[2E]}\times 10^2$ ↗ | 1.975 [1.407] | 2.056 [1.465] | 2.514 [1.791] | 2.750 [1.960] |
| $\propto^{EBT}_{O[E]}\left(\frac{10^2}{cm}\right)$ ↗ | 1.013 [0.721] | 1.060 [0.755] | 1.334 [0.949] | 1.479 [1.052] |
| At **x=0.5**, | | | | |
| $\sigma^{EBT}_{O[E]}\left(\frac{10^2}{\Omega\times cm}\right)$ ↗ | 1.285 [0.942] | 1.311 [0.961] | 1.452 [1.065] | 1.520 [1.114] |
| $\kappa^{EBT}_{O[E]}\times 10^3$ ↗ | 2.589 [1.897] | 2.709 [1.985] | 3.396 [2.488] | 3.757 [2.752] |
| $\varepsilon^{EBT}_{2O[2E]}\times 10^2$ ↗ | 2.275 [1.668] | 2.368 [1.736] | 2.893 [2.122] | 3.164 [2.321] |
| $\propto^{EBT}_{O[E]}\left(\frac{10^2}{cm}\right)$ ↗ | 0.865 [0.634] | 0.906 [0.664] | 1.140 [0.835] | 1.263 [0.925] |
| At **x=1**, | | | | |
| $\sigma^{EBT}_{O[E]}\left(\frac{10^2}{\Omega\times cm}\right)$ ↗ | 1.234 [0.925] | 1.260 [0.944] | 1.395 [1.046] | 1.460 [1.095] |
| $\kappa^{EBT}_{O[E]}\times 10^3$ ↗ | 3.225 [2.416] | 3.374 [2.528] | 4.226 [3.165] | 4.672 [3.498] |
| $\varepsilon^{EBT}_{2O[2E]}\times 10^2$ ↗ | 2.926 [2.194] | 3.046 [2.283] | 3.717 [2.786] | 4.063 [3.046] |
| $\propto^{EBT}_{O[E]}\left(\frac{10^2}{cm}\right)$ ↗ | 0.751 [0.563] | 0.787 [0.589] | 0.990 [0.741] | 1.097 [0.821] |

| **Acceptor** | Ga | Mg | **In** | Cd |
|---|---|---|---|---|
| $r_a$ (nm) ↗ | 0.126 | 0.140 | **0.144** | 0.148 |
| At **x=0**, | | | | |
| $\sigma^{EBT}_{O[E]}\left(\frac{10^3}{\Omega\times cm}\right)$ ↗ | 2.451 [0.305] | 2.622 [0.326] | 2.631 [0.327] | 2.640 [0.328] |
| $\kappa^{EBT}_{O[E]}\times 10^2$ ↗ | 4.038 [0.497] | 4.687 [0.576] | 4.723 [0.581] | 4.759 [0.585] |
| $\varepsilon^{EBT}_{2O[2E]}\times 10^1$ ↗ | 3.429 [0.426] | 3.902 [0.485] | 3.928 [0.488] | 3.955 [0.492] |
| $\propto^{EBT}_{O[E]}\left(\frac{10^3}{cm}\right)$ ↗ | 1.395 [0.172] | 1.523 [0.187] | 1.529 [0.188] | 2.488 [0.306] |
| At **x=0.5**, | | | | |
| $\sigma^{EBT}_{O[E]}\left(\frac{10^3}{\Omega\times cm}\right)$ ↗ | 3.012 [0.330] | 3.223 [0.353] | 3.234 [0.354] | 3.245 [0.355] |
| $\kappa^{EBT}_{O[E]}\times 10^2$ ↗ | 5.819 [0.629] | 6.743 [0.728] | 6.794 [0.733] | 6.846 [0.739] |
| $\varepsilon^{EBT}_{2O[2E]}\times 10^1$ ↗ | 5.107 [0.559] | 5.802 [0.636] | 5.840 [0.640] | 5.879 [0.644] |
| $\propto^{EBT}_{O[E]}\left(\frac{10^3}{cm}\right)$ ↗ | 1.540 [0.166] | 1.681 [0.181] | 1.688 [0.182] | 2.746 [0.296] |
| At **x=1**, | | | | |
| $\sigma^{EBT}_{O[E]}\left(\frac{10^3}{\Omega\times cm}\right)$ ↗ | 3.575 [0.352] | 3.825 [0.376] | 3.838 [0.378] | 3.851 [0.379] |
| $\kappa^{EBT}_{O[E]}\times 10^2$ ↗ | 8.989 [0.873] | 10.38 [1.006] | 10.46 [1.013] | 10.54 [1.021] |
| $\varepsilon^{EBT}_{2O[2E]}\times 10^1$ ↗ | 8.143 [0.801] | 9.222 [0.907] | 9.280 [0.913] | 9.340 [0.919] |
| $\propto^{EBT}_{O[E]}\left(\frac{10^3}{cm}\right)$ ↗ | 1.653 [0.160] | 1.804 [0.175] | 1.812 [0.176] | 2.947 [0.285] |

**Table 6n.** In the X(x)-system, at E=3.2 eV and T=20 K, for given $r_d$ and x, the numerical results of $n_{O[E]}(E)$, $\kappa_{O[E]}(E)$, $\varepsilon_{1O[E]}(E)$ and $\varepsilon_{2O[E]}(E)$, are obtained, as functions of N, by using Equations (17, 19b, 19c and 16), respectively, noting that, with increasing N, $\eta_{o[E]}$ increases [increases], and $E_{gn1\ O[E]}$ increases [decreases], respectively.

| $N\ (10^{18}\ cm^{-3})$ ↗ | 15 | 26 | 60 | 100 |
|---|---|---|---|---|
| **At x=0** | | | | |
| For $\mathbf{r_d = r_{As}}$, | | | | |
| $\eta_{o[E]} \gg 1$ | 185.6 [142.8] | 267.9 [206.1] | 468.1 [360.1] | 658.1 [506.2] |
| $E_{gn1\ O[E]}$ in eV | 0.41 [0.09] | 0.45 [-0.004] | 0.59 [-0.21] | 0.74 [-0.39] |
| $n_{O[E]}$ | 5.24 [5.47] | 5.21 [5.53] | 5.11 [5.67] | 4.99 [5.77] |
| $\kappa_{O[E]}$ | 0.06 [0.04] | 0.10 [0.06] | 0.23 [0.13] | 0.39 [0.21] |
| $\varepsilon_{1O[E]}$ | 27.49 [29.89] | 27.14 [30.61] | 26.03 [32.09] | 24.73 [33.27] |
| $\varepsilon_{2O[E]}$ | 0.65 [0.41] | 1.09 [0.68] | 2.39 [1.49] | 3.87 [2.40] |
| For $\mathbf{r_d = r_{Sb}}$, | | | | |
| $\eta_{o[E]} \gg 1$ | 185.5 [142.7] | 267.9 [206.1] | 468.1 [360.0] | 658.1 [506.2] |
| $E_{gn1\ O[E]}$ in eV | 0.44 [0.12] | 0.49 [0.03] | 0.64 [-0.16] | 0.81 [-0.32] |
| $n_{O[E]}$ | 5.12 [5.37] | 5.08 [5.40] | 4.96 [5.52] | 4.83 [5.62] |
| $\kappa_{O[E]}$ | 0.06 [0.03] | 0.10 [0.06] | 0.22 [0.12] | 0.37 [0.19] |
| $\varepsilon_{1O[E]}$ | 26.17 [28.53] | 25.77 [29.18] | 24.55 [30.51] | 23.16 [31.59] |
| $\varepsilon_{2O[E]}$ | 0.60 [0.38] | 1.01 [0.63] | 2.20 [1.37] | 3.55 [2.21] |
| **At x=0.5** | | | | |
| For $\mathbf{r_d = r_{As}}$, | | | | |
| $\eta_{o[E]} \gg 1$ | 172.0 [135.3] | 248.35 [195.3] | 433.7 [341.1] | 609.8 [479.6] |
| $E_{gn1\ O[E]}$ in eV | 0.27 [-0.02] | 0.30 [-0.12] | 0.41 [-0.33] | 0.53 [-0.51] |
| $n_{O[E]}$ | 5.42 [5.62] | 5.40 [5.69] | 5.32 [5.82] | 5.23 [5.93] |
| $\kappa_{O[E]}$ | 0.05 [0.03] | 0.09 [0.06] | 0.21 [0.12] | 0.34 [0.19] |
| $\varepsilon_{1O[E]}$ | 29.41 [31.63] | 29.17 [32.37] | 28.32 [33.89] | 27.28 [35.10] |
| $\varepsilon_{2O[E]}$ | 0.61 [0.40] | 1.01 [0.66] | 2.21 [1.43] | 3.58 [2.31] |
| For $\mathbf{r_d = r_{Sb}}$, | | | | |
| $\eta_{o[E]} \gg 1$ | 171.9 [135.2] | 248.2 [195.2] | 433.7 [341.1] | 609.7 [479.6] |
| $E_{gn1\ O[E]}$ in eV | 0.30 [0.009] | 0.34 [-0.08] | 0.46 [-0.28] | 0.60 [-0.44] |
| $n_{O[E]}$ | 5.29 [5.49] | 5.26 [5.55] | 5.17 [5.68] | 5.07 [5.78] |
| $\kappa_{O[E]}$ | 0.05 [0.03] | 0.09 [0.05] | 0.20 [0.12] | 0.32 [0.18] |
| $\varepsilon_{1O[E]}$ | 28.01 [30.19] | 27.71 [30.85] | 26.73 [32.23] | 25.59 [33.33] |
| $\varepsilon_{2O[E]}$ | 0.56 [0.37] | 0.93 [0.61] | 2.03 [1.32] | 3.29 [2.13] |
| **At x=1** | | | | |
| For $\mathbf{r_d = r_{As}}$, | | | | |
| $\eta_{o[E]} \gg 1$ | 160.6 [128.5] | 231.9 [185.5] | 405.1 [324.1] | 569.5 [455.6] |
| $E_{gn1\ O[E]}$ in eV | 0.14 [-0.13] | 0.16 [-0.23] | 0.24 [-0.45] | 0.34 [-0.64] |
| $n_{O[E]}$ | 5.59 [5.77] | 5.58 [5.84] | 5.53 [5.97] | 5.46 [6.08] |
| $\kappa_{O[E]}$ | 0.05 [0.03] | 0.08 [0.05] | 0.19 [0.11] | 0.31 [0.18] |
| $\varepsilon_{1O[E]}$ | 31.29 [33.35] | 31.14 [34.11] | 30.51 [35.66] | 29.68 [36.89] |
| $\varepsilon_{2O[E]}$ | 0.57 [0.38] | 0.94 [0.63] | 2.07 [1.38] | 3.35 [2.23] |
| For $\mathbf{r_d = r_{Sb}}$, | | | | |
| $\eta_{o[E]} \gg 1$ | 160.6 [128.5] | 231.8 [185.5] | 405.1 [324.0] | 569.5 [455.6] |
| $E_{gn1\ O[E]}$ in eV | 0.17 [-0.10] | 0.20 [-0.20] | 0.29 [-0.40] | 0.41 [-0.57] |
| $n_{O[E]}$ | 5.46 [5.64] | 5.44 [5.70] | 5.37 [5.82] | 5.29 [5.92] |
| $\kappa_{O[E]}$ | 0.05 [0.03] | 0.08 [0.05] | 0.18 [0.11] | 0.29 [0.17] |
| $\varepsilon_{1O[E]}$ | 29.80 [31.83] | 29.59 [32.51] | 28.83 [33.91] | 27.89 [35.03] |

| | | | | |
|---|---|---|---|---|
| $\varepsilon_{2O[E]}$ | 0.52 [0.35] | 0.87 [0.59] | 1.90 [1.27] | 3.07 [2.05] |
| N ($10^{18}$ $cm^{-3}$) ↗ | 15 | 26 | 60 | 100 |

**Table 6p.** In the X(x)-system, at E=3.2 eV and T=20 K, for given $r_a$ and x, the numerical results of $n_{O[E]}(E)$, $\kappa_{O[E]}(E)$, $\varepsilon_{1O[E]}(E)$ and $\varepsilon_{2O[E]}(E)$, are obtained, as functions of N, by using Equations (17, 19b, 19c and 16), respectively, noting that, with increasing N, $\eta_{o[E]}$ increases [increases], and $E_{gp1\ O[E]}$ increases [decreases], respectively.

| N ($10^{18}$ $cm^{-3}$) ↗ | 15 | 26 | 60 | 100 |
|---|---|---|---|---|
| **At x=0** | | | | |
| For $\mathbf{r_d} = \mathbf{r_{Mg}}$, | | | | |
| $\eta_{o[E]} \gg 1$ | 178.2 [41.11] | 261.8 [60.41] | 463.5 [106.9] | 654.2 [151.0] |
| $E_{gp1\ O[E]}$ in eV | 0.69 [0.38] | 0.82 [0.37] | 1.14 [0.34] | 1.45 [0.32] |
| $n_{O[E]}$ | 5.03 [5.26] | 4.93 [5.27] | 4.66 [5.29] | 4.38 [5.31] |
| $\kappa_{O[E]}$ | 0.06 [0.005] | 0.11 [0.008] | 0.25 [0.017] | 0.44 [0.028] |
| $\varepsilon_{1O[E]}$ | 25.33 [27.7] | 24.28 [27.8] | 21.65 [28.0] | 19.03 [28.2] |
| $\varepsilon_{2O[E]}$ | 0.62 [0.05] | 1.06 [0.09] | 2.36 [0.18] | 3.85 [0.29] |
| For $\mathbf{r_d} = \mathbf{r_{In}}$, | | | | |
| $\eta_{o[E]} \gg 1$ | 178.1 [41.09] | 261.8 [60.39] | 463.4 [106.9] | 654.2 [150.9] |
| $E_{gp1\ O[E]}$ in eV | 0.69 [0.38] | 0.82 [0.37] | 1.14 [0.35] | 1.45 [0.32] |
| $n_{O[E]}$ | 5.03 [5.26] | 4.92 [5.27] | 4.65 [5.29] | 4.38 [5.31] |
| $\kappa_{O[E]}$ | 0.06 [0.005] | 0.11 [0.008] | 0.25 [0.018] | 0.44 [0.027] |
| $\varepsilon_{1O[E]}$ | 25.29 [27.7] | 24.24 [27.8] | 21.61 [28.0] | 19.00 [28.1] |
| $\varepsilon_{2O[E]}$ | 0.62 [0.05] | 1.06 [0.09] | 2.36 [0.19] | 3.84 [0.29] |
| **At x=0.5** | | | | |
| For $\mathbf{r_d} = \mathbf{r_{Mg}}$, | | | | |
| $\eta_{o[E]} \gg 1$ | 163.2 [34.8] | 241.0 [51.44] | 428.2 [91.41] | 605.1 [129.1] |
| $E_{gp1\ O[E]}$ in eV | 0.57 [0.29] | 0.69 [0.28] | 0.99 [0.25] | 1.27 [0.23] |
| $n_{O[E]}$ | 5.21 [5.42] | 5.11 [5.42] | 4.87 [5.44] | 4.62 [5.45] |
| $\kappa_{O[E]}$ | 0.05 [0.004] | 0.09 [0.007] | 0.22 [0.01] | 0.38 [0.02] |
| $\varepsilon_{1O[E]}$ | 27.14 [29.34] | 26.16 [29.43] | 23.69 [29.62] | 21.25 [29.77] |
| $\varepsilon_{2O[E]}$ | 0.56 [0.04] | 0.97 [0.07] | 2.18 [0.15] | 3.55 [0.24] |
| For $\mathbf{r_d} = \mathbf{r_{In}}$, | | | | |
| $\eta_{o[E]} \gg 1$ | 163.1 [34.8] | 241.0 [51.42] | 428.2 [91.40] | 605.1 [129.2] |
| $E_{gp1\ O[E]}$ in eV | 0.57 [0.29] | 0.69 [0.27] | 0.99 [0.25] | 1.27 [0.23] |
| $n_{O[E]}$ | 5.21 [5.41] | 5.11 [5.42] | 4.87 [5.44] | 4.62 [5.45] |
| $\kappa_{O[E]}$ | 0.05 [0.004] | 0.09 [0.007] | 0.22 [0.01] | 0.38 [0.02] |
| $\varepsilon_{1O[E]}$ | 27.10 [29.30] | 26.12 [29.39] | 23.65 [29.57] | 21.21 [29.72] |
| $\varepsilon_{2O[E]}$ | 0.56 [0.04] | 0.97 [0.07] | 2.17 [0.15] | 3.54 [0.24] |
| **At x=1** | | | | |
| For $\mathbf{r_d} = \mathbf{r_{Mg}}$, | | | | |
| $\eta_{o[E]} \gg 1$ | 150.6 [30.1] | 223.6 [44.7] | 398.9 [79.76] | 564.3 [112.8] |
| $E_{gp1\ O[E]}$ in eV | 0.45 [0.19] | 0.56 [0.18] | 0.84 [0.16] | 1.11 [0.14] |
| $n_{O[E]}$ | 5.38 [5.56] | 5.29 [5.57] | 5.07 [5.59] | 4.85 [5.60] |
| $\kappa_{O[E]}$ | 0.05 [0.003] | 0.08 [0.005] | 0.20 [0.01] | 0.34 [0.02] |
| $\varepsilon_{1O[E]}$ | 28.93 [30.97] | 28.01 [31.05] | 25.68 [31.22] | 23.39 [31.36] |

| | | | | |
|---|---|---|---|---|
| $\varepsilon_{2O[E]}$ | 0.52 [0.04] | 0.90 [0.06] | 2.03 [0.13] | 3.31 [0.20] |
| For $\mathbf{r_d} = \mathbf{r_{In}}$, | | | | |
| $\eta_{o[E]} \gg 1$ | 150.5 [30.1] | 223.5 [44.69] | 398.8 [79.75] | 564.2 [112.8] |
| $E_{gp1\ O[E]}$ in eV | 0.45 [0.19] | 0.56 [0.18] | 0.84 [0.16] | 1.11 [0.14] |
| $n_{O[E]}$ | 5.37 [5.56] | 5.29 [5.57] | 5.07 [5.58] | 4.84 [5.59] |
| $\kappa_{O[E]}$ | 0.05 [0.003] | 0.08 [0.005] | 0.20 [0.01] | 0.34 [0.02] |
| $\varepsilon_{1O[E]}$ | 28.89 [30.92] | 27.96 [31.00] | 25.64 [31.17] | 23.35 [31.31] |
| $\varepsilon_{2O[E]}$ | 0.52 [0.04] | 0.90 [0.06] | 2.02 [0.13] | 3.30 [0.20] |
| N ($10^{18}$ cm$^{-3}$) ↗ | 15 | 26 | 60 | 100 |

**Table 7n.** In the X(x)-system, at E=3.2 eV and $N = 10^{20} cm^{-3}$, for given $r_d$ and x, the numerical results of $n_{O[E]}(E)$, $\kappa_{O[E]}(E)$, $\varepsilon_{1O[E]}(E)$ and $\varepsilon_{2O[E]}(E)$, are obtained, as functions of T, by using Equations (17, 19b, 19c and 16), respectively, noting that $\eta_{o[E]}$ and $E_{gn1\ O[E]}$ both decrease with increasing T, respectively.

| T ↗ | 20 K | 50 K | 100 K | 300 K |
|---|---|---|---|---|
| **At x=0** | | | | |
| For $\mathbf{r_d} = \mathbf{r_{As}}$, | | | | |
| $\eta_{o[E]} \gg 1$ | 658.1 [506] | 263.2 [202] | 131.6 [101] | 43.85 [34] |
| $E_{gn1\ O[E]}$ in eV | 0.74 [-0.38] | 0.738 [-0.39] | 0.725 [-0.40] | 0.646 [-0.48] |
| $n_{O[E]}$ | 4.99 [5.772] | 4.992 [5.775] | 5.00 [5.782] | 5.06 [5.828] |
| $\kappa_{O[E]}$ | 0.39 [0.2078] | 0.387 [0.2077] | 0.3868 [0.22075] | 0.3825 [0.2063] |
| $\varepsilon_{1O[E]}$ | 24.73 [33.27] | 24.77 [33.30] | 24.87 [33.39] | 25.50 [33.92] |
| $\varepsilon_{2O[E]}$ | 3.8689 [2.3989] | 3.8690 [2.3991] | 3.8694 [2.3996] | 3.874 [2.405] |
| For $\mathbf{r_d} = \mathbf{r_{Sb}}$, | | | | |
| $\eta_{o[E]} \gg 1$ | 658.1 [506] | 263.2 [202] | 131.6 [101] | 43.85 [34] |
| $E_{gn1\ O[E]}$ in eV | 0.81 [-0.31] | 0.805 [-0.32] | 0.793 [-0.33] | 0.713 [-0.41] |
| $n_{O[E]}$ | 4.82 [5.624] | 4.830 [5.627] | 4.840 [5.634] | 4.90 [5.681] |
| $\kappa_{O[E]}$ | 0.3683 [0.1964] | 0.3680 [0.1963] | 0.3673 [0.1961] | 0.3630 [0.1949] |
| $\varepsilon_{1O[E]}$ | 23.16 [31.59] | 23.19 [31.62] | 23.29 [31.71] | 23.91 [32.23] |
| $\varepsilon_{2O[E]}$ | 3.5555 [2.208] | 3.5557 [2.209] | 3.5561 [2.210] | 3.560 [2.214] |
| **At x=0.5** | | | | |
| For $\mathbf{r_d} = \mathbf{r_{As}}$, | | | | |
| $\eta_{o[E]} \gg 1$ | 609.8 [479] | 243.9 [191] | 121.9 [96] | 40.63 [31.95] |
| $E_{gn1\ O[E]}$ in eV | 0.53 [-0.513] | 0.52 [-0.52] | 0.51 [-0.53] | 0.40 [-0.64] |
| $n_{O[E]}$ | 5.23 [5.93] | 5.24 [5.932] | 5.25 [5.94] | 5.33 [6.00] |
| $\kappa_{O[E]}$ | 0.342 [0.1949] | 0.341 [0.1948] | 0.340 [0.1945] | 0.336 [0.1931] |
| $\varepsilon_{1O[E]}$ | 27.28 [35.10] | 27.33 [35.15] | 27.48 [35.27] | 28.30 [35.96] |
| $\varepsilon_{2O[E]}$ | 3.579 [2.3108] | 3.5796 [2.3109] | 3.5801 [2.3114] | 3.585 [2.3174] |
| For $\mathbf{r_d} = \mathbf{r_{Sb}}$, | | | | |
| $\eta_{o[E]} \gg 1$ | 609.7 [479] | 243.9 [192] | 121.9 [95.9] | 40.63 [31.94] |
| $E_{gn1\ O[E]}$ in eV | 0.60 [-0.44] | 0.59 [-0.45] | 0.57 [-0.47] | 0.47 [-0.57] |
| $n_{O[E]}$ | 5.07 [5.77] | 5.075 [5.78] | 5.089 [5.79] | 5.168 [5.85] |
| $\kappa_{O[E]}$ | 0.3245 [0.1841] | 0.3241 [0.1840] | 0.3232 [0.1837] | 0.3188 [0.1823] |
| $\varepsilon_{1O[E]}$ | 25.59 [33.33] | 25.65 [33.38] | 25.79 [33.50] | 26.60 [34.18] |
| $\varepsilon_{2O[E]}$ | 3.2897 [2.1274] | 3.2898 [2.1275] | 3.2902 [2.1280] | 3.2950 [2.1335] |
| **At x=1** | | | | |
| For $\mathbf{r_d} = \mathbf{r_{As}}$, | | | | |

| | | | | |
|---|---|---|---|---|
| $\eta_{o[E]} \gg 1$ | 569.5 [456] | 227.8 [182] | 113.9 [91] | 37.95 [30] |
| $E_{gn1\ O[E]}$ in eV | 0.34 [-0.64] | 0.33 [-0.65] | 0.30 [-0.67] | 0.18 [-0.80] |
| $n_{O[E]}$ | 5.46 [6.07] | 5.47 [6.08] | 5.48 [6.09] | 5.57 [6.16] |
| $\kappa_{O[E]}$ | 0.306 [0.1833] | 0.306 [0.1831] | 0.305 [0.1828] | 0.301 [0.1813] |
| $\varepsilon_{1O[E]}$ | 29.68 [36.89] | 29.76 [36.95] | 29.95 [37.12] | 30.96 [37.94] |
| $\varepsilon_{2O[E]}$ | 3.3461 [2.2277] | 3.3463 [2.2279] | 3.3468 [2.2285] | 3.352 [2.2349] |
| For $\mathbf{r_d = r_{Sb}}$, | | | | |
| $\eta_{o[E]} \gg 1$ | 569.5 [455] | 227.8 [182] | 113.9 [91] | 37.94 [30] |
| $E_{gn1\ O[E]}$ in eV | 0.41 [-0.566] | 0.40 [-0576] | 0.37 [-0.60] | 0.25 [-0.73] |
| $n_{O[E]}$ | 5.29 [5.92] | 5.30 [5.93] | 5.31 [5.94] | 5.41 [6.01] |
| $\kappa_{O[E]}$ | 0.2901 [0.1731] | 0.290 [0.1730] | 0.289 [0.1726] | 0.285 [0.1711] |
| $\varepsilon_{1O[E]}$ | 27.89 [35.03] | 27.97 [35.10] | 28.16 [35.26] | 29.15 [36.09] |
| $\varepsilon_{2O[E]}$ | 3.0752 [2.0507] | 3.0754 [2.0508] | 3.0758 [2.0514] | 3.0811 [2.0572] |
| T ↗ | 20 K | 50 K | 100 K | 300 K |

**Table 7p**. In the X(x)-system, at E=3.2 eV and $N = 10^{20} cm^{-3}$, for given $r_a$ and x, the numerical results of $n_{O[E]}(E)$, $\kappa_{O[E]}(E)$, $\varepsilon_{1O[E]}(E)$ and $\varepsilon_{2O[E]}(E)$, are obtained, as functions of T, by using Equations (17, 19b, 19c and 16), respectively, noting that $\eta_{o[E]}$ and $E_{gp1\ O[E]}$ both decrease with increasing T, respectively.

| T ↗ | 20 K | 50 K | 100 K | 300 K |
|---|---|---|---|---|
| **At x=0** | | | | |
| For $\mathbf{r_d = r_{Mg}}$, | | | | |
| $\eta_{o[E]} \gg 1$ | 654.2 [151.0] | 261.7 [60.37] | 130.8 [30.17] | 43.59 [9.98] |
| $E_{gn1\ O[E]}$ in eV | 1.45 [0.323] | 1.442 [0.319] | 1.43 [0.306] | 1.35 [0.228] |
| $n_{O[E]}$ | 4.38 [5.310] | 4.39 [5.313] | 4.40 [5.322] | 4.47 [5.378] |
| $\kappa_{O[E]}$ | 0.44 [0.027] | 0.44 [0.027] | 0.44 [0.0276] | 0.43 [0.028] |
| $\varepsilon_{1O[E]}$ | 19.03 [28.20] | 19.07 [28.23] | 19.17 [28.33] | 19.82 [28.92] |
| $\varepsilon_{2O[E]}$ | 3.85 [0.293] | 3.85 [0.2933] | 3.85 [0.2941] | 3.85 [0.302] |
| For $\mathbf{r_d = r_{In}}$, | | | | |
| $\eta_{o[E]} \gg 1$ | 654.2 [150.9] | 261.7 [60.37] | 130.8 [30.16] | 43.59 [9.98] |
| $E_{gn1\ O[E]}$ in eV | 1.45 [0.324] | 1.443 [0.319] | 1.43 [0.307] | 1.35 [0.228] |
| $n_{O[E]}$ | 4.38 [5.306] | 4.38 [5.309] | 4.39 [5.318] | 4.47 [5.374] |
| $\kappa_{O[E]}$ | 0.44 [0.027] | 0.44 [0.027] | 0.43 [0.027] | 0.43 [0.028] |
| $\varepsilon_{1O[E]}$ | 19.00 [28.15] | 19.04 [28.19] | 19.14 [28.28] | 19.79 [28.88] |
| $\varepsilon_{2O[E]}$ | 3.84 [0.292] | 3.84 [0.293] | 3.84 [0.293] | 3.84 [0.301] |
| **At x=0.5** | | | | |
| For $\mathbf{r_d = r_{Mg}}$, | | | | |
| $\eta_{o[E]} \gg 1$ | 605.1 [129.2] | 242.0 [51.66] | 121.0 [25.81] | 40.32 [8.51] |
| $E_{gn1\ O[E]}$ in eV | 1.27 [0.234] | 1.26 [0.227] | 1.247 [0.208] | 1.144 [0.105] |
| $n_{O[E]}$ | 4.62 [5.456] | 4.63 [5.461] | 4.648 [5.474] | 4.740 [5.545] |
| $\kappa_{O[E]}$ | 0.3839 [0.022] | 0.3834 [0.0218] | 0.3821 [0.0219] | 0.3753 [0.0224] |
| $\varepsilon_{1O[E]}$ | 21.25 [29.77] | 21.308 [29.826] | 21.463 [29.968] | 22.32 [30.753] |
| $\varepsilon_{2O[E]}$ | 3.55 [0.238] | 3.552 [0.2387] | 3.5525 [0.2395] | 3.5573 [0.2485] |
| For $\mathbf{r_d = r_{In}}$, | | | | |
| $\eta_{o[E]} \gg 1$ | 605.1 [129.2] | 242.0 [51.65] | 121.0 [25.80] | 40.32 [8.51] |
| $E_{gn1\ O[E]}$ in eV | 1.27 [0.234] | 1.266 [0.227] | 1.247 [0.208] | 1.144 [0.105] |
| $n_{O[E]}$ | 4.62 [5.452] | 4.628 [5.457] | 4.644 [5.470] | 4.735 [5.541] |
| $\kappa_{O[E]}$ | 0.3831 [0.022] | 0.3826 [0.0218] | 0.3813 [0.0218] | 0.374 [0.0224] |

| | | | | |
|---|---|---|---|---|
| $\varepsilon_{1O[E]}$ | 21.21 [29.72] | 21.27 [29.781] | 21.425 [29.923] | 22.28 [30.707] |
| $\varepsilon_{2O[E]}$ | 3.54 [0.238] | 3.541 [0.2381] | 3.5420 [0.2389] | 3.547 [0.2480] |
| **At x=1** | | | | |
| For $\mathbf{r_d = r_{Mg}}$, | | | | |
| $\eta_{o[E]} \gg 1$ | 564.3 [112.8] | 225.7 [45.12] | 112.8 [22.53] | 37.60 [7.41] |
| $E_{gn1\ O[E]}$ in eV | 1.11 [0.141] | 1.10 [0.131] | 1.07 [0.107] | 0.947 [-0.021] |
| $n_{O[E]}$ | 4.85 [5.600] | 4.857 [5.607] | 4.878 [5.624] | 4.986 [5.709] |
| $\kappa_{O[E]}$ | 0.3416 [0.01786] | 0.3410 [0.01787] | 0.3395 [0.0179] | 0.3327 [0.0185] |
| $\varepsilon_{1O[E]}$ | 23.39 [31.36] | 23.472 [31.43] | 23.680 [31.63] | 24.75 [32.59] |
| $\varepsilon_{2O[E]}$ | 3.31 [0.200] | 3.312 [0.2004] | 3.3131 [0.2013] | 3.3185 [0.2113] |
| For $\mathbf{r_d = r_{In}}$, | | | | |
| $\eta_{o[E]} \gg 1$ | 564.2 [112.8] | 225.7 [45.12] | 112.8 [22.53] | 37.59 [7.41] |
| $E_{gn1\ O[E]}$ in eV | 1.11 [0.142] | 1.10 [0.132] | 1.076 [0.107] | 0.948 [-0.020] |
| $n_{O[E]}$ | 4.84 [5.596] | 4.852 [5.603] | 4.874 [5.619] | 4.982 [5.705] |
| $\kappa_{O[E]}$ | 0.3409 [0.0178] | 0.3403 [0.01784] | 0.3389 [0.01787] | 0.332 [0.0185] |
| $\varepsilon_{1O[E]}$ | 23.35 [31.31] | 23.43 [31.39] | 23.64 [31.57] | 24.71 [32.546] |
| $\varepsilon_{2O[E]}$ | 3.30 [0.1997] | 3.303 [0.1999] | 3.3032 [0.2009] | 3.309 [0.2108] |
| T ↗ | 20 K | 50 K | 100 K | 300 K |

**Table 8n.** For T=20K and $N = 10^{20} cm^{-3}$, and for given x and $r_d$, the numerical results of $\sigma_{O[E]}$ (E), $\varepsilon_{2O[2E]}$(E) and $\propto_{O[E]}$ (E) , are obtained by using Equations (18, 19c, 19d), noting that, as given in Eq. (15), $E_{gnE} \equiv E_{gn2} + E_{Fn}$ and $E_{gnO} \equiv E_{gn1} + E_{Fn}$.

| E in eV | $\sigma_{O[E]}\ (\frac{10^5}{\Omega \times cm})$ | $\varepsilon_{2O[2E]}$ | $\propto_{O[E]}\ (\frac{10^5}{cm})$ |
|---|---|---|---|
| At x=0 and $r_d = r_{As}$, | | | |
| $\mathbf{-0.3864} = E_{gn2}$ | **… [0]** | **… [0]** | **… [0]** |
| $\mathbf{0.4861} = E_{gnE}$ | **… [1.1952]** | **… [15.78]** | **… [0.7191]** |
| $\mathbf{0.7424} = E_{gn1}$ | **0** [1.1953] | **0** [10.34] | **0** [0.6831] |
| **1.8767** $=E_{gnO}$ | **1.9278** [1.1955] | **6.5953** [4.0902] | **1.21298** [0.4902] |
| 3 | 1.9282 [1.1956] | 4.127 [2.5588] | 1.084 [0.5075] |
| 3.5 | 1.9283 [1.1956] | 3.537 [2.1933] | 1.652 [1.1783] |
| 4 | 1.9283 [1.1956] | 3.095 [1.9192] | 1.555 [1.0200] |
| 4.5 | 1.9284 [1.1956] | 2.751 [1.7059] | 1.369 [0.8158] |
| 5 | 1.9284 [1.1957] | 2.476 [1.5354] | 3.308 [8.8048] |
| 5.5 | 1.9284 [1.1957] | 2.251 [1.3958] | 26.42 [-2.015] |
| 6 | 1.9285 [1.1957] | 2.064 [1.2795] | 11.64 [-3.084] |
| … | | | |
| $\mathbf{10^{22}}$ | **1.9287 [1.1958]** | **0 [0]** | **2.8963 [1.7957]** |
| At x=0 and $r_d = r_{Sb}$, | | | |
| $\mathbf{-0.3188} = E_{gn2}$ | **… [0]** | **… [0]** | **… [0]** |
| $\mathbf{0.5537} = E_{gnE}$ | **… [0.9939]** | **… [12.761]** | **… [0.680]** |
| $\mathbf{0.8096} = E_{gn1}$ | **0** [0.9940] | **0** [8.7287] | **0** [0.6453] |
| **1.9439** $=E_{gnO}$ | **1.59996** [0.9942] | **5.8517** [3.6360] | **1.1444** [0.4564] |
| 2.5 | 1.6002 [0.9942] | 4.551 [2.8273] | 0.922 [0.3569] |
| 3.5 | 1.6004 [0.9942] | 3.251 [2.0196] | 1.559 [1.1049] |
| 4 | 1.6004 [0.9942] | 2.845 [1.7672] | 1.469 [0.9595] |
| 4.5 | 1.6005 [0.9942] | 2.529 [1.5708] | 1.295 [0.7689] |
| 5 | 1.6005 [0.9943] | 2.276 [1.4138] | 3.109 [8.1379] |
| 5.5 | 1.6005 [0.9943] | 2.069 [1.2852] | 24.53 [-1.898] |
| 6 | 1.6005 [0.9943] | 1.896 [1.1781] | 11.11 [-2.880] |
| … | | | |
| $\mathbf{10^{22}}$ | **1.6007 [0.9943]** | **0 [0]** | **2.8010 [1.7399]** |
| At x=0.5 and $r_d = r_{As}$, | | | |
| $\mathbf{-0.5133} = E_{gn2}$ | **… [0]** | **… [0]** | **… [0]** |

| | | | |
|---|---|---|---|
| $\mathbf{0.3133} = E_{gnE}$ | **... [1.2403]** | **... [23.59]** | **... [0.6789]** |
| $\mathbf{0.5323} = E_{gn1}$ | **0** [1.2404] | **0** [13.89] | **0** [0.652] |
| **1.5833** $=E_{gnO}$ | **1.9214**[1.2406] | **7.2323** [4.6699] | **1.1126** [0.4977] |
| 3.5 | 1.9220 [1.2407] | 3.273 [2.1127] | 1.513 [1.1398] |
| 4 | 1.9220 [1.2407] | 2.864 [1.8486] | 1.411 [0.9755] |
| 4.5 | 1.9220 [1.2408] | 2.545 [1.6433] | 1.229 [0.7724] |
| 5 | 1.9221 [1.2408] | 2.291 [1.4789] | 3.301 [11.76] |
| 5.5 | 1.9221 [1.2408] | 2.083 [1.3445] | -219.6 [-1.7511] |
| 6 | 1.9221 [1.2408] | 1.909 [1.2325] | 17.41 [-2.6379] |
| ... | | | |
| $\mathbf{10^{22}}$ | **1.9223 [1.24087]** | **0 [0]** | **2.5816 [1.6665]** |
| At x=0.5 and $r_d = r_{Sb}$, | | | |
| $\mathbf{-0.4438} = E_{gn2}$ | **... [0]** | **... [0]** | **... [0]** |
| $\mathbf{0.3828} = E_{gnE}$ | **... [1.0312]** | **... [17.778]** | **... [0.6027]** |
| $\mathbf{0.6015} = E_{gn1}$ | **0** [1.0313] | **0** [11.315] | **0** [0.6163] |
| **1.6524**$=E_{gnO}$ | **1.5947** [1.0315] | **6.3689** [4.1195] | **1.0515** [0.4650] |
| 3 | 1.5951 [1.0315] | 3.509 [2.2692] | 0.891 [0.4460] |
| 3.5 | 1.5952 [1.0316] | 3.008 [1.9451] | 1.426 [1.0682] |
| 4 | 1.5952 [1.0316] | 2.632 [1.7019] | 1.332 [0.9174] |
| 4.5 | 1.5952 [1.0316] | 2.339 [1.5128] | 1.161 [0.7278] |
| 5 | 1.5953 [1.0316] | 2.105 [1.3616] | 3.098 [10.767] |
| 5.5 | 1.5953 [1.0316] | 1.914 [1.2378] | -250.1 [-1.6498] |
| 6 | 1.5953 [1.0316] | 1.755 [1.1347] | 16.74 [-2.4657] |
| ... | | | |
| $\mathbf{10^{22}}$ | **1.5954 [1.031681]** | **0 [0]** | **2.4967 [1.6144]** |
| At x=1 and and $r_d = r_{As}$, | | | |
| $\mathbf{-0.6377} = E_{gn2}$ | **... [0]** | **... [0]** | **... [0]** |
| $\mathbf{0.1476} = E_{gnE}$ | **... [1.2815]** | **... [48.291]** | **... [0.6437]** |
| $\mathbf{0.3386} = E_{gn1}$ | **0** [1.2816] | **0** [21.048] | **0** [0.6205] |
| **1.3202** $=E_{gnO}$ | **1.9250** [1.2819] | **8.1078** [5.3993] | **1.0242** [0.4951] |
| 3.5 | 1.9256 [1.2820] | 3.059 [2.0368] | 1.407 [1.1066] |
| 4 | 1.9257 [1.2820] | 2.677 [1.7822] | 1.300 [0.9357] |
| 4.5 | 1.9257 [1.2820] | 2.379 [1.5842] | 1.119 [0.7331] |
| 5 | 1.9257 [1.2820] | 2.142 [1.4258] | 3.361 [19.191] |
| 5.5 | 1.9257 [1.2821] | 1.947 [1.2962] | -18.74 [-1.5337] |
| 6 | 1.9258 [1.2821] | 1.785 [1.1882] | 42.40 [-2.2785] |
| ... | | | |
| $\mathbf{10^{22}}$ | **1.9259 [1.282138]** | **0 [0]** | **2.3311 [1.5518]** |
| At x=1 and $r_d = r_{Sb}$, | | | |
| $\mathbf{-0.5665} = E_{gn2}$ | **... [0]** | **... [0]** | **... [0]** |
| $\mathbf{0.2187} = E_{gnE}$ | **... [1.0653]** | **... [29.989]** | **... [0.6074]** |
| $\mathbf{0.4095} = E_{gn1}$ | **0** [1.0654] | **0** [16.020] | **0** [0.5869] |
| **1.3911**$=E_{gnO}$ | **1.5977** [1.0656] | **7.0720** [4.7168] | **0.9691** [0.4639] |
| 4 | 1.5982 [1.0657] | 2.460 [1.6406] | 1.226 [0.8798] |
| 4.5 | 1.5983 [1.0657] | 2.187 [1.4582] | 1.057 [0.6907] |
| 5 | 1.5983 [1.0658] | 1.968 [1.3125] | 3.150 [17.183] |
| 5.5 | 1.5983 [1.0658] | 1.789 [1.1932] | -17.98 [-1.4450] |
| 6 | 1.5983 [1.0659] | 1.640 [1.0937] | 42.05 [-2.1310] |
| ... | | | |
| $\mathbf{10^{22}}$ | **1.59846 [1.065841]** | **0 [0]** | **2.2544 [1.5032]** |

**Table 8p.** For T=20K and $N = 10^{20} cm^{-3}$, and for given x and $r_d$, the numerical results of $\sigma_{O[E]}$ (E), $\varepsilon_{2O[2E]}$(E) and $\propto_{O[E]}$ (E), are obtained by using Equations (18, 19c, 19d), noting that, as given in Eq. (15), $E_{gpE} \equiv E_{gp2} + E_{Fp}$ and $E_{gpO} \equiv E_{gp1} + E_{Fp}$.

| E in eV | $\sigma_{O[E]}$ $(\frac{10^5}{\Omega \times cm})$ | $\varepsilon_{2O[2E]}$ | $\propto_{O[E]}$ $(\frac{10^5}{cm})$ |
|---|---|---|---|
| At x=0 and $r_a = r_{Mg}$, | | | |
| $\mathbf{0.3233} = E_{gp2}$ | **... [0]** | **... [0]** | **... [0]** |
| $\mathbf{0.5835} = E_{gpE}$ | **... [0.1466]** | **... [1.6075]** | **... [0.0796]** |
| $\mathbf{1.4468} = E_{gp1}$ | **0** [0.1466] | **0** [0.6483] | **0** [0.0664] |
| **2.5744** $=E_{gpO}$ | **1.9246** [0.1466] | **4.7834** [0.3643] | **0.9541** [0.0439] |

| | | | |
|---|---|---|---|
| 3 | 1.9246 [0.1466] | 4.105 [0.3127] | 0.986 [0.0548] |
| 3.5 | 1.9246 [0.1466] | 3.518 [0.2842] | 1.230 [0.0772] |
| 4 | 1.9246 [0.1466] | 3.079 [0.2345] | 1.183 [0.0883] |
| 4.5 | 1.9246 [0.1466] | 2.736 [0.2084] | 1.080 [0.0755] |
| 5 | 1.9246 [0.1466] | 2.463 [0.1876] | 1.885 [0.2464] |
| 5.5 | 1.9246 [0.1466] | 2.239 [0.1705] | 3.845 [-0.7456] |
| 6 | 1.9246 [0.1466] | 2.052 [0.1563] | 3.443 [-6.6788] |
| … | | | |
| $\mathbf{10^{22}}$ | **1.9246 [0.1466]** | **0 [0]** | **2.1440 [0.1633]** |
| At x=0 and $r_a = r_{In}$, | | | |
| $\mathbf{0.3237} = E_{gp2}$ | **… [0]** | **… [0]** | **… [0]** |
| $\mathbf{0.5839} = E_{gpE}$ | **… [0.1457]** | **… [1.6027]** | **… [0.0793]** |
| $\mathbf{1.4471} = E_{gp1}$ | **0** [0.1458] | **0** [0.6467] | **0** [0.0661] |
| **2.5747** $=E_{gpO}$ | **1.9124** [0.1458] | **4.7689** [0.3066] | **0.9488** [0.0332] |
| 3.5 | 1.9124 [0.1458] | 3.508 [0.2674] | 1.223 [0.0955] |
| 4 | 1.9124 [0.1458] | 3.070 [0.2340] | 1.176 [0.0879] |
| 4.5 | 1.9124 [0.1458] | 2.728 [0.2080] | 1.074 [0.0752] |
| 5 | 1.9124 [0.1458] | 2.456 [0.1872] | 1.875 [0.2456] |
| 5.5 | 1.9124 [0.1458] | 2.232 [0.1702] | 3.831 [-0.7368] |
| 6 | 1.9124 [0.1458] | 2.046 [0.1560] | 3.430 [-6.2761] |
| … | | | |
| $\mathbf{10^{22}}$ | **1.9124 [0.1458]** | **0 [0]** | **2.1340 [0.1626]** |
| At x=0.5 and $r_a = r_{Mg}$, | | | |
| $\mathbf{0.2339} = E_{gp2}$ | **… [0]** | **… [0]** | **… [0]** |
| $\mathbf{0.4565} = E_{gpE}$ | **… [0.1284]** | **… [1.6710]** | **… [0.0632]** |
| $\mathbf{1.2730} = E_{gp1}$ | **0** [0.1284] | **0** [0.5993] | **0** [0.0539] |
| **2.3160** $=E_{gpO}$ | **1.9137** [0.1284] | **4.9076** [0.3294] | **0.8779** [0.0379] |
| 3.5 | 1.9137 [0.1284] | 3.247 [0.2180] | 1.103 [0.0781] |
| 4 | 1.9137 [0.1284] | 2.841 [0.1907] | 1.071 [0.0534] |
| 4.5 | 1.9137 [0.1284] | 2.526 [0.1695] | 0.960 [0.0602] |
| 5 | 1.9137 [0.1284] | 2.273 [0.1526] | 1.764 [0.2044] |
| 5.5 | 1.9137 [0.1284] | 2.066 [0.1387] | 3.973 [-05153] |
| 6 | 1.9137 [0.1284] | 1.894 [0.1272] | 3.417 [-2.6458] |
| … | | | |
| $\mathbf{10^{22}}$ | **1.9137 [0.1284]** | **0 [0]** | **1.9065 [0.1280]** |
| At x=0.5 and $r_a = r_{In}$, | | | |
| $\mathbf{0.2343} = E_{gp2}$ | **… [0]** | **… [0]** | **… [0]** |
| $\mathbf{0.4569} = E_{gpE}$ | **… [0.1277]** | **… [1.6659]** | **… [0.0629]** |
| $\mathbf{1.2733} = E_{gp1}$ | **0** [0.1277] | **0** [0.5979] | **0** [0.0536] |
| **2.3163** $=E_{gpO}$ | **1.9015** [0.1277] | **4.8926** [0.3287] | **0.8730** [0.0377] |
| 3.5 | 1.9015 [0.1277] | 3.238 [0.2175] | 1.097 [0.0767] |
| 4 | 1.9015 [0.1277] | 2.833 [0.1903] | 1.052 [0.0703] |
| 4.5 | 1.9015 [0.1277] | 2.518 [0.1692] | 0.955 [0.0599] |
| 5 | 1.9015 [0.1277] | 2.266 [0.1522] | 1.755 [0.2038] |
| 5.5 | 1.9015 [0.1277] | 2.060 [0.1384] | 3.961 [-0.5096] |
| 6 | 1.9015 [0.1277] | 1.889 [0.1269] | 3.405 [-2.5545] |
| … | | | |
| $\mathbf{10^{22}}$ | **1.9015 [0.1277]** | **0 [0]** | **1.8976 [0.1275]** |
| At x=1 and $r_a = r_{Mg}$, | | | |
| $\mathbf{0.1414} = E_{gp2}$ | **… [0]** | **… [0]** | **… [0]** |
| $\mathbf{0.3359} = E_{gpE}$ | **… [0.1155]** | **… [1.9066]** | **… [0.0517]** |
| $\mathbf{1.1101} = E_{gp1}$ | **0** [0.1156] | **0** [0.5769] | **0** [0.0449] |
| **2.0827** $=E_{gpO}$ | **1.9128** [0.1156] | **5.0894** [0.3075] | **0.8136** [0.0334] |
| 4 | 1.9128 [0.1156] | 2.650 [0.1601] | 0.960 [0.0584] |
| 4.5 | 1.9128 [0.1156] | 2.355 [0.1423] | 0.867 [0.0495] |
| 5 | 1.9128 [0.1156] | 2.120 [0.1281] | 1.675 [0.1765] |
| 5.5 | 1.9128 [0.1156] | 1.927 [0.1164] | 4.235 [-0.3682] |
| 6 | 1.9128 [0.1156] | 1.767 [0.1067] | 3.462 [-1.3699] |
| … | | | |
| $\mathbf{10^{22}}$ | **1.9128 [0.1156]** | **0 [0]** | **1.7174 [0.1038]** |
| At x=1 and $r_a = r_{In}$, | | | |
| $\mathbf{0.1117} = E_{gp2}$ | **… [0]** | **… [0]** | **… [0]** |

| | | | |
|---|---|---|---|
| $\mathbf{0.3362} = E_{gpE}$ | **... [0.1149]** | **... [1.9004]** | **... [0.0515]** |
| $\mathbf{1.1104} = E_{gp1}$ | **0** [0.1149] | **0** [0.5755] | **0** [0.0447] |
| **2.0829** $=E_{gpO}$ | **1.9005** [0.1149] | **5.0738** [0.3068] | **0.8091** [0.0332] |
| 4 | 1.9005 [0.1149] | 2.642 [0.1598] | 0.955 [0.0581] |
| 4.5 | 1.9005 [0.1149] | 2.348 [0.1420] | 0.862 [0.0493] |
| 5 | 1.9005 [0.1149] | 2.114 [0.1278] | 1.667 [0.1760] |
| 5.5 | 1.9005 [0.1149] | 1.921 [0.1162] | 4.224 [-0.3643] |
| 6 | 1.9005 [0.1149] | 1.761 [0.1065] | 3.451 [-1.3364] |
| … | | | |
| $\mathbf{10^{22}}$ | **1.9005 [0.1149]** | **0 [0]** | **1.7094 [0.1034]** |

**Table 9n:** For given x, $r_d$, and T=(4.2 K and 77 K), the numerical results of $\sigma_{O[E]}$, $\mu_{O[E]}$ and $D_{O[E]}$, expressed respectively in $\left(\frac{10^4}{ohm\times cm}, \frac{10^3\times cm^2}{V\times s}, \frac{10^3\times cm^2}{s}\right)$, and as functions of N, are obtained by using Equations (20a, 22 and 24), suggesting that, for a given N, they decrease [decrease], with increasing $r_d$.

| Donor | As | Sb |
|---|---|---|
| $r_d$ (nm) ↗ | 0.118 | 0.140 |
| For x=0 and at T=4.2 K | | |
| N ($10^{19}$ $cm^{-3}$) | | |
| 3 | 6.221 [3.891], 12.95 [8.102], 4.388 [2.111] | 5.178 [3.248], 10.78 [6.766], 3.653 [1.763] |
| 7 | 13.77 [8.559], 12.28 [7.634], 7.324 [3.501] | 11.44 [7.124], 10.20 [6.355], 6.083 [2.914] |
| 10 | 19.28 [11.95], 12.03 [7.462], 9.101 [4.340] | 16.00 [9.939], 9.990 [6.205], 7.554 [3.609] |
| For x=0.5 and at T=4.2 K | | |
| N ($10^{19}$ $cm^{-3}$) | | |
| 3 | 6.201 [4.035], 12.91 [8.401], 4.053 [2.074] | 5.162 [3.368], 10.75 [7.014], 3.374 [1.731] |
| 7 | 13.73 [8.880], 12.24 [7.920], 6.763 [3.441] | 11.40 [7.390], 10.17 [6.592], 5.618 [2.864] |
| 10 | 19.21 [12.40], 11.99 [7.743], 8.405 [4.267] | 15.95 [10.31], 9.957 [6.438], 6.976 [3.548] |
| For x=1 and at T=4.2 K | | |
| N ($10^{19}$ $cm^{-3}$) | | |
| 3 | 6.212 [4.166], 12.93 [8.675], 3.792 [2.034] | 5.172 [3.477], 10.77 [7.240], 3.157 [1.698] |
| 7 | 13.75 [9.174], 12.27 [8.182], 6.329 [3.377] | 11.42 [7.634], 10.19 [6.809], 5.257 [2.810] |
| 10 | 19.25 [12.81], 12.02 [8.000], 7.865 [4.188] | 15.98 [10.65], 9.975 [6.651], 6.528 [3.482] |
| For x=0 and at T=77 K | | |
| N ($10^{19}$ $cm^{-3}$) | | |
| 3 | 6.663 [4.231], 13.87 [8.809], 4.699 [2.295] | 5.546 [3.532], 11.55 [7.357], 3.912 [1.916] |
| 7 | 14.09 [8.800], 12.57 [7.849], 7.491 [3.599] | 11.70 [7.325], 10.44 [6.534], 6.222 [2.996] |
| 10 | 19.55 [12.16], 12.21 [7.592], 9.230 [4.416] | 16.23 [10.11], 10.13 [6.314], 7.661 [3.672] |
| For x=0.5 and at T=77 K | | |
| N ($10^{19}$ $cm^{-3}$) | | |
| 3 | 6.642 [4.387], 13.83 [9.135], 4.339 [2.254] | 5.529 [3.662], 11.51 [7.627], 3.613 [1.882] |
| 7 | 14.04 [9.130], 12.52 [8.144], 6.918 [3.537] | 11.66 [7.599], 10.40 [6.778], 5.746 [2.944] |
| 10 | 19.49 [12.62], 12.17 [7.879], 8.524 [4.341] | 16.17 [10.49], 10.10 [6.551], 7.075 [3.610] |
| For x=1 and at T=77 K | | |
| N ($10^{19}$ $cm^{-3}$) | | |
| 3 | 6.654 [4.531], 13.85 [9.433], 4.061 [2.211] | 5.540 [3.781], 11.54 [7.874], 3.381 [1.846] |
| 7 | 14.07 [9.433], 12.55 [8.413], 6.474 [3.472] | 11.69 [7.849], 10.42 [7.002], 5.377 [2.889] |
| 10 | 19.55 [13.04], 12.19 [8.141], 7.976 [4.262] | 16.20 [10.84], 10.12 [6.768], 6.620 [3.543] |

**Table 9p:** For given x, $r_a$, and T=(4.2 K and 77 K), the numerical results of $\sigma_{O[E]}$, $\mu_{O[E]}$ and $D_{O[E]}$, expressed respectively in $\left(\frac{10^4}{ohm\times cm}, \frac{10^4\times cm^2}{V\times s}, \frac{10^3\times cm^2}{s}\right)$, and as functions of N, are obtained by using Equations (20a, 22 and 24), suggesting that, for a given N, they decrease [decrease] with increasing $r_a$.

| Acceptor | Mg | In |
|---|---|---|
| $r_a$ (nm) ↗ | 0.140 | 0.144 |
| For x=0 and at T=4.2 K | | |
| N ($10^{19}$ $cm^{-3}$) | | |

| | | |
|---|---|---|
| 3 | 6.089 [0.509], 1.306 [0.109], 4.338 [0.084] | 6.049 [0.506], 1.298 [0.108], 4.310 [0.083] |
| 5 | 9.937 [0.795], 1.263 [0.101], 5.946 [0.110] | 9.873 [0.791], 1.255 [0.100], 5.910 [0.109] |
| 10 | 19.24 [1.466], 1.212 [0.092], 9.112 [0.160] | 19.12 [1.457], 1.204 [0.091], 9.054 [0.159] |
| For x=0.5 and at T=4.2 K | | |
| N ($10^{19}$ $cm^{-3}$) | | |
| 3 | 6.021 [0.447], 1.303 [0.097], 3.986 [0.063] | 5.982 [0.445], 1.295 [0.096], 3.960 [0.062] |
| 5 | 9.857 [0.698], 1.260 [0.089], 5.475 [0.083] | 9.794 [0.695], 1.252 [0.088], 5.440 [0.082] |
| 10 | 19.13 [1.284], 1.208 [0.081], 8.402 [0.120] | 19.01 [1.277], 1.201 [0.080], 8.349 [0.119] |
| For x=1 and at T=4.2 K | | |
| N ($10^{19}$ $cm^{-3}$) | | |
| 3 | 5.984 [0.403], 1.306 [0.088], 3.710 [0.050] | 5.944 [0.401], 1.298 [0.087], 3.686 [0.049] |
| 5 | 9.829 [0.630], 1.262 [0.081], 5.107 [0.065] | 9.765 [0.626], 1.254 [0.080], 4.616 [0.064] |
| 10 | 19.13 [1.155], 1.211 [0.073], 7.850 [0.095] | 19.00 [1.149], 1.203 [0.072], 7.800 [0.094] |
| For x=0 and at T=77 K | | |
| N ($10^{19}$ $cm^{-3}$) | | |
| 3 | 6.095 [0.519], 1.308 [0.111], 4.341 [0.085] | 6.056 [0.516], 1.300 [0.110], 4.314 [0.084] |
| 5 | 9.942 [0.803], 1.264 [0.102], 5.949 [0.111] | 9.878 [0.798], 1.256 [0.101], 5.911 [0.110] |
| 10 | 19.25 [1.471], 1.212 [0.093], 9.114 [0.160] | 19.12 [1.463], 1.205 [0.092], 9.056 [0.159] |
| For x=0.5 and at T=77 K | | |
| N ($10^{19}$ $cm^{-3}$) | | |
| 3 | 6.028 [0.459], 1.304 [0.099], 3.990 [0.0645] | 5.989 [0.457], 1.296 [0.098], 3.964 [0.0642] |
| 5 | 9.863 [0.708], 1.260 [0.090], 5.477 [0.084] | 9.800 [0.704], 1.252 [0.089], 5.442 [0.083] |
| 10 | 19.14 [1.291], 1.208 [0.0815], 8.404 [0.121] | 19.02 [1.283], 1.201 [0.0810], 8.350 [0.120] |
| For x=1 and at T=77 K | | |
| N ($10^{19}$ $cm^{-3}$) | | |
| 3 | 5.992 [0.418], 1.308 [0.0911], 3.715 [0.0514] | 5.953 [0.415], 1.300 [0.0907], 3.691 [0.0511] |
| 5 | 9.836 [0.640], 1.263 [0.082], 5.110 [0.066] | 9.772 [0.637], 1.255 [0.0818], 5.077 [0.065] |
| 10 | 19.13 [1.163], 1.211 [0.0736], 7.852 [0.095] | 19.01 [1.156], 1.203 [0.0732], 7.802 [0.094] |

**Table 10n:** For given x, $r_d$, T=(3K and 80K) and N, the numerical results of various thermoelectric coefficients: $\sigma_{Th.O[E]}$, $S_{O[E]}$, $VC1_{O[E]}$, $VC2_{O[E]}$, $Ts_{O[E]}$, $Pt_{O[E]}$ and $ZT_{O[E]}$, are obtained by using Equations (21, 25, 27, 28, 29, 30 and 26), respectively. Further, their variations with increasing $r_d$ are represented by the arrows: ↗ (increase), and ↘ (decrease).

| Donor | P | **As** | Sb |
|---|---|---|---|
| For **x=0** and **N=$3.233\times10^{18}$ cm$^{-3}$**, | | | |
| $\xi_{n(T=3K)}$ ↘ | 443.221 [340.940] | 443.085 [340.836] | 442.266 [340.206] |
| $\xi_{n(T=80K)}$ ↘ | 16.695 [12.883] | 16.690 [12.879] | 16.660 [12.856] |
| $\sigma_{Th.O[E]]\,(3K)}$ $(\frac{10^{-4}\times W}{cm\times K})$ ↘ | 6.051 [3.891] | 5.842 [3.760] | 4.902 [3.173] |
| $\sigma_{Th.O[E]]\,(80K)}$ $(\frac{10^{-1}\times W}{cm\times K})$ ↘ | 0.574 [0.341] | 0.555 [0.330] | 0.467 [0.256] |
| $-S_{O[E]\,(3K)}$ $(\frac{10^{-6}\times V}{K})$ ↘ | 1.279 [1.663] | 1.280 [1.664] | 1.282 [1.666] |
| $-S_{O[E]\,(80K)}$ $(\frac{10^{-5}\times V}{K})$ ↘ | 3.356 [4.315] | 3.357 [4.316] | 3.363 [4.324] |
| $-VC1_{O[E]\,(3K)}$ $(\frac{10^{-7}\times V}{K})$ ↘ | 8.528 [11.08] | 8.530 [11.09] | 8.546 [11.11] |
| $-VC1_{O[E]\,(80K)}$ $\left(\frac{10^{-5}\times V}{K}\right)$ ↘ | 2.165 [2.722] | 2.166 [2.723] | 2.170 [2.727] |
| $-VC2_{O[E]\,(3K)}$ $(\frac{10^{-6}\times V}{K})$ ↘ | 2.558 [3.325] | 2.559 [3.326] | 2.564 [3.333] |
| $-VC2_{O[E]\,(80K)}$ $\left(\frac{10^{-3}\times V}{K}\right)$ ↘ | 1.732 [2.178] | 1.733 [2.179] | 1.736 [2.182] |
| $-Ts_{O[E]\,(3K)}$ $(\frac{10^{-6}\times V}{K})$ ↘ | 1.279 [1.662] | 1.280 [1.663] | 1.282 [1.666] |
| $-Ts_{O[E]\,(80K)}$ $\left(\frac{10^{-5}\times V}{K}\right)$ ↘ | 3.248 [4.083] | 3.249 [4.084] | 3.255 [4.091] |
| $-Pt_{O[E]\,(3K)}(10^{-6}\times V)$ ↘ | 3.837 [4.998] | 3.838 [4.999] | 3.846 [5.000] |
| $-Pt_{O[E]\,(80K)}(10^{-3}\times V)$ ↘ | 2.685 [3.452] | 2.686 [3.453] | 2.691 [3.459] |

| | | | | |
|---|---|---|---|---|
| $ZT_{O[E]\,(3K)}\ (10^{-5})$ | ↗ | 6.698 [11.32] | 6.702 [11.327] | 6.727 [11.369] |
| $ZT_{O[E]\,(80K)}(10^{-2})$ | ↗ | 4.611 [7.623] | 4.614 [7.628] | 4.631 [7.656] |
| For **x=0.5** and **N=$3.6294 \times 10^{18}$ cm$^{-3}$**, one has: | | | | |
| $\xi_{n(T=3K)}$ | ↘ | 443.931 [349.160] | 443.817 [349.071] | 443.131 [348.531] |
| $\xi_{n(T=80K)}$ | ↘ | 16.722 [13.189] | 16.718 [13.185] | 16.692 [13.165] |
| $\sigma_{Th.O[E]]\,(3K)}\ (\frac{10^{-4}\times W}{cm\times K})$ | ↘ | 6.705 [4.465] | 6.472 [4.314] | 5.430 [3.637] |
| $\sigma_{Th.O[E]]\,(80K)}\ (\frac{10^{-1}\times W}{cm\times K})$ | ↘ | 0.428 [0.324] | 0.413 [0.313] | 0.347 [0.265] |
| $-S_{O[E]\,(3K)}\ (\frac{10^{-6}\times V}{K})$ | ↘ | 1.277 [1.624] | 1.278 [1.625] | 1.279 [1.627] |
| $-S_{O[E]\,(80K)}\ (\frac{10^{-5}\times V}{K})$ | ↘ | 3.351 [4.219] | 3.352 [4.220] | 3.357 [4.226] |
| $-VC1_{O[E]\,(3K)}\ (\frac{10^{-7}\times V}{K})$ | ↘ | 8.514 [10.82] | 8.516 [10.83] | 8.532 [10.84] |
| $-VC1_{O[E]\,(80K)}\ \left(\frac{10^{-5}\times V}{K}\right)$ | ↘ | 2.162 [2.668] | 2.163 [2.669] | 2.166 [2.673] |
| $-VC2_{O[E]\,(3K)}\ (\frac{10^{-6}\times V}{K})$ | ↘ | 2.554 [3.247] | 2.555 [3.248] | 2.559 [3.253] |
| $-VC2_{O[E]\,(80K)}\ \left(\frac{10^{-3}\times V}{K}\right)$ | ↘ | 1.730 [2.134] | 1.731 [2.135] | 1.733 [2.138] |
| $-Ts_{O[E]\,(3K)}\ (\frac{10^{-6}\times V}{K})$ | ↘ | 1.277 [1.623] | 1.278 [1.624] | 1.279 [1.627] |
| $-Ts_{O[E]\,(80K)}\ \left(\frac{10^{-5}\times V}{K}\right)$ | ↘ | 3.244 [4.002] | 3.245 [4.003] | 3.249 [4.009] |
| $-Pt_{O[E]\,(3K)}(10^{-6}\times V)$ | ↘ | 3.831 [4.871] | 3.832 [4.872] | 3.838 [4.880] |
| $-Pt_{O[E]\,(80K)}(10^{-3}\times V)$ | ↘ | 2.681 [3.375] | 2.682 [3.376] | 2.686 [3.381] |
| $ZT_{O[E]\,(3K)}\ (10^{-5})$ | ↗ | 6.677 [10.79] | 6.681 [10.80] | 6.701 [10.83] |
| $ZT_{O[E]\,(80K)}(10^{-2})$ | ↗ | 4.597 [7.286] | 4.599 [7.290] | 4.613 [7.312] |
| For **x=1** and **N=$4.0078 \times 10^{18}$ cm$^{-3}$**, one has: | | | | |
| $\xi_{n(T=3K)}$ | ↘ | 443.222 [354.579] | 443.125 [354.501] | 442.538 [354.031] |
| $\xi_{n(T=80K)}$ | ↘ | 16.696 [13.391] | 16.692 [13.388] | 16.670 [13.370] |
| $\sigma_{Th.O[E]]\,(3K)}\ (\frac{10^{-4}\times W}{cm\times K})$ | ↘ | 7.354 [5.031] | 7.098 [4.860] | 5.953 [4.094] |
| $\sigma_{Th.O[E]]\,(80K)}\ (\frac{10^{-1}\times W}{cm\times K})$ | ↘ | 0.436 [0.336] | 0.420 [0.325] | 0.353 [0.274] |
| $-S_{O[E]\,(3K)}\ (\frac{10^{-6}\times V}{K})$ | ↘ | 1.279 [1.599] | 1.280 [1.5994] | 1.281 [1.601] |
| $-S_{O[E]\,(80K)}\ (\frac{10^{-5}\times V}{K})$ | ↘ | 3.356 [4.158] | 3.357 [4.159] | 3.361 [4.164] |
| $-VC1_{O[E]\,(3K)}\ (\frac{10^{-7}\times V}{K})$ | ↘ | 8.528 [10.659] | 8.530 [10.66] | 8.541 [10.67] |
| $-VC1_{O[E]\,(80K)}\ \left(\frac{10^{-5}\times V}{K}\right)$ | ↘ | 2.166 [2.634] | 2.167 [2.635] | 2.169 [2.637] |
| $-VC2_{O[E]\,(3K)}\ (\frac{10^{-6}\times V}{K})$ | ↘ | 2.558 [3.198] | 2.559 [3.1985] | 2.562 [3.203] |
| $-VC2_{O[E]\,(80K)}\ \left(\frac{10^{-3}\times V}{K}\right)$ | ↘ | 1.732 [2.107] | 1.733 [2.108] | 1.735 [2.110] |
| $-Ts_{O[E]\,(3K)}\ (\frac{10^{-6}\times V}{K})$ | ↘ | 1.279 [1.599] | 1.280 [1.5992] | 1.281 [1.601] |
| $-Ts_{O[E]\,(80K)}\ \left(\frac{10^{-5}\times V}{K}\right)$ | ↘ | 3.248 [3.951] | 3.249 [3.952] | 3.253 [3.956] |
| $-Pt_{O[E]\,(3K)}(10^{-6}\times V)$ | ↘ | 3.838 [4.797] | 3.839 [4.798] | 3.844 [4.804] |
| $-Pt_{O[E]\,(80K)}(10^{-3}\times V)$ | ↘ | 2.685 [3.326] | 2.686 [3.327] | 2.689 [3.331] |
| $ZT_{O[E]\,(3K)}\ (10^{-5})$ | ↗ | 6.698 [10.46] | 6.701 [10.47] | 6.719 [10.50] |
| $ZT_{O[E]\,(80K)}(10^{-2})$ | ↗ | 4.611 [7.077] | 4.613 [7.080] | 4.625 [7.098] |

**Table 10p:** For given x, $r_a$, T=(3K and 80K) and N, the numerical results of various thermoelectric coefficients: $\sigma_{Th.O[E]}$, $S_{O[E]}$, $VC1_{O[E]}$, $VC2_{O[E]}$, $Ts_{O[E]}$, $Pt_{O[E]}$ and $ZT_{O[E]}$, are obtained by using Equations (21, 25, 27, 28, 29, 30 and 26), respectively. Further, their variations with increasing $r_a$ are represented by the arrows: ↗ (increase), and ↘ (decrease.

| Acceptor | | Ga | Mg | In |
|---|---|---|---|---|
| **For x=0** and **N=$2.4 \times 10^{19}$ cm$^{-3}$** one has: | | | | |
| $\xi_{n(T=3K)}$ | ↘ | 1659.6 [382.991] | 1651.7 [381.157] | 1651.2 [381.054] |

| | | | | |
|---|---|---|---|---|
| $\xi_{n(T=80K)}$ | ↘ | 62.255 [14.449] | 61.957 [14.380] | 61.941 [14.377] |
| $\sigma_{Th.O[E]]\,(3K)}\ (\frac{10^{-3}\times W}{cm\times K})$ | ↘ | 4.089 [0.342] | 3.598 [0.307] | 3.574 [0.305] |
| $\sigma_{Th.O[E]]\,(80K)}\ (\frac{10^{-2}\times W}{cm\times K})$ | ↘ | 10.920 [0.939] | 9.608 [0.842] | 9.546 [0.837] |
| $-S_{O[E]\,(3K)}\ (\frac{10^{-7}\times V}{K})$ | ↘ | 3.416 [14.804] | 3.432 [14.875] | 3.434 [14.879] |
| $-S_{O[E]\,(80K)}\ (\frac{10^{-6}\times V}{K})$ | ↘ | 9.100 [38.632] | 9.143 [38.810] | 9.146 [38.820] |
| $-VC1_{O[E]\,(3K)}\ (\frac{10^{-7}\times V}{K})$ | ↘ | 2.277 [9.869] | 2.288 [9.916] | 2.289 [9.919] |
| $-VC1_{O[E]\,(80K)}\ \left(\frac{10^{-6}\times V}{K}\right)$ | ↘ | 6.052 [24.652] | 6.081 [24.755] | 6.083 [24.761] |
| $-VC2_{O[E]\,(3K)}\ (\frac{10^{-7}\times V}{K})$ | ↘ | 6.833 [29.606] | 6.865 [29.748] | 6.867 [29.757] |
| $-VC2_{O[E]\,(80K)}\ \left(\frac{10^{-4}\times V}{K}\right)$ | ↘ | 4.842 [19.722] | 4.865 [19.804] | 4.866 [19.809] |
| $-Ts_{O[E]\,(3K)}\ (\frac{10^{-7}\times V}{K})$ | ↘ | 3.416 [14.803] | 3.432 [14.874] | 3.434 [14.878] |
| $-Ts_{O[E]\,(80K)}\ \left(\frac{10^{-6}\times V}{K}\right)$ | ↘ | 9.078 [36.979] | 9.121 [37.133] | 9.124 [37.142] |
| $-Pt_{O[E]\,(3K)}(10^{-6}\times V)$ | ↘ | 1.025 [4.441] | 1.029 [4.462] | 1.030 [4.464] |
| $-Pt_{O[E]\,(80K)}(10^{-4}\times V)$ | ↘ | 7.280 [30.906] | 7.314 [31.048] | 7.317 [31.056] |
| $ZT_{O[E]\,(3K)}\ (10^{-6})$ | ↗ | 4.778 [89.710] | 4.823 [90.575] | 4.826 [90.625] |
| $ZT_{O[E]\,(80K)}(10^{-3})$ | ↗ | 3.389 [61.092] | 3.422 [61.656] | 3.424 [61.688] |
| **For x=0.5** and **N=$\mathbf{2.702\times 10^{19}}$ cm$^{-3}$** one has: | | | | |
| $\xi_{n(T=3K)}$ | ↘ | 1659.6 [354.300] | 1650.6 [352.378] | 1650.1 [352.269] |
| $\xi_{n(T=80K)}$ | ↘ | 62.255 [13.380] | 61.917 [13.309] | 61.898 [13.305] |
| $\sigma_{Th.O[E]]\,(3K)}\ (\frac{10^{-3}\times W}{cm\times K})$ | ↘ | 4.535 [0.334] | 3.986 [0.299] | 3.960 [0.298] |
| $\sigma_{Th.O[E]]\,(80K)}\ (\frac{10^{-2}\times W}{cm\times K})$ | ↘ | 12.112 [0.919] | 10.645 [0.825] | 10.575 [0.820] |
| $-S_{O[E]\,(3K)}\ (\frac{10^{-7}\times V}{K})$ | ↘ | 3.416 [16.003] | 3.435 [16.090] | 3.436 [16.095] |
| $-S_{O[E]\,(80K)}\ (\frac{10^{-6}\times V}{K})$ | ↘ | 9.100 [41.611] | 9.149 [41.826] | 9.152 [41.839] |
| $-VC1_{O[E]\,(3K)}\ (\frac{10^{-7}\times V}{K})$ | ↘ | 2.277 [10.668] | 2.290 [10.726] | 2.291 [10.729] |
| $-VC1_{O[E]\,(80K)}\ \left(\frac{10^{-6}\times V}{K}\right)$ | ↘ | 6.052 [26.358] | 6.085 [26.480] | 6.087 [26.487] |
| $-VC2_{O[E]\,(3K)}\ (\frac{10^{-7}\times V}{K})$ | ↘ | 6.833 [32.003] | 6.870 [32.177] | 6.872 [32.188] |
| $-VC2_{O[E]\,(80K)}\ \left(\frac{10^{-4}\times V}{K}\right)$ | ↘ | 4.842 [21.087] | 4.868 [21.184] | 4.870 [21.190] |
| $-Ts_{O[E]\,(3K)}\ (\frac{10^{-7}\times V}{K})$ | ↘ | 3.416 [16.002] | 3.435[16.089] | 3.436 [16.094] |
| $-Ts_{O[E]\,(80K)}\ \left(\frac{10^{-6}\times V}{K}\right)$ | ↘ | 9.078 [39.538] | 9.127 [39.720] | 9.131 [39.731] |
| $-Pt_{O[E]\,(3K)}(10^{-6}\times V)$ | ↘ | 1.025 [4.801] | 1.030 [4.827] | 1.031 [4.828] |
| $-Pt_{O[E]\,(80K)}(10^{-4}\times V)$ | ↘ | 7.280 [33.288] | 7.319 [33.461] | 7.322 [33.471] |
| $ZT_{O[E]\,(3K)}\ (10^{-6})$ | ↗ | 4.778 [104.82] | 4.830 [105.97] | 4.833 [106.04] |
| $ZT_{O[E]\,(80K)}(10^{-3})$ | ↗ | 3.389 [70.875] | 3.426 [71.612] | 3.429 [71.654] |
| **For x=1** and **N=$\mathbf{3.0034\times 10^{19}}$ cm$^{-3}$**, one has: | | | | |
| $\xi_{n(T=3K)}$ | ↘ | 1659.6 [331.928] | 1649.8 [329.957] | 1649.2 [329.846] |
| $\xi_{n(T=80K)}$ | ↘ | 62.256 [12.548] | 61.886 [12.474] | 61.865 [12.470] |
| $\sigma_{Th.O[E]]\,(3K)}\ (\frac{10^{-3}\times W}{cm\times K})$ | ↘ | 5.000 [0.330] | 4.391 [0.296] | 4.361 [0.294] |
| $\sigma_{Th.O[E]]\,(80K)}\ (\frac{10^{-2}\times W}{cm\times K})$ | ↘ | 13.354 [0.913] | 11.726 [0.819] | 11.65 [0.815] |
| $-S_{O[E]\,(3K)}\ (\frac{10^{-7}\times V}{K})$ | ↘ | 3.416 [17.081] | 3.436 [17.183] | 3.438 [17.189] |
| $-S_{O[E]\,(80K)}\ (\frac{10^{-6}\times V}{K})$ | ↘ | 9.0997 [44.262] | 9.154 [44.511] | 9.157 [44.525] |
| $-VC1_{O[E]\,(3K)}\ (\frac{10^{-7}\times V}{K})$ | ↘ | 2.277 [11.386] | 2.291 [11.454] | 2.292 [11.458] |
| $-VC1_{O[E]\,(80K)}\ \left(\frac{10^{-6}\times V}{K}\right)$ | ↘ | 6.052 [27.840] | 6.088 [27.977] | 6.090 [27.985] |
| $-VC2_{O[E]\,(3K)}\ (\frac{10^{-7}\times V}{K})$ | ↘ | 6.833 [34.16] | 6.873 [34.36] | 6.876 [34.37] |

| | | | | |
|---|---|---|---|---|
| $-VC2_{O[E]\,(80K)}\left(\frac{10^{-4}\times V}{K}\right)$ | ↘ | 4.842 [22.272] | 4.870 [22.381] | 4.872 [22.388] |
| $-Ts_{O[E]\,(3K)}\left(\frac{10^{-7}\times V}{K}\right)$ | ↘ | 3.416 [17.080] | 3.436 [17.181] | 3.438 [17.188] |
| $-Ts_{O[E]\,(80K)}\left(\frac{10^{-6}\times V}{K}\right)$ | ↘ | 9.078 [41.760] | 9.132 [41.966] | 9.135 [41.978] |
| $-Pt_{O[E]\,(3K)}(10^{-6}\times V)$ | ↘ | 1.025 [5.124] | 1.0310 [5.155] | 1.0314 [5.157] |
| $-Pt_{O[E]\,(80K)}(10^{-4}\times V)$ | ↘ | 7.280 [35.409] | 7.323 [35.609] | 7.326 [35.620] |
| $ZT_{O[E]\,(3K)}\,(10^{-6})$ | ↗ | 4.778 [119.43] | 4.835 [120.86] | 4.838 [120.94] |
| $ZT_{O[E]\,(80K)}(10^{-3})$ | ↗ | 3.389 [80.194] | 3.430 [81.100] | 3.432 [81.152] |

**Table 11:** Here, in the O-EP [E-OP] and for given physical conditions: x, $r_{d(a)}$, N (or T), the same values of $\xi_{n(p)}$ decrease, according to the increasing T (or to the decreasing N), and other thermoelectric coefficients are in variations, as indicated by the arrows as: (increase: ↗, decrease: ↘). One notes here that (i) for $\xi_{n(p)} \simeq 1.8138$, while the numerical results of $S_{O[E]}$ present a same minimum $S_{O[E]\,min.}\left(\simeq -1.563\times 10^{-4}\,\frac{V}{K}\right)$, those of $ZT_{O[E]}$ show a same maximum $ZT_{O[E]\,max.} = 1$, (ii) for $\xi_p = 1$, those of $S_{O[E]}$, $ZT_{O[E]}$, $ZT_{O[E]Mott}$, $VC1_{E[O]}$, and $Ts_{O[E]}$ 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 $\xi_p \simeq 1.8138$, $(ZT)_{O[E]\,Mott} = 1$.

| | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| $\xi_{n(p)}$ | ↘ | 1.880 [1.880] | | **1.8138 [1.8138]** | | 1.750 [1.750] | | **1 [1]** | | 0.998 [0.998] |
| $S_{O[E]}\left(10^{-4}\,\frac{V}{K}\right)$ | | −1.562 [−1.562] | ↘ | **−1.563** [**−1.563**] | ↗ | −1.562 [−1.562] | ↗ | **−1.322** [**−1.322**] | ↗ | −1.320 [−1.320] |
| $ZT_{O[E]}$ | | 0.999 [0.999] | ↗ | **1** [1] | ↘ | 0.999 [0.999] | ↘ | **0.715** [**0.715**] | ↘ | 0.713 [0.713] |
| $(ZT)_{O[E]\,Mott}$ | ↗ | 0.931 [0.931] | | **1** [1] | | 1.074 [1.074] | | **3.290 [3.290]** | | 3.306 [3.306] |
| $VC1_{E[O]}\left(10^{-4}\,\frac{V}{K}\right)$ | | −0.061[−0.061] | ↗ | 0 [0] | ↗ | 0.063 [0.063] | ↗ | **1.105 [1.105]** | ↗ | 1.109 [1.109] |
| $Ts_{O[E]}\left(10^{-4}\,\frac{V}{K}\right)$ | | −0.092 [−0.092] | ↗ | 0 [0] | ↗ | 0.094 [0.094] | ↗ | **1.657 [1.657]** | ↗ | 1.663 [1.663] |