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OPTICAL COEFFICIENTS IN THE N(P)-TYPE DEGENERATE GaAs(1-x) Sb(x)-CRYSTALLINE ALLOY, DUE TO THE NEW STATIC DIELECTRIC CONSTANT-LAW AND THE GENERALIZED MOTT CRITERIUM IN THE METAL-INSULATOR TRANSITION. (2)

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ABTRACT

In the n(p)-type $GaAs_{1-x}Sb_{x^{-}}$ crystalline alloy, with $0 \le x \le 1$, basing on our two recent works^[1,2], for a given x, and with an increasing $\mathbf{r}_{d(a)}$, the optical coefficients have been determined, as functions of the photon energy E, total impurity density N, the donor (acceptor) radius $\mathbf{r}_{d(a)}$, concentration x, and temperature T. Those results have been affected by (i) the important new $\varepsilon(\mathbf{r}_{d(a)}, \mathbf{x})$ -law, developed in Equations (8a, 8b), stating that, for a given x, due to the impurity-size effect, ε decreases (Σ) with an increasing (Σ) $\mathbf{r}_{d(a)}$, and then by (ii) the generalized Mott critical d(a)-density defined in the metal-insulator transition (MIT), $\mathbf{N}_{CDn(NDp)}(\mathbf{r}_{d(a)}, \mathbf{x})$, as observed in Equations (8c, 9a).

Furthermore, we also showed that $^{N_{CDn(NDp)}}$ is just the density of carriers localized in exponential band tails, with a precision of the order of 2.9×10^{-7} , as that given in Table 4 of Ref.^[1], according to a definition of the effective density of electrons (holes) given in parabolic conduction (valence) bands by: $N^*(N, r_{d(a)}, x) \equiv N - N_{CDn(NDp)}(r_{d(a)}, x)$, as defined in Eq. (9d). In summary, due to the new $^{*(r_{d(a)}, x)}$ -law and to the effective density of electrons (holes) given in parabolic conduction (valence) bands $^{N^*(N, r_{d(a)}, x)}$, for a given x, and with an increasing $r_{d(a)}$, the numerical results of all the optical coefficients, obtained in appropriated physical conditions (E, N, T), and calculated by using Equations (15, 16, 20,

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21), are reported in Tables 1, 2, 3n, 3p, 4n, 4p, 5n, and 5p in Appendix 1.

KEYWORS: GaAs_{1-x}Sb_x- crystalline alloy; impurity-size effect; Mott critical impurity density in the MIT, optical coefficients.

INTRODUCTION

Here, basing on our two recent works^[1,2] and also other ones^[3-8], all the optical coefficients given in the n(p)-type $X(x) \equiv GaAs_{1-x}Sb_x$ - crystalline alloy, with $0 \le x \le 1$, are investigated, as functions of the photon energy E, total impurity density N, the donor (acceptor) radius $r_{d(a)}$, concentration x, and temperature T.

Then, for a given x, and with an increasing $\mathbf{r}_{d(a)}$, the numerical results of all the optical coefficients, obtained in appropriated physical conditions (E, N, T), and calculated by using Equations (15, 16, 20, 21), are reported in Tables 1, 2, 3n, 3p, 4n, 4p, 5n, and 5p in Appendix 1.

ENERGY BAND STUCTURE PARAMETERS

First of all, in the $n^+(p^+) - p(n) X(x)$ - crystalline alloy at T=0 K, we denote the donor (acceptor) d(a)- radius by $r_{d(a)}$, and also the intrinsic one by: $r_{do(ao)} = r_{As(Ga)} = 0.118$ nm (0.126 nm).

A. Effect of x- concentration

Here, the intrinsic energy-band-structure parameters^[1], are expressed as functions of x, are given in the following.

(i)-The unperturbed relative effective electron (hole) mass in conduction (valence) bands are given by:

$$m_{c(v)}(x)/m_o = 0.047(0.3) \times x + 0.066(0.291) \times (1-x)$$
 (1)

(ii)-The unperturbed relative static dielectric constant of the intrinsic of the single crystalline X- alloy is found to be defined by:

$$\varepsilon_{o}(x) = 15.69 \times x + 13.13 \times (1 - x).$$
 (2)

(iii)-Finally, the unperturbed band gap at 0 K is found to be given by:

$$E_{go}(x) = 0.81 \times x + 1.52 \times (1 - x).$$
 (3)

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

$$E_{do(ao)}(x) = \frac{13600 \times [m_{c(v)}(x)/m_0]}{[\epsilon_0(x)]^2} \text{ meV},$$
 (4)

and then, the isothermal bulk modulus, by:

$$B_{do(ao)}(x) \equiv \frac{E_{do(ao)}(x)}{\left(\frac{4\pi}{s}\right) \times \left(r_{do(ao)}\right)^{s}}.$$
 (5)

B. Effect of Impurity $r_{d(a)}$ -size, with a given x

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

At $r_{d(a)} = r_{do(ao)}$, the needed boundary conditions are found to be, for the impurity-atom volume $V = (4\pi/3) \times (r_{d(a)})^3$, $V_{do(ao)} = (4\pi/3) \times (r_{do(ao)})^3$, for the pressure p, $p_o = 0$, and for the deformation potential energy (or the strain energy) σ , $\sigma_o = 0$. Further, the two important equations^[1,7], used to determine the σ -variation, $\Delta \sigma \equiv \sigma - \sigma_o = \sigma$, are defined by: $\frac{dp}{dv} = \frac{B}{v}$ and $p = \frac{d\sigma}{dv}$. giving: $\frac{d\sigma}{dv} = \frac{B}{v}$. Then, by an integration, one gets:

$$\left[\Delta\sigma(r_{d(a)},x)\right]_{n(p)} = B_{do(ao)}(x) \times (V - V_{do(ao)}) \times \ln\left(\frac{V}{V_{do(ao)}}\right) = E_{do(ao)}(x) \times \left[\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^2 - 1\right] \times \ln\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^2 \ge 0. \tag{6}$$

Furthermore, we also shown 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: $\pm \left[\Delta\sigma(r_{d(a)},x)\right]_{n(p)}$,

$$\begin{split} & E_{gno(gpo)}(r_{d(a)},x) - E_{go}(x) = E_{d(a)}(r_{d(a)},x) - E_{do(ao)}(x) = E_{do(ao)}(x) \times \left[\left(\frac{\epsilon_{o}(x)}{\epsilon(r_{d(a)})} \right)^2 - 1 \right] = + \left[\Delta \sigma(r_{d(a)},x) \right]_{n(p)}, \\ & \text{for } r_{d(a)} \geq r_{do(ao)}, \text{ and for } r_{d(a)} \leq r_{do(ao)}, \\ & E_{gno(gpo)}(r_{d(a)},x) - E_{go}(x) = E_{d(a)}(r_{d(a)},x) - E_{do(ao)}(x) = E_{do(ao)}(x) \times \left[\left(\frac{\epsilon_{o}(x)}{\epsilon(r_{d(a)})} \right)^2 - 1 \right] = - \left[\Delta \sigma(r_{d(a)},x) \right]_{n(p)}. \end{split}$$

Therefore, from Equations (6) and (7), one obtains the expressions for relative dielectric constant $\varepsilon(\mathbf{r}_{d(a)},\mathbf{x})$ and energy band gap $\mathbf{E}_{\mathsf{gn}(\mathsf{gp})}(\mathbf{r}_{d(a)},\mathbf{x})$, as:

$$\text{(i)-for } r_{d(a)} \geq r_{do(ao)}, \text{ since } \epsilon(r_{d(a)}\textbf{,}\textbf{x}) = \sqrt{1 + \left[\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^s - 1\right] \times \ln\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^s} \\ \leq \epsilon_0(\textbf{x}), \text{ being a new } \epsilon(r_{d(a)}\textbf{,}\textbf{x}) - law,$$

$$E_{gno(gpo)} \big(r_{d(a)'} x \big) - E_{go}(x) = E_{d(a)} \big(r_{d(a)'} x \big) - E_{do(ao)}(x) = E_{do(ao)}(x) \\ \times \left[\Big(\frac{r_{d(a)}}{r_{do(ao)}} \Big)^3 - 1 \right] \\ \times \ln \Big(\frac{r_{d(a)}}{r_{do(ao)}} \Big)^3 \\ \geq 0, \\ (8a)^{\frac{1}{2}} \left(\frac{r_{d(a)}}{r_{do(ao)}} \right)^3 \\ = 0,$$

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

 $\text{(ii)-for } r_{d(a)} \leq r_{do(ao)} \text{, since } \epsilon (r_{d(a)} \textbf{,} \textbf{x}) = \sqrt{1 - \left[\left(\frac{r_{d(a)}}{r_{do(ao)}} \right)^s - 1 \right] \times \ln \left(\frac{r_{d(a)}}{r_{do(ao)}} \right)^s} \\ \geq \epsilon_o(\textbf{x}), \text{ with a condition,}$ given by:

$$\begin{split} &\left[\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 - 1\right] \times \ln\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 < 1, \text{ being a new } \mathbf{E}(\mathbf{r_{d(a)}}, \mathbf{x})\text{-law}, \\ & E_{gno(gpo)}(r_{d(a)}, \mathbf{x}) - E_{go}(\mathbf{x}) = E_{d(a)}(r_{d(a)}, \mathbf{x}) - E_{do(ao)}(\mathbf{x}) = -E_{do(ao)}(\mathbf{x}) \times \left[\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 - 1\right] \times \ln\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^2 \leq 0. \end{split} \tag{8b}$$

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

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

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

$$N_{\text{CDn}(\text{CDp})}(r_{d(a)},x)^{1/3} \times a_{\text{Bn}(\text{Bp})}(r_{d(a)},x) = M_{n(p)}, M_{n(p)} = 0.25,$$
 depending thus on our **new** $\varepsilon(r_{d(a)},x)$ -law. (9a)

This excellent one can be explained from the definition of the reduced effective Wigner-Seitz (WS) radius $^{\Gamma_{gn}(gp)}$, characteristic of interactions, by:

$$r_{\text{sn}\,(\text{sp})}\big(N, r_{\text{d(a)}}, x\big) \equiv \left(\frac{3}{4\pi N}\right)^{1/3} \times \frac{1}{a_{\text{Bn}\,(\text{Bp})}(r_{\text{d(a)}}, x)} = 1.1723 \times 10^8 \times \left(\frac{1}{N}\right)^{1/3} \times \frac{m_{\text{c(v)}}(x)/m_{\text{o}}}{\epsilon(r_{\text{d(a)}}, x)}, \tag{9b}$$

being equal to, in particular, at $N=N_{CDn(CDp)}(r_{d(a)},x)$: $r_{sn(sp)}(N_{CDn(CDp)}(r_{d(a)},x),r_{d(a)},x)=$ **2.4814**, for any $(r_{d(a)},x)$ -values. So, from Eq. (9b), one also has:

$$N_{CDn(CDp)}(r_{d(a)},x)^{1/3} \times a_{Bn(Bp)}(r_{d(a)},x) = \left(\frac{3}{4\pi}\right)^{\frac{1}{3}} \times \frac{1}{24814} = 0.25 = (WS)_{n(p)} = M_{n(p)}. \tag{9c}$$

Thus, the above Equations (9a, 9b, 9c) confirm our new $\varepsilon(\mathbf{r}_{d(a)},\mathbf{x})$ -law, given in Equations (8a, 8b). Furthermore, by using $\mathbf{M}_{\mathbf{n}(\mathbf{p})} = \mathbf{0.25}$, according to the empirical Heisenberg parameter $\mathbf{\mathcal{H}}_{\mathbf{n}(\mathbf{p})} = \mathbf{0.47137}$, as those given in Equations (8, 15) of the Ref. [1], we have also showed that $\mathbf{N}_{CDn(CDp)}$ is just the density of electrons (holes) localized in the exponential conduction (valence)-band tail, with a precision of the order of $\mathbf{2.9} \times \mathbf{10}^{-7}$. Therefore, the

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

$$N^*(N, r_{d(a)}, x) \equiv N - N_{CDn(NDp)}(r_{d(a)}, x).$$
 (9d)

C. Effect of temperature T, with given x and $\mathbf{r}_{d(a)}$

Here, the intrinsic band $gap^{\mathbb{E}_{gni(gpi)}(\mathbf{r}_{d(a)}, X, T)}$ at any T is given by:

$$\begin{split} E_{gni(gpi)}(r_{d(a)},x,T) \text{ in eV} &= E_{gno(gpo)}(r_{d(a)},x) - 10^{-4} \times T^2 \times \left\{ \frac{7.205 \times x}{T+94\,\text{K}} + \frac{5.405 \times (1-x)}{T+204\,\text{K}} \right\}, \\ \text{suggesting that, for given x and } r_{d(a)}, E_{gni(gpi)} \text{ decreases with an increasing } T. \end{split} \tag{10}$$

Then, in the following, for the study of optical phenomena, one denote the conduction (valence)-band density of states by $N_{c(v)}(T,x)$ as:

$$N_{c(v)}(T,x) = 2 \times g_{c(v)}(x) \times \left(\frac{m_T(x) \times k_B T}{2\pi \hbar^2}\right)^{\frac{3}{2}} (cm^{-3}), g_v(x) \equiv 1 \times x + 1 \times (1-x) = 1,$$
 (11)

where $m_r(x)/m_a$ is the reduced effective mass $m_r(x)/m_a$, defined by :

$$m_r(x) \equiv [m_c(x) \times m_v(x)]/[m_c(x) + m_v(x)].$$

D. Heavy Doping Effect, with given T, x and $r_{d(a)}$

Here, as given in our previous works^[1,2], the Fermi energy $E_{Fn}(-E_{Fp})$, and the band gap narrowing are reported in the following.

First, the reduced Fermi energy $\eta_{n(p)}$ or the Fermi energy $E_{Fn}(-E_{Fp})$, obtained for any T and any effective d(a)-density, $N^*(N,r_{d(a)},x)=N^*$, defined in Eq. (9d), for a simplicity of presentation, being investigated in our previous paper^[8], with a precision of the order of 2.11×10^{-4} , is found to be given by:

$$\eta_{n(p)}(u) \equiv \frac{E_{Fn}(u)}{k_BT}(\frac{-E_{Fp}(u)}{k_BT}) = \frac{G(u) + Au^BF(u)}{1 + Au^B}, \ A = 0.0005372 \ \text{and} \ B = 4.82842262, \eqno(12)$$

where u is the reduced electron density, $u(N, r_{d(a)}, x, T) \equiv \frac{N^a}{N_{C(b)}(T, x)}$, $F(u) = au^{\frac{a}{a}} \left(1 + bu^{-\frac{a}{a}} + cu^{-\frac{a}{a}}\right)^{-\frac{a}{a}}$.

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

 $d=2^{3/2}\left[\frac{1}{\sqrt{27}}-\frac{8}{16}\right]>0$. Therefore, from Eq. (12), the Fermi energies are expressed as functions of variables: $N_r r_{d(a)} x$, and T.

Here, one notes that: (i) as $u \gg 1$, according to the HD [d(a)-X(x)- alloy] ER-case, or to the degenerate case, Eq. (12) is reduced to the function F(u), and in particular at T=0 and as

 $N^*=0$, according to the metal- insulator transition (MIT), one has: $+E_{Fn}(-E_{Fp})=\frac{\hbar^2}{2\times m_r(x)}\times (3\pi^2N^*)^{2/3}=0, \text{ and (ii)}$

 $\frac{E_{Fn}(u\ll 1)}{k_BT}(\frac{-E_{Fp}(u\ll 1)}{k_BT})\ll -1$, to the LD [a(d)- X(x)- alloy] BR-case, or to the non-degenerate case, Eq. (12) is reduced to the function G(u), noting that the notations: **HD(LD)** and **ER(BR)** denote the heavily doped (lightly doped)-cases and emitter (base)-regions, respectively.

Now, in Eq. (9b), in which one replaces $m_{c(v)}(x)$ by $m_r(x)$, the effective Wigner-Seitz radius becomes as:

$$r_{sn(sp)}(N, r_{d(a)}, x) = 1.1723 \times 10^8 \times \left(\frac{g_{c(v)}(x)}{N^*}\right)^{1/3} \times \frac{m_r(x)}{g(r_{d(a)}, x)},$$
 (13a)

the correlation energy of an effective electron gas, $E_{cn(cp)}(N,r_{d(a)},x)$, is given as:

$$E_{\rm cn(cp)}\big({\rm N,r_{d(a)},x}\big) = \frac{-0.87553}{0.0908 + {\rm r_{sn(sp)}}} + \frac{\frac{0.87558}{0.0908 + {\rm r_{sn(sp)}}} + \left(\frac{2[1 - \ln(2)]}{\pi^2}\right) \times \ln({\rm r_{sn(sp)}}) - 0.093288}{1 + 0.03847728 \times {\rm r_{sn(sp)}^{1.67878876}}} \ . \tag{13b}$$

Then, taking into account various spin-polarized chemical potential-energy contributions such as: exchange energy of an effective electron (hole) gas, majority-carrier correlation energy of an effective electron (hole) gas, minority hole (electron) correlation energy, majority electron (hole)-ionized d(a) interaction screened Coulomb potential energy, and finally minority hole (electron)-ionized d(a) interaction screened Coulomb potential energy, the band gap narrowings are given in the following.

In the n-type HD X(x)- alloy, the BGN is found to be given by:

$$\begin{split} \Delta E_{gn}(N,r_d,x) &\simeq a_1 \times \frac{\epsilon_0(x)}{\epsilon(r_d,x)} \times N_r^{1/3} + a_2 \times \frac{\epsilon_0(x)}{\epsilon(r_d,x)} \times N_r^{\frac{1}{8}} \times (2.503 \times [-E_{cn}(r_{gn}) \times r_{sn}]) + a_3 \times \left[\frac{\epsilon_0(x)}{\epsilon(r_d,x)}\right]^{5/4} \times \\ \sqrt{\frac{m_v}{m_r}} \times N_r^{1/4} + a_4 \times \sqrt{\frac{\epsilon_0(x)}{\epsilon(r_d,x)}} \times N_r^{1/2} \times 2 + a_5 \times \left[\frac{\epsilon_0(x)}{\epsilon(r_d,x)}\right]^{\frac{8}{8}} \times N_r^{\frac{1}{6}} \\ , N_r &\equiv \left(\frac{N^*}{N_{CDm}(r_{d,x})}\right). \end{split} \tag{14n}$$

where
$$a_1 = 3.8 \times 10^{-3} (eV)$$
, $a_2 = 6.5 \times 10^{-4} (eV)$, $a_3 = 2.8 \times 10^{-3} (eV)$, $a_4 = 5.597 \times 10^{-3} (eV)$ and $a_5 = 8.1 \times 10^{-4} (eV)$, and in the p-type HD X(x)- alloy, as:

$$\begin{split} \Delta E_{gp}(N,r_{a},x) &\simeq a_{1} \times \frac{\epsilon_{0}(x)}{\epsilon(r_{B}x)} \times N_{r}^{1/3} + a_{2} \times \frac{\epsilon_{0}(x)}{\epsilon(r_{B}x)} \times N_{r}^{\frac{1}{2}} \times \left(2.503 \times \left[-E_{cp}(r_{sp}) \times r_{sp}\right]\right) + a_{3} \times \left[\frac{\epsilon_{0}(x)}{\epsilon(r_{B}x)}\right]^{5/4} \times \\ \sqrt{\frac{m_{c}}{m_{r}}} \times N_{r}^{1/4} + 2a_{4} \times \sqrt{\frac{\epsilon_{0}(x)}{\epsilon(r_{B}x)}} \times N_{r}^{1/2} + a_{5} \times \left[\frac{\epsilon_{0}(x)}{\epsilon(r_{B}x)}\right]^{\frac{1}{2}} \times N_{r}^{\frac{1}{2}} \\ N_{r} &\equiv \left(\frac{N^{*}}{N_{CDp}(r_{B}x)}\right), \end{split} \tag{14p}$$

where
$$a_1 = 3.15 \times 10^{-3} (eV)$$
, $a_2 = 5.41 \times 10^{-4} (eV)$, $a_3 = 2.32 \times 10^{-3} (eV)$, $a_4 = 4.12 \times 10^{-3} (eV)$ and $a_5 = 9.8 \times 10^{-5} (eV)$.

One also remarks that, as $N^*=0$, according to the MIT, $\Delta E_{gn(gp)}(N, r_{d(a)}, x)=0$.

OPTICAL BAND GAP

Here, the optical band gap is found to be defined by:

$$E_{gn1(gp1)}(N, r_{d(a)}, x, T) \equiv E_{gni(gpi)}(r_{d(a)}, x, T) - \Delta E_{gn(gp)}(N, r_{d(a)}, x) + (-)E_{Fn(Fp)}(N, r_{d(a)}, x, T), \quad (15)$$

where $E_{gin(gip)}$, $[+E_{Fn}, -E_{Fp}] \ge 0$, and $\Delta E_{gn(gp)}$ are respectively determined in Equations [10, 12, 14n(p)], respectively. So, as noted above, at the MIT, Eq. (15) thus becomes: $E_{gn1(gp1)}(r_{d(a)},x) = E_{gn0(gp0)}(r_{d(a)},x)$, according to: $N = N_{CDn(NDp)}(r_{d(a)},x)$.

OPTICAL COEFFICIENTS

The optical properties of any medium can be described by the complex refraction index \mathbb{N} and the complex dielectric function $\mathbf{\epsilon}$, $\mathbb{N} \equiv \mathbf{n} - i \mathbf{\kappa}$ and $\mathbf{\epsilon} \equiv \mathbf{\epsilon}_1 - i \mathbf{\epsilon}_2$, where $i^2 = -1$ and $\mathbf{\epsilon} \equiv \mathbb{N}^2$. Therefore, the real and imaginary parts of $\mathbf{\epsilon}$ denoted by $\mathbf{\epsilon}_1$ and $\mathbf{\epsilon}_2$ can thus be expressed in terms of the refraction index \mathbf{n} and the extinction coefficient $\mathbf{\kappa}$ as: $\mathbf{\epsilon}_1 \equiv \mathbf{n}^2 - \mathbf{\kappa}^2$ and $\mathbf{\epsilon}_2 \equiv 2 \mathbf{n} \mathbf{\kappa}$. One notes that the optical absorption coefficient $\mathbf{\alpha}$ is related to $\mathbf{\epsilon}_2$, \mathbf{n} , $\mathbf{\kappa}$, and the optical conductivity $\mathbf{\sigma}_0$, by [2]

$$\alpha(E,N,r_{d(a)},x,T) \equiv \frac{\hbar q^2 \times |v(E)|^2}{n(E) \times \epsilon_{\texttt{measurece}} \times cE} \times J(E^*) = \frac{\epsilon \times \epsilon_2(E)}{\hbar cn(E)} \equiv \frac{\epsilon E \times \kappa(E)}{\epsilon_n(E) \times \epsilon_{\texttt{measurece}}} \equiv \frac{4\pi \sigma_O(E)}{\epsilon_n(E) \times \epsilon_{\texttt{measurece}}} \; , \; \epsilon_1 \equiv n^2 - \kappa^2 \; \text{ and } \; \epsilon_2 \equiv 2n\kappa, \quad (16)$$

where, since $E \equiv \hbar \omega$ is the photon energy, the effective photon energy: $E^* = E - E_{gn1(gp1)}(N, r_{d(a)}, x, T)$ is thus defined as the reduced photon energy.

Here, -q, \hbar , $|\mathbf{v}(E)|$, ω , $\epsilon_{free\,space}$, \mathbf{c} and $J(E^*)$ respectively represent: the electron charge, Dirac's constant, matrix elements of the velocity operator between valence (conduction)-and-conduction (valence) bands in n(p)-type semiconductors, photon frequency, permittivity of free space, velocity of light, and joint density of states. It should be noted that, if the three functions such as: $|\mathbf{v}(E)|^2$, $J(E^*)$ and n(E) are known, then the other optical dispersion functions as those given in Eq. (16) can thus be determined. Moreover, the normal-incidence reflectance, R(E), can be expressed in terms of $\kappa(E)$ and n(E) as:

$$R(E, N, r_{d(a)}, x, T) = \frac{[n(E)-1]^2 + \kappa(E)^2}{[n(E)+1]^2 + \kappa(E)^2}.$$
(17)

From Equations (16, 17), if the two optical functions, ε_1 and ε_2 , (or **n** and κ), are both known, the other ones defined above can thus be determined, noting also that:

 $\mathbf{E}_{\mathbf{gn1}(\mathbf{gp1})}(\mathbf{N}, \mathbf{r}_{\mathbf{d(a)}}, \mathbf{x}, \mathbf{T}) = \mathbf{E}_{\mathbf{gn1}(\mathbf{gp1})}$, for a presentation simplicity.

Then, one has: -at low values of $E \gtrsim E_{gn1(gp1)}$,

$$J_{n(p)}\big(\text{E},\text{N},\text{r}_{\text{d(a)}},\text{x},\text{T}\big) = \frac{1}{2\pi^2} \times \left(\frac{2m_r}{\hbar^2}\right)^{3/2} \times \frac{(\text{E}-\text{E}_{\text{gn1}(\text{gp1})})^{a-(1/2)}}{\text{E}_{\text{gn1}(\text{gpi})}^{a-1}} = \frac{1}{2\pi^2} \times \left(\frac{2m_r}{\hbar^2}\right)^{3/2} \times (\text{E}-\text{E}_{\text{gn1}(\text{gp1})})^{1/2}, \text{ for a=1, } (18)$$

and at large values of $E > E_{gn1(gp1)}$,

$$J_{n(p)}\left(\text{E},\text{N},r_{d(a)},\text{x},\text{T}\right) = \frac{1}{2\pi^2} \times \left(\frac{2m_r}{\hbar^2}\right)^{3/2} \times \frac{\left(\text{E}-\text{E}_{gn1}(gp1)\right)^{a-(1/2)}}{\text{E}_{gni}^{a-1}(gpi)} = \frac{1}{2\pi^2} \times \left(\frac{2m_r}{\hbar^2}\right)^{3/2} \times \frac{\left(\text{E}-\text{E}_{gn1}(gp1)\right)^2}{\text{E}_{gni}^{3/2}(gpi)}^{3/2} \\ \text{a=5/2}. \tag{19}$$

Further, one notes that, as $E \to \infty$, Forouhi and Bloomer (FB)^[4] claimed that $\kappa(E \to \infty) \to a$ constant, while the $\kappa(E)$ -expressions, proposed by Van Cong^[2] quickly go to 0 as E^{-3} , and consequently, their numerical results of the optical functions such as: $\sigma_0(E)$ and $\alpha(E)$, given in Eq. (16), both go to 0 as E^{-2} .

Now, an improved Forouhi-Bloomer parameterization model (FB-PM), used to determine the expressions of the optical coefficients in the degenerate $\mathbf{n^+(p^+)} - \mathbf{p(n)} \, \mathbf{X(x)}$ - crystalline alloy, is now proposed as follows. Then, if denoting the functions G(E) and F(E) and by: $G(E) \equiv \sum_{i=1}^4 \frac{A_i}{\mathbf{E^2} - \mathbf{B_i E + C_i}} \text{ and } F(E) \equiv \sum_{i=1}^4 \frac{A_i}{\mathbf{E^2} \times (1+10^{-4} \times \mathbf{E}) - \mathbf{B_i E + C_i}}, \text{ we propose:}$

$$\kappa(E, N, r_{d(a)}, x, T) = G(E) \times E_{gni(gpi)}^{3/2} \times (E^* \equiv E - E_{gn1(gp1)})^{1/2}, \text{ for } E_{gni(gpi)} \le E \le 2.3 \text{ eV},$$

 $= F(E) \times (E^* \equiv E - E_{gn1(gp1)})^2, \text{ for } E \ge 2.3 \text{ eV},$ (20)

being equal to 0 for $E^*=0$ (or for $E=E_{gn1(gp1)}$), and also going to 0 as E^{-1} as $E\to\infty$, and further, $n(E,N,r_{d(a)},x,T)=n_{\infty}(r_{d(a)},x)+\sum_{i=1}^4\frac{x_i(E_{gn1(gp1)})\times E+y_i(E_{gn1(gp1)})}{E^2-B_iE+C_i}$ 21) going to a constant as $E\to\infty$, since $n(E\to\infty,r_{d(a)},x)\to n_{\infty}(r_{d(a)},x)=\sqrt{\epsilon(r_{d(a)},x)}\times\frac{\omega_T}{\omega_L}$, $\omega_L=8.9755\times 10^{13}~s^{-1}$ [5] and $\omega_L=8.9755\times 10^{13}~s^{-1}$.

Here, the other parameters are determined by: $X_i \left(E_{\texttt{gn1(gp1)}} \right) = \frac{A_i}{O_i} \times \left[-\frac{B_i^2}{2} + E_{\texttt{gn1(gp1)}} B_i - E_{\texttt{gn1(gp1)}}^2 + C_i \right],$

$$\begin{split} Y_i \Big(E_{\texttt{gn1}(\texttt{gp1})} \Big) &= \frac{A_i}{Q_i} \times \left[\frac{B_i \times (E_{\texttt{gn1}(\texttt{gp1})}^2 + C_i)}{2} - 2 E_{\texttt{gn1}(\texttt{gp1})} C_i \right], \quad Q_i = \frac{\sqrt{4 C_i - B_i^2}}{2}, \\ \text{for} & i = (1, \qquad 2, \qquad 3, \qquad \text{and} \qquad 4), \end{split}$$

 $A_i = 1.154 \times A_{i(FB)} = 4.7314 \times 10^{-4}$, 0.2314, 0.1118 and 0.0116

$$B_i \equiv B_{i(FB)} = 5.871, 6.154, 9.679$$
 and 13.232, and $C_i \equiv C_{i(FB)} = 8.619, 9.784, 23.803, and 44.119.$

Then, as noted above, if the two optical functions, \mathbf{n} and \mathbf{k} , are both known, the other ones defined in Equations (16, 17) can also be determined.

NUMERICAL RESULTS

Now, some numerical results of those optical functions are investigated in the n(p)-type $X(x) \equiv GaAs_{1-x}Sb_x$ crystalline alloy, as follows.

A. Metal-insulator transition (MIT)-case

As discussed above, the physical conditions used for the MIT are found to be given by: T=0K, $N^*=0$ or $N=N_{\mathtt{CDn}(\mathtt{CDp})}$, giving rise to: $E_{\mathtt{gn1}(\mathtt{gp1})}(N^*=0,r_{\mathtt{d(a)}},x,T=0)=E_{\mathtt{gn1}(\mathtt{gp1})}(r_{\mathtt{d(a)}},x)=E_{\mathtt{gno}(\mathtt{gpo})}(r_{\mathtt{d(a)}},x)$.

Then, in this MIT-case, if $E = E_{gn1(gp1)}(r_{d(a)},x) = E_{gno(gpo)}(r_{d(a)},x)$, which can be defined as the critical photon energy: $E \equiv E_{CPE}(r_{d(a)},x)$, one obtains: $\kappa_{MIT}(r_{d(a)},x) = 0$ from Eq. (20), and from Eq. (16): $\epsilon_{2(MIT)}(r_{d(a)},x) = 0$, $\sigma_{O(MIT)}(r_{d(a)},x) = 0$ and $\alpha_{MIT}(r_{d(a)},x) = 0$, and the other functions such as: $n_{MIT}(r_{d(a)},x)$ from Eq. (21), and $\epsilon_{1(MIT)}(r_{d(a)},x)$ and $R_{MIT}(r_{d(a)},x)$ from Eq. (16) decrease with increasing $r_{d(a)}$ and E_{CPE} , as those investigated in Table 1 in Appendix 1.

B. Optical coefficients, obtained as $E \rightarrow \infty$

In Eq. (21), at any T, the choice of the real refraction index:

 $n(E \to \infty, \mathbf{r}_{d(\mathbf{a})}, x, T) = n_{\infty}(\mathbf{r}_{d(\mathbf{a})}, x) = \sqrt{\varepsilon(\mathbf{r}_{d(\mathbf{a})}, x)} \times \frac{\omega_T}{\omega_L}$ $\omega_T = 5.1 \times 10^{13} \text{ s}^{-1[5]}$ and $\omega_L = 8.9755 \times 10^{13} \text{ s}^{-1}$, was obtained from the Lyddane-Sachs-Teller relation^[5], from which T(L) represent the transverse (longitudinal) optical phonon modes. Then, from Equations (16, 17, 20), from such the asymptotic behavior $(E \to \infty)$, we obtain: $\kappa_{\infty}(\mathbf{r}_{d(\mathbf{a})}, x) \to 0$ and $\varepsilon_{2,\infty}(\mathbf{r}_{d(\mathbf{a})}, x) \to 0$, as E^{-1} , so that $\varepsilon_{1,\infty}(\mathbf{r}_{d(\mathbf{a})}, x)$, $\sigma_{0,\infty}(\mathbf{r}_{d(\mathbf{a})}, x)$, $\sigma_{\infty}(\mathbf{r}_{d(\mathbf{a})}, x)$ and $\sigma_{\infty}(\mathbf{r}_{d(\mathbf{a})}, x)$ go to their appropriate limiting constants, as those investigated in Table 2 in Appendix 1.

C. Variations of some optical coefficients, obtained in P(B)-X(x)-system, as functions of E

In the P(B)-X(x)-system, at T=0K and N = $N_{CDn(CDp)}(r_{P(B)}, x)$, our numerical results of n, κ , ε_1 and ε_2 are obtained from Equations (21, 20, 16), respectively, and expressed as functions of $E [\geq E_{CPE}(r_{d(a)}, x)]$ and for given x, as those reported in Tables 3n and 3p in Appendix 1.

D. Variations of various optical coefficients, as functions of N

In the X(x)-system, at E=3.2 eV and T=20 K, for given $\mathbf{r}_{d(a)}$ and x, and from Equations (12, 15, 21, 20, 16), respectively, we can determine the variations of $\eta_{n(p)}(\gg 1$, degenerate case), $\mathbf{E}_{gn1(gp1)}$, n, κ , ε_1 and ε_2 , obtained as functions of N, being represented by the arrows: \nearrow and \searrow , as those tabulated in Tables 4n and 4p in Appendix 1.

E. Variations of various optical coefficients as functions of T

In the X(x)-system, at E=3.2 eV and N = 10^{20} cm⁻³, for given $r_{d(a)}$ and x, and from Equations (12, 15, 21, 20, 16), respectively, we can determine the variations of $\eta_{n(p)}(\gg 1$, degenerate case), $E_{gn1(gp1)}$, n, κ , ε_1 and ε_2 , obtained as functions of T, being represented by the arrows: \nearrow and \searrow , as those tabulated in Tables 5n and 5p in Appendix 1.

CONCLUDING REMARKS

In the n(p)-type $X(x) \equiv GaAs_{1-x}Sb_x$ - crystalline alloy, by basing on our two recent works^[1,2], for a given x, and with an increasing $\mathbf{r}_{d(a)}$, the optical coefficients have been determined, as functions of the photon energy E, total impurity density N, the donor (acceptor) radius $\mathbf{r}_{d(a)}$, concentration x, and temperature T. Those results have been affected by (i) the important new $\mathbf{\epsilon}(\mathbf{r}_{d(a)},\mathbf{x})$ -law, developed in Equations (8a, 8b), stating that, for a given x, due to the impurity-size effect, $\mathbf{\epsilon}$ decreases (\mathbf{k}) with an increasing (\mathbf{k}) $\mathbf{r}_{d(a)}$, and then by (ii) the generalized Mott critical d(a)-density defined in the metal-insulator transition (MIT), $\mathbf{N}_{CDn(NDp)}(\mathbf{r}_{d(a)},\mathbf{x})$, as observed in Equations (8c, 9a).

Further, we also showed that $N_{CDn(NDp)}$ is just the density of carriers localized in exponential band tails, with a precision of the order of 2.9×10^{-7} , as that given in Table 4 of Ref.^[1], according to a definition of the effective density of electrons (holes) given inparabolic conduction (valence) bands by: $N^*(N, r_{d(a)}, x) \equiv N - N_{CDn(NDp)}(r_{d(a)}, x)$, as defined in Eq. (9d).

In summary, due to the new $\varepsilon(\mathbf{r_{d(a)}}, \mathbf{x})$ -law and to the effective density of electrons (holes) given in parabolic conduction (valence) bands $\mathbf{N^*}(\mathbf{N}, \mathbf{r_{d(a)}}, \mathbf{x})$, for a given x, and with an increasing $\mathbf{r_{d(a)}}$, the numerical results of all the optical coefficients, obtained in appropriated physical conditions (E, N, T), and calculated by using Equations (15, 16, 20, 21), are reported in Tables 1, 2, 3n, 3p, 4n, 4p, 5n, and 5p in Appendix 1.

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APPENDIX 1

Table 1: In the MIT-case, T=0K, $N=N_{CDn(p)}(r_{d(a)},x)$, and the critical photon energy $E_{CPE}=E=E_{gno(gpo)}(r_{d(a)},x)$, if $E=E_{gn1(gp1)}(r_{d(a)},x)=E_{CPE}(r_{d(a)},x)$, the numerical results of optical functions such as: $n_{MIT}(r_{d(a)},x)$, obtained from Eq. (21), and those of other ones: $\epsilon_{1(MIT)}(r_{d(a)},x)$ and $R_{MIT}(r_{d(a)},x)$, from Eq. (16decrease (1) with increasing (2) $r_{d(a)}$

Donor		P	As	Te	Sb	Sn	
r _d (nm) [4]	7	0.110	0.118	0.132	0.136	0.140	
At x=0 ,							
E _{CPE} in meV	7	1519.8	1520	1520.7	1521.2	1521.8	
n _{MIT}	\sqrt	3.437	3.416	3.352	3.313	3.268	
$\varepsilon_{1(MIT)}$	7	11.81	11.67	11.23	10.98	10.68	
R_{MIT}	\searrow	0.302	0.299	0.292	0.288	0.282	
At x=0.5 ,							
$E_{\text{CPE}}\mathrm{in}\;\mathrm{meV}$	7	1664.8	1665	1665.5	1665.8	1666.3	
n _{MIT}	7	3.446	3.424	3.356	3.316	3.269	
$\varepsilon_{1(MIT)}$	7	11.87	11.72	11.27	10.99	10.69	
R _{MIT}	7	0.303	0.300	0.292	0.288	0.282	
At x=1 ,							
$E_{\text{CPE}}\mathrm{in}\;\mathrm{meV}$	7	1809.9	1810	1810.3	1810	.6 1810.9	
n _{MIT}	7	3.450	3.427	3.357	3.315	3.266	
$\varepsilon_{1(MIT)}$	7	11.90	11.74	11.27	10.99	9 10.67	
R_{MIT}	7	0.303	0.300	0.293	0.288	8 0.282	
Acceptor		В	Ga	Mg	In	Cd	
r _a (nm)	7	0.088	0.126	0.140	0.144	0.148	
At x=0 ,							
E _{CPE} in meV	7	1503.7	1520	1523	1524	1527	
n _{MIT}	~	4.173	3.416	3.358	3.323	3.281	
$\varepsilon_{1(MIT)}$	~	17.41	11.67	11.27	6 11.04	10.77	
R_{MIT}	7	0.376	0.299	0.293	0.289	9 0.284	

At $x=0.5$,						
E _{CPE} in me	V Z	1651	1665	1667	1669	1671
n _{MIT}	7	4.215	3.424	3.363	3.326	3.283
$\varepsilon_{1(MIT)}$	7	17.76	11.72	11.31	11.06	10.78
R_{MIT}	7	0.380	0.300	0.293	0.289	0.284
At x=1 ,						
E _{CPE} in meV	7	1798	1810	1812	1813	1815
n _{MIT}	7	4.251	3.427	3.364	3.326	3.281
$\varepsilon_{1(MIT)}$	7	18.07	11.74	11.32	11.06	10.77
R_{MIT}	7	0.383	0.300	0.293	0.289	0.284

Table 2: Here, as $E \to \infty$, the numerical results of $n_{\infty}(r_{d(a)},x)$, $\mathcal{E}_{1,\infty}(r_{d(a)},x)$, $\sigma_{0,\infty}(r_{d(a)},x)$, $\sigma_{0,\infty}(r_{d(a)},x)$, $\sigma_{0,\infty}(r_{d(a)},x)$ and $\sigma_{\infty}(r_{d(a)},x)$ go to their appropriate limiting constants.

Donor	P	As	Te	Sb	Sn	
At x =0,						
n_{∞}	2.08	2.0589	1.9950	1.9566	1.9124	
ε _{1,∞} \	4.327	4.2392	3.9800	3.8284	3.6571	
$\sigma_{O,\infty} \text{ in } \frac{10^2}{\Omega \times cm}$	9.4915	9.3951	9.1033	8.9282	8.7263	
oc in (10° × cm ⁻¹) 2.	160 2.160	2.160	2.160	2.160		
R _∞ \	0.123	0.120	0.110	0.105	0.098	
At x=0.5 ,						
n _∞ ≥	2.179	2.157	2.090	2.050	2.003	
ε _{1,∞} \	4.748	4.652	4.368	4.202	4.014	
$\sigma_{O,\infty}$ in $\frac{10^5}{\Omega \times cm}$	9.943	9.842	9.537	9.353	9.142	
oc _∞ in (10° × cm ⁻¹) 2.	2.160	2.160	2.160	2.160		
R _∞ ≽	0.137	0.134	0.124	0.118	0.112	

At x=1 ,						
n _{so}	2.274 2	.251	2.181	2.139	2.090	
ε _{1,∞} ∨	5.170	5.066	4.756	4.575	4.370	
$\sigma_{O,\infty}$ in $\frac{10^2}{\Omega \times cm}$	10.37	0.27	9.951	9.760	9.539	
∝ in (10° × cm ⁻¹) 2.160	2.160	2.160	2.160	2.16	50	
R _∞ ∨	0.151 0	.148	0.138	0.132	0.124	
Acceptor	В	Ga	Mg	In	Cd	
At x=0 ,						
n_{∞}	2.806 2.	059	2.002	1.968	1.928	
ε _{1,ee} \	7.872 4.	239	4.010	3.874	3.719	
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega \times cm}$	12.80 9	395	9.138	8.981	8.799	
α_{∞} in $(10^9 \times cm^{-1})$	2.160 2.	160	2.160	2.160	2.160	
R_{∞}	0.225 0.	120	0.111	0.106	0.100	
At x=0.5,						
n_{∞}	2.939	2.15	7 2.09	98	2.062	2.020
ε _{1,00}	8.639	4.652	2 4.40	01	4.252	4.081
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega \times cm}$	13.41	9.842	9.57	3	9.409	9.218
\propto_{∞} in $(10^9 \times cm^{-1})$	2.160	2.160	2.16	0	2.160	2.160
R _∞ \	0.242	0.134	4 0.12	5	0.120	0.114
At x=1 ,						
n _∞ \	3.067	2.251	2.189)	2.152	2.108
ε _{1,∞}	9.407	5.066	4.792	2	4.629	4.444
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega \times cm}$	13.99	10.27	9.98	9	9.818	9.619
α_{∞} in $(10^9 \times cm^{-1})$	2.160	2.160	2.16	50	2.160	2.160
R _∞ ≥	0.258	0.148	0.13	9	0.133	0.127

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Table 3n: In the P-X(x)-system, and at T=0K and N = N_{CDn}(r_p,x), according to the MIT, our numerical results of n, κ , ϵ_1 and ϵ_2 are obtained from Equations (21, 20, 16), respectively, and expressed as functions of $E \geq E_{CPE}(r_p,x)$ and x, noting that (i) $\kappa = 0$

=0, 3 = 1.5198
3.489 0.055 12.172 0.508 3.823 0.222 14.570 1.698 4.498 0.364 20.097 3.272 4.521 1.800 17.197 16.272 3.676 2.042 9.347 15.013 3.822 1.862 11.140 14.232 4.183 2.890 9.143 24.178 2.422 4.049 -10.524 19.614 1.203 2.865 -6.762 6.896 1.331 2.140 -2.807 5.696 2.080 0 4.3266 0
3.823 0.222 14.570 1.698 4.498 0.364 20.097 3.272 4.521 1.800 17.197 16.272 3.676 2.042 9.347 15.013 3.822 1.862 11.140 14.232 4.183 2.890 9.143 24.178 2.422 4.049 -10.524 19.614 1.203 2.865 -6.762 6.896 1.331 2.140 -2.807 5.696 2.080 0 4.3266 0
4.498 0.364 20.097 3.272 4.521 1.800 17.197 16.272 3.676 2.042 9.347 15.013 3.822 1.862 11.140 14.232 4.183 2.890 9.143 24.178 2.422 4.049 -10.524 19.614 1.203 2.865 -6.762 6.896 1.331 2.140 -2.807 5.696 2.080 0 4.3266 0 2.080 0 11.875 0
4.521 1.800 17.197 16.272 3.676 2.042 9.347 15.013 3.822 1.862 11.140 14.232 4.183 2.890 9.143 24.178 2.422 4.049 -10.524 19.614 1.203 2.865 -6.762 6.896 1.331 2.140 -2.807 5.696 2.080 0 4.3266 0 2=0.5, E=1.6648 3.446 0 11.875 0
3.676 2.042 9.347 15.013 3.822 1.862 11.140 14.232 4.183 2.890 9.143 24.178 2.422 4.049 -10.524 19.614 1.203 2.865 -6.762 6.896 1.331 2.140 -2.807 5.696 2.080 0 4.3266 0 2.080 0 11.875 0
3.822 1.862 11.140 14.232 4.183 2.890 9.143 24.178 2.422 4.049 -10.524 19.614 1.203 2.865 -6.762 6.896 1.331 2.140 -2.807 5.696 2.080 0 4.3266 0 x=0.5, E=1.6648 3.446 0 11.875 0
4.183 2.890 9.143 24.178 2.422 4.049 -10.524 19.614 1.203 2.865 -6.762 6.896 1.331 2.140 -2.807 5.696 2.080 0 4.3266 0 x=0.5, E=1.6648 3.446 0 11.875 0
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E = 1.6648 3.446 0 11.875 0
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3.697 0.213 13.624 1.573
4.293 0.264 18.358 2.267
4.409 1.464 17.295 12.912
3.735 1.754 10.876 13.100
3.872 1.650 12.268 12.782
4.207 2.616 10.855 22.007
2 .600 3 .718 - 7.063 19 .338
1.459 2.660 -4.948 7.763
1.561 2.003 -1.576 6.256

10 ²²	2.179	0	4.7484	0	
At x=1,					
$E_{CPE} = 1.8099$	3.450	0	11.905	0	
2	3.582	0.182	12.801	1.301	
2.5	4.103	0.180	16.804	1.480	
3	4.296	1.163	17.102	9.996	
3.5	3.779	1.487	12.067	11.241	
4	3.910	1.452	13.179	11.353	
4.5	4.221	2.355	12.271	19.880	
5	2.763	3.402	-3.937	18.800	
5.5	1.698	2.463	-3.183	8.363	
6	1.777	1.872	-0.345	6.652	

10 ²²	2.274	0	5.170	0	
in eV	n	κ	ϵ_1	ε_2	

Table 3p: In the B-X(x)-system, and at T=0K and N = N_{CDp}(r_B, x), according to the MIT, our numerical results of n, κ , ϵ_1 and ϵ_2 are obtained from Equations (21, 20, 16), respectively, and expressed as functions of E [\geq E_{CPE}(r_B, x)] and x, noting that (i) κ = 0 and ϵ_2 = 0 at E = E_{CPE}(r_B, x), and κ \rightarrow 0 and ϵ_2 \rightarrow 0 as E \rightarrow ∞ .

E in eV	n	к	ε_1	ε_2	
At x=0,					
$E_{CPE} = 1.5037$	4.173	0	17.414	0	
1.6	4.236	0.059	17.939	0.502	
2	4.575	0.222	20.883	2.033	
2.5	5.258	0.376	27.509	3.952	
3	5.270	1.839	24.390	19.384	
3.5	4.406	2.075	15.110	18.286	
4	4.552	1.886	17.168	17.174	
4.5	4.916	2.921	15.638	28.727	
5	3.138	4.086	-6.847	25.649	
5.5	1.911	2.888	-4.692	11.040	
6	2.041	2.155	-0.477	8.799	

10 ²²	2.8057	0	7.8719	0	

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At $x=0.5$,					
$E_{CPE} = 1.6512$	4.2147	0	17.763	0	
2	4.478	0.214	20.005	1.920	
2.5	5.081	0.273	25.738	2.771	
3	5.189	1.494	24.690	15.507	
3.5	4.499	1.780	17.079	16.016	
4	4.637	1.670	18.715	15.486	
4.5	4.974	2.641	17.769	26.272	
5	3.354	3.748	-2.805	25.143	
5.5	2.205	2.679	-2.316	11.816	
6	2.310	2.016	1.270	9.312	
10 ²²	2.9393	0	8.6393	0	
At x=1,					
$\mathbf{E}_{CPE} = 1.7982$	4.2508	0	18.0698	0	
2	4.392	0.185	19.255	1.628	
2.5	4.918	0.186	24.158	1.834	
3	5.106	1.186	24.662	12.114	
3.5	4.576	1.508	18.671	13.803	
4	4.708	1.467	20.012	13.817	
4.5	5.021	2.375	19.567	23.853	
5	3.551	3.427	0.869	24.339	
5.5	2.480	2.478	0.007	12.293	
6	2.561	1.882	3.016	9.639	
10 ²²	3.0670	0	9.4067	0	
E in eV	n	κ	ε_1	ϵ_2	

Table 4n: In the X(x)-system, at E=3.2 eV and T=20 K, for given r_d and x, and from Equations (12, 15, 21, 20, 16), respectively, we can determine the variations of $\eta_n(\gg 1, \text{degenerate case})$, E_{gn1} , n, κ , ε_1 and ε_2 , obtained as functions of N, being represented by the arrows: \nearrow and \searrow , noting that both η_n and E_{gn1} increase with increasing N.

N (10 ¹⁸ cm ⁻³	h 7	15	26	60	100		
	•		x=0				
For $\mathbf{r_d} = \mathbf{r_{As}}$,							
$\eta_n\gg 1$	7	238	345	602	847		
Egn1 in eV	7	1.475	1.525	1.686	1.870		
n	7	4.247	4.201	4.046	3.865		
ĸ	\mathbf{V}	2.206	2.080	1.698	1.311		
ε_1	7	13.175	13.319	13.489	13.221		
ε_2	7	18.736	17.473	13.744	10.137		
For $\mathbf{r_d} = \mathbf{r_{Te}}$,						 •	
$\eta_n \gg 1$	7	239	345	602	847		
E _{gn1} in eV		1.497	1.554	1.731	1.928		
n	7	4.163	4.109	3.939	3.743		
κ	V	2.149	2.008	1.600	1.200		
ε_1	7	12.708	12.853	12.957	12.571		
ε_2	7	17.892	16.500	12.602	8.983		
For $\mathbf{r_d} = \mathbf{r_{Sn}}$,	,					 _	
	7	239	345	602	847		
Egn1 in eV	7	1.525	1.591	1.786	1.999		
n	7	4.054	3.992	3.802	3.587		
ĸ	7	2.080	1.920	1.481	1.068		
ε_1		12.109	▶ 12.249	12.260	11.727		
ε_2	7	16.864	15.327	11.261	7.664		
			x=0.5			_	
For $\mathbf{r_d} = \mathbf{r_{As}}$,	,					 _	
$\eta_n\gg 1$		131	189	329	463		
Egn1 in eV	\sqrt	1.252	1.163	1.004	0.895		

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n	7	4.054	3.992	3.802	3.587		
K	7	2.080	1.920	1.481	1.068		
ε1		12.109	₹ 12.249 N	12.260	11.727		
ε ₂	7	16.864	15.327	11.261	7.664		
-			x=0.5				
For $\mathbf{r_d} = \mathbf{r_{As}}$,	307.076						
$\eta_n \gg 1$		131	189	329	463		
E _{gn1} in eV		1.252	1.163	1.004	0.895		
n	7	4.548	4.627	4.764	4.855		
ĸ	7		3.074				
ε1	1		11.953		8.050		
ε_2	7	25.585			38.256		
For $\mathbf{r_d} = \mathbf{r_{Te}}$,						•	
$\eta_n \gg 1$		131	189	329	463		
Egn1 in eV		1.284	1.206		0.979		
n	7	4.452	4.522	4.641	4.718		
κ	1		2.947		3.657		
ε_1	7		11.766				
ε_2		24.219	26.650	31.251	34.505		
For $\mathbf{r_d} = \mathbf{r_{Sn}}$,							
		131	189	329	463		
E _{gn1} in eV			1.259	1.150	1.084		
n	7	4.329		4.485	4.542		
K	7	2.606	2.791		3.320		
 ε ₁	7	11.951	11.465	10.409			
ε_2	7	22.570	24.501	27.942	30.156		
2			x=1		***		
For $\mathbf{r_d} = \mathbf{r_{As}}$,							20001-000
$\eta_n \gg 1$	7	94	135	236	332		
Egn1 in eV	7	1.040	0.834	0.412	0.075		
l I	7		5.000	- 11			
c	7	3.457	4.151	5.760			
5 ₁	1	11.342	7.758				
2	7	33.377	41.500				
For m. — m							
For $\mathbf{r_d} = \mathbf{r_{Te}}$,	94	135	236	332		
η _n ≫ 1 E _{gn1} in eV	-		0.898	0.510			
n gni m c v	7	67-00-00-00-00-00-00-00-00-00-00-00-00-00	4.876	5000000	0 00-00-00-00-00-00-00-00-00-00-00-00-00		
	7	3.303	3.929				
·	100						
ε ₁	7	11.319	8.344	-1.896	-15.191		

Cong.

ε2	7	31.154	38.315	55.582	72.085
For $\mathbf{r_d} = \mathbf{r_5}$	n,				
$\eta_n \gg 1$	7	94	135	236	332
Egn1 in eV	7	1.149	0.978	0.632	0.359
n	7	4.572	4.719	4.999	5.204
K	1	3.117	3.661	4.888	5.983
ε ₁	7	11.191	8.871	1.099	-8.714
$\frac{\varepsilon_1}{\varepsilon_2}$	7	28.504	34.555	48.867	62.282
N (10 ¹⁸ cm	-3 ₎ /	15	26	60	100

Table 4p: In the X(x)-system, at E=3.2 eV and T=20 K, for given r_d and x, and from Equations (12, 15, 21, 20, 16), respectively, we can determine the variations of $\eta_p(\gg 1, \text{degenerate case})$, E_{gp1} , n, κ , ε_1 and ε_2 , obtained as functions of N, being represented by the arrows: \mathcal{F} and \mathcal{L} , noting that both η_p and E_{gp1} increase with increasing N.

N (10 ¹⁸ cm ⁻	³) /	15	26	60	100	
			x=0			
For $\mathbf{r_a} = \mathbf{r_{Ga}}$,					
$\eta_p \gg 1$	7	227	335	595	840	
E _{gp1} in eV	7	1.869	2.043	2.466	2.869	
n	7	3.866	3.690	3.234	2.772	
κ	\	1.313	0.992	0.399	0.081	
ε_1	7	13.223	12.623	10.303	7.676	
ε ₂	7	10.156	7.320	2.581	0.450	
For $\mathbf{r_a} = \mathbf{r_{In}}$,	,					_
η _p ≫ 1	7	223	332	592	838	
E _{gp1} in eV	7	1.869	2.045	2.472	2.876	
n	7	3.775	3.596	3.138	2.672	
κ	\	1.312	0.988	0.393	0.077	
ε_1	7	12.529	11.953	9.692	7.135	
ε_2	\	9.909	7.106	2.468	0.415	

For r ₂ = r _{Cd} .						
$\eta_p \gg 1$	1	221	330	592	837	
Egp1 in eV	1	1.869	2.046	2.474	2.880	
n	7	3.735	3.555	3.095	2.628	
κ	>	1.313	0.987	0.391	0.076	
ε_1	1	12.230	11.664	9.430	6.904	
ε_2	4	9.808	7.016	2.420	0.400	
			x=0.5			
For $\mathbf{r_2} = \mathbf{r_{G2}}$,	5855 O		81982			
$\eta_p \gg 1$	1	125	184	326	460	
Egp1 in eV	1	1.833	1.921	2.138	2.346	
n	١.	4.000	3.911	3.687	3.465	
κ	4	1.385	1.212	0.836	0.540	
ε_1	1	14.083	13.831	12.901	11,712	
ε_2	>	11.077	9.482	6.165	3.743	
For r ₂ = r _{ln} ,						
$\eta_p \gg 1$	1	124	183	325	459.6	
Egp1 in eV	7	1.837	1.926	2.14	6 2.356	
n	V	3.901	3.811	3.58	5 3.359	
ĸ	>	1.377	1.202		4 0.528	
ε_1	1	13.323	13.081		2 11.006	
ε_2	1	10.743				
For $\mathbf{r_2} = \mathbf{r_{Cd}}$						
$\eta_p \gg 1$	1		182.9			
Egp1 in eV	1	1.837	1.926	2.146	2.356	
n	7	3.901	3.811	3.585		
κ	7	1.377	1.202	0.824		
ε_1		13.323	13.081	12.172	2 11.006	
ε2	\sim	10.743	9.165	5.908	3,550	
			x=1			
For $\mathbf{r_2} = \mathbf{r_{G_2}}$,						
$\eta_p \gg 1$	1	90.6	132.7	234.2	330.3	
Egp1 in eV	1	1.912	1.970	2.114	2,254	
n	7	4.014	3.956	3.806	3.658	
κ		1.229	1.121	0.874	0.663	
€1	7	14.604	14.390	13.725	12.940	
£2	>	9.867	8.871	6.651	4.848	
For $\mathbf{r_2} = \mathbf{r_{ln}}$.						
$\eta_p \gg 1$	2	89.6	131.9	233.6	329.8	
Eppi in eV	1	1.917	1.976	2.123	2.265	
n	5	3.910	3.850	3.698	3.548	
κ		1.220	1.110	0.860	0.648	
ε,		13.803	13,593	12.939	12.165	
ε_2	¥	9.541	8.551	6.364	4.600	

For $\mathbf{r_2} = \mathbf{r_{Cd}}$, $\eta_p \gg 1$,	89.1	131.4	233.3	329.5	

N (10 ¹⁸	cm ⁻³) /	15	26	60	100	
€2	- 1	9.398	8.412	6.238	4.493	
£1		13.457	13.249	12.600	11.831	
K	1	1.216	1.106	0.854	0.642	
n	~	3.865	3.804	3.651	3.499	

Table 5n: In the X(x)-system, at E=3.2 eV and N = 10^{20}cm^{-3} , for given r_d and x, and from Equations (12, 15, 21, 20, 16), respectively, we can determine the variations of $\eta_n(\gg 1, \text{degenerate case})$, E_{gn1} , n, κ , ε_1 and ε_2 , obtained as functions of T, being represented by the arrows: \mathcal{F} and \mathcal{F} , noting that both η_n and E_{gn1} decrease with increasing T.

T in K		2 0	50)	100	300	
			X	=0			
For $\mathbf{r_d} = \mathbf{r_l}$	4s,						
$\eta_n \gg 1$	7	847	33	39	169	56	
Egn1 in eV	7	1.870	1.866	1.853	1.774		
n	7	3.865	3.870		3.882	3.961	
κ	7	1.311	1.320	1.345	1.507		
ε ₁	1	13.221	13.232	13.263	13.415		
ε ₂	7	10.132	10.215	10.441	11.940		
For $\mathbf{r_d} = \mathbf{r_{Te}}$,					833883900	
Carlot Co.	7	847	339	169	56		
Egn1 in eV	7	1.928	1.923	1.911	1.832		
n	7	3.743	3.747	3.760	3.839		
K	7	1.200	1.208	1.232	1.388		
€1	7	12.571	12.584	12.621	12.816		
ε2	7	8.983	9.055	9.264	10.656		
For $\mathbf{r_d} = \mathbf{r_{Sn}}$,						
	7	847	339	169	56		
Egn1 in eV	7	1.999	1.995	1.983	1.904		
n	7	3.587	3.592	3.604	3.685		
K	1	1.068	1.076	1.098	1.246		
€1	7	11.727	11.742	11.785	12.026		
ε_2	7	7.664	7.729	7.919	9.181		

For $\mathbf{r_d} = \mathbf{r_A}$, is			2.5	~ 4	
$\eta_n \gg 1$,	463	185		31	
Egn1 in eV		0.895	0.887	0.869	0.765	
n	7	4.855	4.861	4.876	4.960	
K	7	3.940	3.964			
ε_1	>	8.050	7.914	7.551	5.292	
ε_2	7	38.256	38.542	39.287	43.600	
For $\mathbf{r_d} = \mathbf{r_T}$	`a,					
$\eta_n\gg 1$,	463	185	93	31	
Egn1 in eV	1	0.979	0.972			
n	1	4.718	4.724		4.825	
K	1	3.657	3.680	3.742	4.096	
ε_1	1	8.886	8.769		6.508	
ε2	7	34.505	34.773	35.472	39.525	
For $\mathbf{r_d} = \mathbf{r_S}$	n,					o de la companya del companya de la companya de la companya del companya de la companya del la companya de la c
		463	185	93	31	
Egn1 in eV			1.077			
n		4.542	4.548	4.564	4.652	
κ	Ź		3.342			
ε_1			9.517			
ε_2	7		30.403			
-4						
			x=1			
For $\mathbf{r_d} = \mathbf{r_{As}}$	ς,					
$\eta_n \gg 1$	7	332	133	66	22	
E _{gn1} in eV	7	0.075	0.065	0.040	-0.088	
n	7	5.564	5.571	5.587	5.672	
κ	7	7.241	7.287	7.402	8.016	
ε_1	\	-21.467	-22.067			
ε_2	7	80.578	81.193		90.929	
For $\mathbf{r_d} = \mathbf{r_{Te}}$						
$\eta_n \gg 1$	1	332	133	66	22	
E _{gn1} in eV	1	0.201	0.191	0.167	0.038	
II .	7	5.407	5.414	5.431	5.519	
κ	,	6.665	6.710	6.821	7.410	
ε ₁		-15.191			-24.451	
ε ₂		72.085	72.660	74.093	81.787	
						<u> </u>
For $\mathbf{r}_d = \mathbf{r}_{5n}$	0	225	122	EE	22	
$\eta_n \gg 1$		0.359	133 0.349	66 0.324	22 0.196	
Egni in eV	- 4					
n	'	5.204	5.212	5.230	5.321	
K	1	5.983	6.026	6.130	6.690	
ε1		-8.714 62.282			-16.443 71.189	
E ₂		62.282	62.809	64.122	71.189	
T in K	1	20	50	100	300	

Table 5p: In the X(x)-system, at E=3.2 eV and N = 10^{20} cm⁻³, for given r_a and x, and from Equations (12, 15, 21, 20, 16), respectively, we can determine the variations of $\eta_p(\gg 1, \text{degenerate case}), E_{gp1}, n, \kappa, \varepsilon_1 \text{ and } \varepsilon_2, \text{ obtained as functions of T, being represented by}$ the arrows: \nearrow and \searrow , noting that both η_p and E_{gp1} decrease with increasing T.

T in K	7		20	50	100	300			
				x=0					
For $\mathbf{r_a} = \mathbf{r_{Ga}}$,								
$\eta_p \gg 1$	7	84	10	336	168	56			
E _{gp1} in eV	7	2.	869	2.865	2.852	2.773			
n	7	2.	.772	2.777		2.792	2.885		
K	7		.081	0.083	0.090	0.135			
ε_1	7		.676	7.704	7.785	8.303			
ε ₂	7	0.	.450	0.463	0.501	0.779			
For $\mathbf{r_2} = \mathbf{r_{ln}}$,									
η _p ≫ 1		8	38	335	168	56			
E _{gp1} in eV	7	2.	876	2.872	2.860	2.780			
n	7	2.	.672	2.677		2.692	2.785		
κ	7	0.	.077	0.080	0.086	0.130			
ε ₁	7		.135	7.162	7.241	7.741			
ε_2	7	0.	.415	0.427	0.462	0.726			
For $\mathbf{r_2} = \mathbf{r_0}$	Cd,								
17.55	7	r:	837	3	35	167	56		
Egp1 in eV		7	2.880	2.	875	2.863	2.784		
n		7	2.628	2.	634		2.648	2.742	
K	,	7	0.076	0.	078	0.084	0.128		
ε_1		7	6.904	6.	931	7.008	7.500		
ε ₂		7	0.400	0.	412	0.446	0.704		
99				x=0.5					
For $\mathbf{r_2} = \mathbf{r_0}$:a,	*****							
$\eta_p \gg 1$	7		460	1	84	92	31		
E _{gp1} in eV		7	2.346	2.3	339	2.320	2.217		

n						
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	n					
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$						
For $\mathbf{r_a} = \mathbf{r_{ln}}$, $\eta_p \gg 1$ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \	-					
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	ε ₂		3.743	3.815	4.005	5.165
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	For $\mathbf{r_2} = \mathbf{r_{ln}}$,				
	$\eta_p\gg 1$	7	460	184	92	30.6
κ	E _{gp1} in eV	7	2.356	2.349	2.330	2.226
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	n	7	3.359	3.367	3.387	3.499
$ ε_2 $ / 3.550 3.619 3.801 4.919 For $\mathbf{r_2} = \mathbf{r_{Cd}}$, $η_p \gg 1$ 459 184 92 30 $ \mathbf{E_{gp1}}$ in eV ≥ 2.360 2.353 2.334 2.230 n / 3.313 3.321 3.341 3.453 κ / 0.523 0.532 0.556 0.697 $ε_1$ / 10.702 10.745 10.854 11.437 $ε_2$ / 3.466 3.534 3.713 4.812 Tell For $\mathbf{r_2} = \mathbf{r_{G_2}}$, $η_p \gg 1$ 330 132 66 22 $ \mathbf{E_{gp1}}$ in eV ≥ 2.254 2.244 2.220 2.091 n / 3.658 3.668 3.695 3.830 κ / 0.663 0.677 0.712 0.911 $ε_1$ / 12.940 13.000 13.145 13.842 $ε_2$ / 4.848 4.966 5.263 6.978 For $\mathbf{r_2} = \mathbf{r_{In}}$, $η_p \gg 1$ 330 132 66 22 $ \mathbf{E_{gp1}}$ in eV ≥ 2.255 2.255 2.230 2.102 n / 3.548 3.558 3.585 3.720 κ / 0.648 0.662 0.697 0.894 $ε_1$ / 12.165 12.223 12.365 13.043 $ε_2$ / 4.600 4.713 5.000 6.653 For $\mathbf{r_2} = \mathbf{r_{Id}}$, $η_p \gg 1$ 329 132 66 22 $ \mathbf{E_{gp1}}$ in eV ≥ 2.269 2.259 2.235 2.106 n / 3.499 3.510 3.536 3.672 κ / 0.642 0.656 0.691 0.887 $ε_1$ / 11.831 11.889 12.028 12.698 $ε_2$ / 4.493 4.604 4.886 6.512						
For $\mathbf{r_2} = \mathbf{r_{Cd}}$, $\eta_p \gg 1$	-					
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	ε_2		3.550	3.619	3.801	4.919
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	For $\mathbf{r}_2 = \mathbf{r}_{Cd}$,				
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$			459	184	92	30
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	-			2.353	2.334	2.230
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$						
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	κ	7	0.523			0.697
For $\mathbf{r_2} = \mathbf{r_{G_2}}$, $\eta_p \gg 1$ 330 132 66 22 $\mathbf{E_{gp1}}$ in eV 2.254 2.244 2.220 2.091 $\mathbf{r_1}$ 3.658 3.668 3.695 3.830 $\mathbf{r_2}$ 7.0.663 0.677 0.712 0.911 $\boldsymbol{\epsilon_1}$ 7.12.940 13.000 13.145 13.842 $\boldsymbol{\epsilon_2}$ 7.4.848 4.966 5.263 6.978 $\mathbf{r_2} = \mathbf{r_{In}}$, $\eta_p \gg 1$ 330 132 66 22 $\mathbf{E_{gp1}}$ in eV 2.265 2.255 2.230 2.102 $\mathbf{r_1}$ 7.3.548 3.558 3.585 3.720 $\mathbf{r_2}$ 8.7 12.165 12.223 12.365 13.043 $\boldsymbol{\epsilon_2}$ 7.4.600 4.713 5.000 6.653 $\mathbf{r_2}$ 8.7 4.600 4.713 5.000 6.653 $\mathbf{r_2}$ 8.7 4.600 4.713 5.000 6.653 $\mathbf{r_2}$ 8.7 0.642 0.656 0.691 0.887 $\boldsymbol{\epsilon_1}$ 7.1.831 11.889 12.028 12.698 $\boldsymbol{\epsilon_2}$ 7.4.493 4.604 4.886 6.512	ε_1			10.745	10.854	11.437
For $\mathbf{r_2} = \mathbf{r_{G_2}}$, $\eta_p \gg 1$ 330 132 66 22 $\mathbf{E_{gp1}}$ in eV 2.254 2.244 2.220 2.091 \mathbf{r} 3.658 3.668 3.695 3.830 \mathbf{r} 7.0.663 0.677 0.712 0.911 $\mathbf{\epsilon_1}$ 7.12.940 13.000 13.145 13.842 $\mathbf{\epsilon_2}$ 7.4.848 4.966 5.263 6.978 $\mathbf{r_2} = \mathbf{r_{In}}$, $\eta_p \gg 1$ 330 132 66 22 $\mathbf{E_{gp1}}$ in eV 2.265 2.255 2.230 2.102 \mathbf{r} 3.548 3.558 3.585 3.720 \mathbf{r} 7.0.648 0.662 0.697 0.894 $\mathbf{\epsilon_1}$ 7.12.165 12.223 12.365 13.043 $\mathbf{\epsilon_2}$ 7.4.600 4.713 5.000 6.653 $\mathbf{r_2} = \mathbf{r_{In}}$, $\eta_p \gg 1$ 329 132 66 22 $\mathbf{E_{gp1}}$ in eV 2.269 2.259 2.235 2.106 $\mathbf{r_2} = \mathbf{r_{In}}$, $\mathbf{r_{I}} \gg 1$ 329 132 66 22 $\mathbf{E_{gp1}}$ in eV 2.269 2.259 2.235 2.106 $\mathbf{r_2} = \mathbf{r_{In}}$, $\mathbf{r_{I}} \gg 1$ 329 132 66 22 $\mathbf{r_{I}} \gg 1$ 329 132 66 25 $\mathbf{r_{I}} \gg 1$ 329 132 66 25 $\mathbf{r_{I}} \gg 1$ 329 132 66 25 $\mathbf{r_{I}} \gg 1$ 329 132 66 6 653 $\mathbf{r_{I}} \gg 1$ 329 132 66 6 25 $\mathbf{r_{I}} \gg 1$ 329 132 66 6 25 $\mathbf{r_{I}} \gg 1$ 3499 3.510 3.536 3.672 $\mathbf{r_{I}} \gg 1$ 3499 4.604 4.886 6.512	ε_2	7	3.466	3.534	3.713	4.812
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$				x=1		
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	For $\mathbf{r}_{-} = \mathbf{r}_{-}$	<u> </u>				
E _{gp1} in eV 2.254 2.244 2.220 2.091 n			330	132	66	22
n	The second secon					
$ε_1$		1470	886000000000000000000000000000000000000	12: 100/4/0-03	5-481 BASA11	0.0000000000000000000000000000000000000
$ε_1$						
For $\mathbf{r_2} = \mathbf{r_{ln}}$, $\eta_p \gg 1$ 330 132 66 22 $\mathbf{E_{gp1}}$ in eV 2.265 2.255 2.230 2.102 \mathbf{r} 3.548 3.558 3.585 3.720 \mathbf{r} 9.648 0.662 0.697 0.894 \mathbf{r} 9.12.165 12.223 12.365 13.043 \mathbf{r} 9.2 4.600 4.713 5.000 6.653 \mathbf{r} 9.3 4.600 4.713 5.000 6.653 \mathbf{r} 9.3 4.99 3.510 3.536 3.672 \mathbf{r} 9.642 0.656 0.691 0.887 \mathbf{r} 11.831 11.889 12.028 12.698 \mathbf{r} 11.831 11.889 12.028 12.698 \mathbf{r} 12.493 4.604 4.886 6.512						
For $\mathbf{r_2} = \mathbf{r_{ln}}$, $\eta_p \gg 1$ 330 132 66 22 $\mathbf{E_{gp1}}$ in eV 2.265 2.255 2.230 2.102 \mathbf{r} 3.548 3.558 3.585 3.720 \mathbf{r} 0.648 0.662 0.697 0.894 $\mathbf{\epsilon_1}$ 7.12.165 12.223 12.365 13.043 $\mathbf{\epsilon_2}$ 7.4.600 4.713 5.000 6.653 $\mathbf{r_3} = \mathbf{r_{Cd}}$, $\eta_p \gg 1$ 329 132 66 22 $\mathbf{E_{gp1}}$ in eV 2.269 2.259 2.235 2.106 $\mathbf{r_1}$ $\mathbf{r_2} = \mathbf{r_{Cd}}$, $\mathbf{r_3}$ 0.642 0.656 0.691 0.887 $\mathbf{\epsilon_1}$ 7.11.831 11.889 12.028 12.698 $\mathbf{\epsilon_2}$ 7.4.493 4.604 4.886 6.512	100					
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$		0.7.0			87,67743	
E_{gp1} in eV 2.265 2.255 2.230 2.102 n 3.548 3.558 3.585 3.720 κ 0.648 0.662 0.697 0.894 ε_1 12.165 12.223 12.365 13.043 ε_2 4.600 4.713 5.000 6.653 For $\mathbf{r_2} = \mathbf{r_{Cd}}$, $\eta_p \gg 1$ 329 132 66 22 E_{gp1} in eV 2.269 2.259 2.235 2.106 n 3.499 3.510 3.536 3.672 κ 0.642 0.656 0.691 0.887 ε_1 11.831 11.889 12.028 12.698 ε_2 4.493 4.604 4.886 6.512						
E_{gp1} in eV 2.265 2.255 2.230 2.102 n 3.548 3.558 3.585 3.720 κ 0.648 0.662 0.697 0.894 ε_1 12.165 12.223 12.365 13.043 ε_2 4.600 4.713 5.000 6.653 For $\mathbf{r_2} = \mathbf{r_{Cd}}$, $\eta_p \gg 1$ 329 132 66 22 E_{gp1} in eV 2.269 2.259 2.235 2.106 n 3.499 3.510 3.536 3.672 κ 0.642 0.656 0.691 0.887 ε_1 11.831 11.889 12.028 12.698 ε_2 4.493 4.604 4.886 6.512	$\eta_p\gg 1$	7	330	132	66	22
n						
$ε_1$ $?$ 0.648 0.662 0.697 0.894 $ε_1$ $?$ 12.165 12.223 12.365 13.043 $ε_2$ $?$ 4.600 4.713 5.000 6.653 For $\mathbf{r_2} = \mathbf{r_{Cd}}$, $η_p \gg 1$ 329 132 66 22 $\mathbf{E_{gp1}}$ in eV 2.269 2.259 2.235 2.106 n $?$ 3.499 3.510 3.536 3.672 κ $?$ 0.642 0.656 0.691 0.887 $ε_1$ $?$ 11.831 11.889 12.028 12.698 $ε_2$ $?$ 4.493 4.604 4.886 6.512			3.548	3.558	3.585	3.720
$ε_1$ / 12.165 12.223 12.365 13.043 $ε_2$ / 4.600 4.713 5.000 6.653 For $\mathbf{r_2} = \mathbf{r_{Cd}}$, $η_p \gg 1$ 329 132 66 22 $\mathbf{E_{gp1}}$ in eV 2.269 2.259 2.235 2.106 In / 3.499 3.510 3.536 3.672 κ / 0.642 0.656 0.691 0.887 $ε_1$ / 11.831 11.889 12.028 12.698 $ε_2$ / 4.493 4.604 4.886 6.512						
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$\begin{array}{c ccccccccccccccccccccccccccccccccccc$						
E_{gp1} in eV 2.269 2.259 2.235 2.106 n 3.499 3.510 3.536 3.672 k 0.642 0.656 0.691 0.887 ε_1 11.831 11.889 12.028 12.698 ε_2 4.493 4.604 4.886 6.512	For $\mathbf{r_a} = \mathbf{r_{Cd}}$					
n \nearrow 3.499 3.510 3.536 3.672 \nearrow 0.642 0.656 0.691 0.887 ε_1 \nearrow 11.831 11.889 12.028 12.698 ε_2 \nearrow 4.493 4.604 4.886 6.512	$\eta_p\gg 1$				66	22
κ \nearrow 0.642 0.656 0.691 0.887 ε_1 \nearrow 11.831 11.889 12.028 12.698 ε_2 \nearrow 4.493 4.604 4.886 6.512	Egp1 in eV	7	2.269	2.259	2.235	2.106
κ \nearrow 0.642 0.656 0.691 0.887 ε_1 \nearrow 11.831 11.889 12.028 12.698 ε_2 \nearrow 4.493 4.604 4.886 6.512	11	7	3 499	3 510	3 536	3 672
ε_1 \nearrow 11.831 11.889 12.028 12.698 ε_2 \nearrow 4.493 4.604 4.886 6.512						
ε ₂						
	ε_2					
1 m K / 20 50 100 300			20	50	100	200
	I in K		20	50	100	300