



**OPTICAL COEFFICIENTS IN THE N(P)-TYPE DEGENERATE  
CdTe(1-x)S(x)-CRYSTALLINE ALLOY, DUE TO THE NEW STATIC  
DIELECTRIC CONSTANT-LAW AND THE GENERALIZED MOTT  
CRITERIUM IN THE METAL-INSULATOR TRANSITION (9)**

**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.

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**\*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.

**ABSTRACT**

In the n(p)-type  $\text{CdTe}_{1-x}\text{S}_x$ - crystalline alloy, with  $0 \leq x \leq 1$ , basing on our two recent works<sup>[1,2]</sup>, for a given  $x$ , and with an increasing  $r_{d(a)}$ , the optical coefficients have been determined, as functions of the photon energy  $E$ , total impurity density  $N$ , the donor (acceptor) radius  $r_{d(a)}$ , concentration  $x$ , and temperature  $T$ . Those results have been affected by (i) the important new  $\varepsilon(r_{d(a)}, x)$ -law, developed in Equations (8a, 8b), stating that, for a given  $x$ , due to the impurity-size effect,  $\varepsilon$  decreases ( $\searrow$ ) with an increasing ( $\nearrow$ )  $r_{d(a)}$ , and then by (ii) the generalized Mott critical d(a)-density defined in the metal-insulator transition (MIT),  $N_{CDn(NDp)}(r_{d(a)}, x)$ , 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  $2.82 \times 10^{-7}$ , as that given in Table 4 of Ref.<sup>[1]</sup>, 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  $\varepsilon(r_{d(a)}, x)$ -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, 21), are reported in Tables 1, 2, 3n, 3p, 4n, 4p, 5n, and 5p in Appendix 1.

**KEYWORDS:** CdTe<sub>1-x</sub>S<sub>x</sub>- crystalline alloy; impurity-size effect; Mott critical impurity density in the MIT, optical coefficients.

## INTRODUCTION

Here, basing on our two recent works<sup>[1,2]</sup> and also other ones<sup>[3-8]</sup>, all the optical coefficients given in the n(p)-type  $X(x) \equiv \text{CdTe}_{1-x}\text{S}_x$  - crystalline alloy, with  $0 \leq x \leq 1$ , 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  $r_{d(a)}$ , 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 STRUCTURE 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:  $r_{do(ao)} = r_{Te(Cd)} = 0.132$  nm (0.148 nm).

### A. Effect of x- concentration

Here, the intrinsic energy-band-structure parameters<sup>[1]</sup>, 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:

$$m_{c(v)}(x)/m_o = 0.197 (0.801) \times x + 0.095 (0.82) \times (1 - x). \quad (1)$$

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

$$\epsilon_o(x) = 9 \times x + 10.31 \times (1 - x). \quad (2)$$

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

$$E_{go}(x) = 2.58 \times x + 1.62 \times (1 - x). \quad (3)$$

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

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

and then, the isothermal bulk modulus, by:

$$B_{do(ao)}(x) \equiv \frac{E_{do(ao)}(x)}{\left(\frac{4\pi}{3}\right) \times (r_{do(ao)})^3}. \tag{5}$$

**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  $\epsilon(r_{d(a)}, x)$ , 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  $p$ ,  $p_0 = 0$ , and for the deformation potential energy (or the strain energy)  $\sigma$ ,  $\sigma_0 = 0$ . Further, the two important equations [1, 7], used to determine the  $\sigma$ -variation,  $\Delta\sigma \equiv \sigma - \sigma_0 = \sigma$ , are defined by:

$\frac{dp}{dV} = -\frac{B}{V}$  and  $p = -\frac{d\sigma}{dV}$ . giving:  $\frac{d}{dV}\left(\frac{d\sigma}{dV}\right) = \frac{B}{V}$ . Then, by an integration, one gets:

$$\left[\Delta\sigma(r_{d(a)}, x)\right]_{n(p)} = B_{do(ao)}(x) \times (V - V_{do(ao)}) \times \ln\left(\frac{V}{V_{do(ao)}}\right) = E_{do(ao)}(x) \times \left[\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 - 1\right] \times \ln\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 \geq 0. \tag{6}$$

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:  $\pm [\Delta\sigma(r_{d(a)}, x)]_{n(p)}$ ,

$$E_{gno(gp)}(r_{d(a)}, x) - E_{go}(x) = E_{d(a)}(r_{d(a)}, x) - E_{do(ao)}(x) = E_{do(ao)}(x) \times \left[ \left(\frac{\epsilon_0(x)}{\epsilon(r_{d(a)})}\right)^2 - 1 \right] = + [\Delta\sigma(r_{d(a)}, x)]_{n(p)},$$

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

$$E_{gno(gp)}(r_{d(a)}, x) - E_{go}(x) = E_{d(a)}(r_{d(a)}, x) - E_{do(ao)}(x) = E_{do(ao)}(x) \times \left[ \left(\frac{\epsilon_0(x)}{\epsilon(r_{d(a)})}\right)^2 - 1 \right] = - [\Delta\sigma(r_{d(a)}, x)]_{n(p)}. \tag{7}$$

Therefore, from Equations (6) and (7), one obtains the expressions for relative dielectric constant  $\epsilon(r_{d(a)}, x)$  and energy band gap  $E_{gn(gp)}(r_{d(a)}, x)$ , as:

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

$\epsilon(r_{d(a)}, x)$ -law,

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

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  $\epsilon(r_{d(a)}, x) = \frac{\epsilon_o(x)}{\sqrt{1 - \left[ \left( \frac{r_{d(a)}}{r_{do(ao)}} \right)^3 - 1 \right] \times \ln \left( \frac{r_{d(a)}}{r_{do(ao)}} \right)^3}} \geq \epsilon_o(x)$ , 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**  $\epsilon(r_{d(a)}, x)$ -law,

$$E_{gno(gp)}(r_{d(a)}, x) - E_{go}(x) = E_{d(a)}(r_{d(a)}, x) - E_{do(ao)}(x) = -E_{do(ao)}(x) \times \left[ \left( \frac{r_{d(a)}}{r_{do(ao)}} \right)^3 - 1 \right] \times \ln \left( \frac{r_{d(a)}}{r_{do(ao)}} \right)^3 \leq 0, \tag{8b}$$

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:

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

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:

$$N_{CDn(CDp)}(r_{d(a)}, x)^{1/3} \times a_{Bn(Bp)}(r_{d(a)}, x) = M_{n(p)}, \quad M_{n(p)} = 0.25, \tag{9a}$$

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

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

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

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:

$$N_{CDn(CDP)}(r_{d(a)}, x)^{1/3} \times a_{Bn(Bp)}(r_{d(a)}, x) = \left(\frac{3}{4\pi}\right)^{1/3} \times \frac{1}{2.4814} = 0.25 = (WS)_{n(p)} = M_{n(p)}. \quad (9c)$$

Thus, the above Equations (9a, 9b, 9c) confirm our new  $\varepsilon(r_{d(a)}, x)$ -law, given in Equations (8a, 8b).

Furthermore, by using  $M_{n(p)} = 0.25$ , according to the empirical Heisenberg parameter  $\mathcal{H}_{n(p)} = 0.47137$ , as those given in Equations (8, 15) of the Ref.<sup>[1]</sup>, we have also showed that  $N_{CDn(CDP)}$  is just the density of electrons (holes) localized in the exponential conduction (valence)-band tail, with a precision of the order of  $2.82 \times 10^{-7}$ . Therefore, the density of electrons (holes) given in parabolic conduction (valence) bands can be defined, as that given in compensated materials, by:

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

### C. Effect of temperature T, with given x and $r_{d(a)}$

Here, the intrinsic band gap  $E_{gni(gpi)}(r_{d(a)}, x, T)$  at any T is given by:

$$E_{gni(gpi)}(r_{d(a)}, x, T) \text{ in eV} = E_{gno(gpo)}(r_{d(a)}, x) - 10^{-4} \times T^2 \times \left\{ \frac{5.405 \times x}{T+204 \text{ K}} + \frac{3.065 \times (1-x)}{T+94 \text{ K}} \right\}, \quad (10)$$

suggesting that, for given x and  $r_{d(a)}$ ,  $E_{gni(gpi)}$  decreases with an increasing T.

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:

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

where  $m_r(x)/m_o$  is the reduced effective mass  $m_r(x)/m_o$ , 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<sup>[1,2]</sup>, 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<sup>[8]</sup>, with a precision of the order of  $2.11 \times 10^{-4}$ , is found to be given by:

$$\eta_{n(p)}(u) \equiv \frac{E_{Fn}(u)}{k_B T} \left( \frac{-E_{Fp}(u)}{k_B T} \right) = \frac{G(u) + Au^B F(u)}{1 + Au^B}, \quad A = 0.0005372 \text{ and } B = 4.82842262, \quad (12)$$

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

$$F(u) = au^{\frac{2}{3}} \left( 1 + bu^{-\frac{4}{3}} + cu^{-\frac{8}{3}} \right)^{\frac{2}{3}}, \quad a = [(3\sqrt{\pi}/4) \times u]^{2/3}, \quad b = \frac{1}{8} \left( \frac{\pi}{a} \right)^2, \quad c = \frac{62.3739855}{1920} \left( \frac{\pi}{a} \right)^4,$$

and  $G(u) \simeq \text{Ln}(u) + 2^{-\frac{3}{2}} \times u \times e^{-du}$ ;  $d = 2^{3/2} \left[ \frac{1}{\sqrt{27}} - \frac{3}{16} \right] > 0$ . Therefore, from Eq. (12), the Fermi energies are expressed as functions of variables :  $N, r_{d(a)}, x$ , 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:  $+E_{Fn}(-E_{Fp}) = \frac{\hbar^2}{2 \times m_r(x)} \times (3\pi^2 N^*)^{2/3} = 0$ , and (ii)  $\frac{E_{Fn}(u \ll 1)}{k_B T} \left( \frac{-E_{Fp}(u \ll 1)}{k_B T} \right) \ll -1$ , 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:

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

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

$$E_{cn(cp)}(N, r_{d(a)}, x) = \frac{-0.87553}{0.0908 + r_{sn(sp)}} + \frac{\frac{0.87553}{0.0908 + r_{sn(sp)}} + \left( \frac{2[1 - \ln(2)]}{\pi^2} \right) \times \ln(r_{sn(sp)}) - 0.093288}{1 + 0.03847728 \times r_{sn(sp)}^{1.67378876}}. \quad (13b)$$

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:

$$\Delta E_{\text{gno}}(N, r_d, x) = a_1 \times \frac{\varepsilon_0(x)}{\varepsilon(r_d, x)} \times N_r^{1/3} + a_2 \times \frac{\varepsilon_0(x)}{\varepsilon(r_d, x)} \times N_r^{1/3} \times (2.503 \times [-E_{\text{cn}}(r_{\text{sn}}) \times r_{\text{sn}}]) +$$

$$a_3 \times \left[ \frac{\varepsilon_0(x)}{\varepsilon(r_d, x)} \right]^{5/4} \times \sqrt{\frac{m_v}{m_r}} \times N_r^{1/4} + a_4 \times \sqrt{\frac{\varepsilon_0(x)}{\varepsilon(r_d, x)}} \times N_r^{1/2} \times 2 + a_5 \times \left[ \frac{\varepsilon_0(x)}{\varepsilon(r_d, x)} \right]^2 \times N_r^{1/6}$$

$$, N_r \equiv \left( \frac{N^*}{N_{\text{CDn}}(r_d, x)} \right),$$

$$\Delta E_{\text{gn}}(N, r_d, x) = \Delta E_{\text{gno}}(N, r_d, x) \times \{2.8 \times x + 2 \times (1 - x)\}, \quad (14n)$$

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

$$\Delta E_{\text{gpo}}(N, r_a, x) = a_1 \times \frac{\varepsilon_0(x)}{\varepsilon(r_a, x)} \times N_r^{1/3} + a_2 \times \frac{\varepsilon_0(x)}{\varepsilon(r_a, x)} \times N_r^{1/3} \times (2.503 \times [-E_{\text{cp}}(r_{\text{sp}}) \times r_{\text{sp}}]) +$$

$$a_3 \times \left[ \frac{\varepsilon_0(x)}{\varepsilon(r_a, x)} \right]^{5/4} \times \sqrt{\frac{m_c}{m_r}} \times N_r^{1/4} + 2a_4 \times \sqrt{\frac{\varepsilon_0(x)}{\varepsilon(r_a, x)}} \times N_r^{1/2} + a_5 \times \left[ \frac{\varepsilon_0(x)}{\varepsilon(r_a, x)} \right]^2 \times N_r^{1/6}$$

$$, N_r \equiv \left( \frac{N^*}{N_{\text{CDp}}(r_a, x)} \right), \Delta E_{\text{gp}}(N, r_a, x) = \Delta E_{\text{gpo}}(N, r_a, x) \times \{50 \times x + 100 \times (1 - x)\}, \quad (14p)$$

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

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

**OPTICAL BAND GAP**

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

$$E_{\text{gn1(gp1)}}(N, r_{d(a)}, x, T) \equiv$$

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

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

**OPTICAL COEFFICIENTS**

The optical properties of any medium can be described by the complex refraction index  $\mathbb{N}$  and the complex dielectric function  $\varepsilon$ ,  $\mathbb{N} \equiv n - i\kappa$  and  $\varepsilon \equiv \varepsilon_1 - i\varepsilon_2$ , where  $i^2 = -1$  and  $\varepsilon \equiv \mathbb{N}^2$ . Therefore, the real and imaginary parts of  $\varepsilon$  denoted by  $\varepsilon_1$  and  $\varepsilon_2$  can thus be expressed in terms of the refraction index  $n$  and the extinction coefficient  $\kappa$  as:  $\varepsilon_1 \equiv n^2 - \kappa^2$

and  $\epsilon_2 \equiv 2n\kappa$ . One notes that the optical absorption coefficient  $\alpha$  is related to  $\epsilon_2$ ,  $n$ ,  $\kappa$ , and the optical conductivity  $\sigma_0$ , by<sup>[2]</sup>

$$\alpha(E, N, r_{d(a)}, \mathbf{x}, T) \equiv \frac{\hbar q^2 \times |v(E)|^2}{n(E) \times \epsilon_{\text{free space}} \times c E} \times J(E^*) = \frac{E \times \epsilon_2(E)}{\hbar c n(E)} \equiv \frac{2E \times \kappa(E)}{\hbar c} \equiv \frac{4\pi \sigma_0(E)}{c n(E) \times \epsilon_{\text{free space}}},$$

$$\epsilon_1 \equiv n^2 - \kappa^2 \text{ and } \epsilon_2 \equiv 2n\kappa, \tag{16}$$

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

Here,  $-q$ ,  $\hbar$ ,  $|v(E)|$ ,  $\omega$ ,  $\epsilon_{\text{free space}}$ ,  $c$  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:  $|v(E)|^2$ ,  $J(E^*)$  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:

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

From Equations (16, 17), if the two optical functions,  $\epsilon_1$  and  $\epsilon_2$ , (or  $n$  and  $\kappa$ ), are both known, the other ones defined above can thus be determined, noting also that:  $E_{gn1(gp1)}(N, r_{d(a)}, \mathbf{x}, T) = E_{gn1(gp1)}$ , for a presentation simplicity.

Then, one has:

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

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

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

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

Further, one notes that, as  $E \rightarrow \infty$ , Forouhi and Bloomer (FB)<sup>[4]</sup> claimed that  $\kappa(E \rightarrow \infty) \rightarrow$  a constant, while the  $\kappa(E)$  -expressions, proposed by Van Cong<sup>[2]</sup> 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  $n^+(p^+) - p(n)$  X(x)- crystalline alloy, is now proposed as follows. Then, if denoting the functions G(E) and F(E) and by:

$$G(E) \equiv \sum_{i=1}^4 \frac{A_i}{E^2 - B_i E + C_i} \text{ and } F(E) \equiv \sum_{i=1}^4 \frac{A_i}{E^2 \times (1 + 10^{-4} \times \frac{E}{e}) - B_i E + C_i}, \text{ we propose:}$$

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

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

being equal to 0 for  $E^* = 0$  (or for  $E = E_{gn1(gp1)}$ ), and also going to 0 as  $E^{-1}$  as  $E \rightarrow \infty$ , and further,

$$n(E, N, r_{d(a)}, x, T) = n_{\infty}(r_{d(a)}, x) + \sum_{i=1}^4 \frac{X_i(E_{gn1(gp1)}) \times E + Y_i(E_{gn1(gp1)})}{E^2 - B_i E + C_i}. \tag{21}$$

going to a constant as  $E \rightarrow \infty$ , since  $n(E \rightarrow \infty, r_{d(a)}, x) \rightarrow n_{\infty}(r_{d(a)}, x) = \sqrt{\epsilon(r_{d(a)}, x)} \times \frac{\omega_T}{\omega_L}$ ,  $\omega_T = 5.1 \times 10^{13} \text{ s}^{-1}$  [5] and  $\omega_L = 8.9755 \times 10^{13} \text{ s}^{-1}$ .

Here, the other parameters are determined by:

$$X_i(E_{gn1(gp1)}) = \frac{A_i}{Q_i} \times \left[ -\frac{B_i^2}{2} + E_{gn1(gp1)} B_i - E_{gn1(gp1)}^2 + C_i \right],$$

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

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

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

Then, as noted above, if the two optical functions, n and  $\kappa$ , 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  $X(x) \equiv \text{CdTe}_{1-x}\text{S}_x$ - 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  $N = N_{CDn(CDp)}$ , giving rise to:  $E_{gn1(gp1)}(N^* = 0, r_{d(a)}, x, T = 0) = E_{gn1(gp1)}(r_{d(a)}, x) = E_{gno(gp0)}(r_{d(a)}, x)$ .

Then, in this MIT-case, if  $E = E_{gn1(gp1)}(r_{d(a)}, x) = E_{gno(gp0)}(r_{d(a)}, x)$ , 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):  $\varepsilon_{2(MIT)}(r_{d(a)}, x) = 0$ ,  $\sigma_{O(MIT)}(r_{d(a)}, x) = 0$  and  $\alpha_{MIT}(r_{d(a)}, x) = 0$ , and the other functions such as:  $n_{MIT}(r_{d(a)}, x)$  from Eq. (21), and  $\varepsilon_{1(MIT)}(r_{d(a)}, x)$  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:  $n(E \rightarrow \infty, r_{d(a)}, x, T) = n_{\infty}(r_{d(a)}, x) = \sqrt{\varepsilon(r_{d(a)}, x)} \times \frac{\omega_T}{\omega_L}$ ,  $\omega_T = 5.1 \times 10^{13} s^{-1}$  [5] and  $\omega_L = 8.9755 \times 10^{13} s^{-1}$ , was obtained from the Lyddane-Sachs-Teller relation<sup>[5]</sup>, from which T(L) represent the transverse (longitudinal) optical phonon modes. Then, from Equations (16, 17, 20), from such the asymptotic behavior ( $E \rightarrow \infty$ ), we obtain:  $\kappa_{\infty}(r_{d(a)}, x) \rightarrow 0$  and  $\varepsilon_{2,\infty}(r_{d(a)}, x) \rightarrow 0$ , as  $E^{-1}$ , so that  $\varepsilon_{1,\infty}(r_{d(a)}, x)$ ,  $\sigma_{O,\infty}(r_{d(a)}, x)$ ,  $\alpha_{\infty}(r_{d(a)}, x)$  and  $R_{\infty}(r_{d(a)}, x)$  go to their appropriate limiting constants for T=0K, as those investigated in Table 2 in Appendix 1.

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

In the P(Ga)-X(x)-system, at T=0K and  $N = N_{CDn(CDp)}(r_{P(Ga)}, x)$ , our numerical results of n,  $\kappa$ ,  $\varepsilon_1$  and  $\varepsilon_2$  are obtained from Equations (21, 20, 16), respectively, and expressed as functions of  $E [\geq E_{CPE}(r_{P(Ga)}, x)]$  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  $r_{d(a)}$  and x, and from Equations (12, 15, 21, 20, 16), respectively, we can determine the variations of  $\eta_{n(p)}(>> 1, \text{degenerate case})$ ,  $E_{gn1(gp1)}$ , n,  $\kappa$ ,  $\varepsilon_1$  and  $\varepsilon_2$ , obtained as functions of N, being represented by the arrows: ↗ and ↘, 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  $N = 10^{20} \text{cm}^{-3}$ , for given  $r_{d(a)}$  and  $x$ , and from Equations (12, 15, 21, 20, 16), respectively, we can determine the variations of  $\eta_{n(p)} (>> 1, \text{degenerate case})$ ,  $E_{gn1(gp1)}$ ,  $n$ ,  $\kappa$ ,  $\varepsilon_1$  and  $\varepsilon_2$ , 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  $\mathbf{X(x)} \equiv \text{CdTe}_{1-x}\mathbf{S_x}$  crystalline alloy, by basing on our two recent works<sup>[1,2]</sup>, for a given  $x$ , and with an increasing  $r_{d(a)}$ , the optical coefficients have been determined, as functions of the photon energy  $E$ , total impurity density  $N$ , the donor (acceptor) radius  $r_{d(a)}$ , concentration  $x$ , and temperature  $T$ .

Those results have been affected by (i) the important new  $\varepsilon(r_{d(a)}, x)$ -law, developed in Equations (8a, 8b), stating that, for a given  $x$ , due to the impurity-size effect,  $\varepsilon$  decreases ( $\searrow$ ) with an increasing ( $\nearrow$ )  $r_{d(a)}$ , and then by (ii) the generalized Mott critical  $d(a)$ -density defined in the metal-insulator transition (MIT),  $N_{CDn(NDp)}(r_{d(a)}, x)$ , 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  $2.82 \times 10^{-7}$ , as that given in Table 4 of Ref.<sup>[1]</sup>, 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  $\varepsilon(r_{d(a)}, x)$ -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, 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  $E_{CPE} = E = E_{gno(gp0)}(r_{d(a)}, x)$ , 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. (16), decrease ( $\searrow$ ) with increasing ( $\nearrow$ )  $r_{d(a)}$  and  $E_{CPE}$ .

Donor		P	Te	Sb	Sn
$r_d$ (nm) [4]	$\nearrow$	0.110	0.132	0.136	0.140
-----					
At $x=0$ ,					
$E_{CPE}$ in meV	$\nearrow$	1617.2	1620	1620.1	1620.4
$n_{MIT}$	$\searrow$	3.245	3.119	3.115	3.104
$\epsilon_{1(MIT)}$	$\searrow$	10.53	9.73	9.71	9.63
$R_{MIT}$	$\searrow$	0.280	0.265	0.264	0.263
-----					
At $x=0.5$ ,					
$E_{CPE}$ in meV	$\nearrow$	2095.1	2100	2100.2	2100.7
$n_{MIT}$	$\searrow$	2.884	2.761	2.757	2.746
$\epsilon_{1(MIT)}$	$\searrow$	8.32	7.62	7.60	7.54
$R_{MIT}$	$\searrow$	0.235	0.219	0.219	0.217
-----					
At $x=1$ ,					
$E_{CPE}$ in meV	$\nearrow$	2572.4	2580	2580.3	2581.1
$n_{MIT}$	$\searrow$	2.521	2.401	2.397	2.386
$\epsilon_{1(MIT)}$	$\searrow$	6.36	5.77	5.75	5.69
$R_{MIT}$	$\searrow$	0.187	0.170	0.169	0.168
-----					
Acceptor		Ga	In	Cd	
$r_a$ (nm)	$\nearrow$	0.126	0.144	0.148	
-----					
At $x=0$ ,					
$E_{CPE}$ in meV	$\nearrow$	1600.6	1619.3	1620	

$n_{MIT}$	↘	3.227	3.123	3.119
$\epsilon_{1(MIT)}$	↘	10.41	9.75	9.73
$R_{MIT}$	↘	0.277	0.265	0.265

At  $x=0.5$ ,

$E_{CPE}$ in meV	↗	2078.1	2099.2	2100
$n_{MIT}$	↘	2.867	2.765	2.761
$\epsilon_{1(MIT)}$	↘	8.22	7.64	7.62
$R_{MIT}$	↘	0.233	0.220	0.219

At  $x=1$ ,

$E_{CPE}$ in meV	↗	2555.1	2579.1	2580
$n_{MIT}$	↘	2.506	2.405	2.401
$\epsilon_{1(MIT)}$	↘	6.28	5.78	5.77
$R_{MIT}$	↘	0.184	0.170	0.1697

**Table 2:** Here, as  $T=0K$  and  $N=N_{CDn(p)}(r_{d(a)}, x)$ , and for  $E \rightarrow \infty$  the numerical results of  $n_{\infty}(r_{d(a)}, x)$ ,  $\epsilon_{1,\infty}(r_{d(a)}, x)$ ,  $\sigma_{O,\infty}(r_{d(a)}, x)$ ,  $\alpha_{\infty}(r_{d(a)}, x)$  and  $R_{\infty}(r_{d(a)}, x)$  go to their appropriate limiting constants.

Donor		P	Te	Sb	Sn
At $x=0$ ,					
$n_{\infty}$	↘	1.9479	1.8245	1.8207	1.8093
$\epsilon_{1,\infty}$	↘	3.7945	3.3287	3.3149	3.2734
$\sigma_{O,\infty}$ in $\frac{10^5}{\Omega \times cm}$	↘	8.8887	8.3253	8.3079	8.2558
$\alpha_{\infty}$ in $(10^9 \times cm^{-1})=$		2.1602			
$R_{\infty}$	↘	0.1034	0.0852	0.0846	0.0830
At $x=0.5$ ,					
$n_{\infty}$	↘	1.8851	1.7656	1.7619	1.7508
$\epsilon_{1,\infty}$	↘	3.5535	3.1173	3.1043	3.0655

$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega \times cm}$	↘	8.6017	8.0565	8.0397	7.9892
$\alpha_\infty$ in $(10^9 \times cm^{-1})=$		2.1602			
$R_\infty$	↘	0.0940	0.0766	0.0761	0.0745

At x=1,

$n_\infty$	↘	1.8200	1.7046	1.7011	1.6904
$\epsilon_{1,\infty}$	↘	3.3124	2.9058	2.8937	2.8575
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega \times cm}$	↘	8.3048	7.7784	7.7622	7.7135
$\alpha_\infty$ in $(10^9 \times cm^{-1})=$		2.1602			
$R_\infty$	↘	0.0845	0.0679	0.0674	0.0658

Acceptor

Ga

In

Cd

At x=0,

$n_\infty$	↘	1.920	1.827	1.824
$\epsilon_{1,\infty}$	↘	3.687	3.340	3.329
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega \times cm}$	↘	8.762	8.339	8.325
$\alpha_\infty$ in $(10^9 \times cm^{-1})=$		2.1602		
$R_\infty$	↘	0.099	0.086	0.085

At x=0.5,

$n_\infty$	↘	1.858	1.768	1.765
$\epsilon_{1,\infty}$	↘	3.453	3.127	3.117
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega \times cm}$	↘	8.479	8.069	8.056
$\alpha_\infty$ in $(10^9 \times cm^{-1})=$		2.1602		
$R_\infty$	↘	0.090	0.077	0.0766

At x=1,

$n_\infty$	↘	1.794	1.707	1.705
$\epsilon_{1,\infty}$	↘	3.218	2.915	2.906
$\sigma_{0,\infty}$ in $\frac{10^5}{\Omega \times cm}$	↘	8.186	7.791	7.778

$$\alpha_{\infty} \text{ in } (10^9 \times \text{cm}^{-1})=2.1602$$

$$R_{\infty} \quad \searrow \quad 0.081 \quad 0.068 \quad 0.0679$$

**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  $n$ ,  $\kappa$ ,  $\epsilon_1$  and  $\epsilon_2$  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)  $\kappa = 0$  and  $\epsilon_2 = 0$  at  $E = E_{CPE}(r_p, x)$ , and  $\kappa \rightarrow 0$  and  $\epsilon_2 \rightarrow 0$  as  $E \rightarrow \infty$ .

E in eV	$n$	$\kappa$	$\epsilon_1$	$\epsilon_2$
<b>At x=0,</b>				
<b><math>E_{CPE} = 1.6172</math></b>	<b>3.2446</b>	<b>0</b>	<b>10.5273</b>	<b>0</b>
2	3.538	0.218	12.473	1.540
2.5	4.159	0.295	17.213	2.454
3	4.247	1.571	15.568	13.340
3.5	3.518	1.846	8.972	12.989
4	3.658	1.718	10.426	12.573
4.5	4.001	2.704	8.694	21.639
5	2.344	3.825	-9.135	17.937
5.5	1.178	2.729	-6.048	6.424
6	1.288	2.048	-2.534	5.276
...				
<b><math>10^{22}</math></b>	<b>1.9479</b>	<b>0</b>	<b>3.7945</b>	<b>0</b>
<b>At x=0.5,</b>				
<b><math>E_{CPE} = 2.0951</math></b>	<b>2.8839</b>	<b>0</b>	<b>8.3169</b>	<b>0</b>
2	2.828	0.160	8.024	0.905
2.5	3.213	0.062	10.319	0.399
3	3.508	0.673	11.853	4.719
3.5	3.258	1.028	9.562	6.698
4	3.386	1.098	10.259	7.438
4.5	3.659	1.882	9.844	13.771
5	2.476	2.821	-1.826	13.968

5.5	1.556	2.097	-1.976	6.524
6	1.596	1.625	-0.094	5.189
...				
<b>10<sup>22</sup></b>	<b>1.8851</b>	<b>0</b>	<b>3.5535</b>	<b>0</b>

At x=1,

<b>E<sub>CPE</sub> =2.5724</b>	<b>2.5214</b>	<b>0</b>	<b>6.3576</b>	<b>0</b>
3	2.801	0.150	7.825	0.841
3.5	2.881	0.448	8.100	2.582
4	3.026	0.617	8.778	3.734
4.5	3.257	1.209	9.150	7.878
5	2.485	1.970	2.294	9.791
5.5	1.795	1.550	0.820	5.566
6	1.790	1.252	1.637	4.484
...				
<b>10<sup>22</sup></b>	<b>1.8200</b>	<b>0</b>	<b>3.3124</b>	<b>0</b>

E in eV	<i>n</i>	<i>κ</i>	<i>ε</i> <sub>1</sub>	<i>ε</i> <sub>2</sub>
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**Table 3p:** In the Ga-X(x)-system, and at T=0K and  $N = N_{CDP}(r_{Ga}, x)$ , according to the MIT, our numerical results of *n*, *κ*, *ε*<sub>1</sub> and *ε*<sub>2</sub> are obtained from Equations (21, 20, 16), respectively, and expressed as functions of  $E [\geq E_{CPE}(r_{Ga}, x)]$  and x, noting that (i)  $\kappa = 0$  and  $\epsilon_2 = 0$  at  $E = E_{CPE}(r_{Ga}, x)$ , and  $\kappa \rightarrow 0$  and  $\epsilon_2 \rightarrow 0$  as  $E \rightarrow \infty$ .

E in eV	<i>n</i>	<i>κ</i>	<i>ε</i> <sub>1</sub>	<i>ε</i> <sub>2</sub>
At x=0,				
<b>E<sub>CPE</sub> =1.6006</b>	<b>3.2271</b>	<b>0</b>	<b>10.4143</b>	<b>0</b>
2	3.536	0.219	12.456	1.548
2.5	4.166	0.306	17.262	2.552
3	4.243	1.609	15.415	13.651
3.5	3.495	1.878	8.689	13.133
4	3.636	1.743	10.182	12.671
4.5	3.982	2.735	8.371	21.785

5	2.308	3.863	-9.595	17.830
5.5	1.132	2.750	-6.281	6.228
6	1.245	2.063	-2.706	5.140
...				
<b>10<sup>22</sup></b>	<b>1.9201</b>	<b>0</b>	<b>3.6870</b>	<b>0</b>

At x=0.5,

<b>E<sub>CPE</sub> =2.0781</b>	<b>2.8675</b>	<b>0</b>	<b>8.2229</b>	<b>0</b>
2.5	3.214	0.067	10.323	0.433
3	3.504	0.698	11.794	4.893
3.5	3.241	1.053	9.394	6.823
4	3.368	1.118	10.094	7.531
4.5	3.643	1.909	9.626	13.905
5	2.444	2.854	-2.170	13.950
5.5	1.515	2.118	-2.188	6.419
6	1.558	1.640	-0.261	5.109
...				
<b>10<sup>22</sup></b>	<b>1.8581</b>	<b>0</b>	<b>3.4527</b>	<b>0</b>

At x=1,

<b>E<sub>CPE</sub> =2.5551</b>	<b>2.5062</b>	<b>0</b>	<b>6.2810</b>	<b>0</b>
3	2.800	0.162	7.802	0.910
3.5	2.868	0.465	8.012	2.667
4	3.012	0.632	8.676	3.802
4.5	3.245	1.231	9.013	7.988
5	2.458	1.998	2.052	9.824
5.5	1.761	1.568	0.639	5.523
6	1.757	1.265	1.486	4.445
...				
<b>10<sup>22</sup></b>	<b>1.7940</b>	<b>0</b>	<b>3.2185</b>	<b>0</b>

E in eV

*n*

*κ*

*ε*<sub>1</sub>

*ε*<sub>2</sub>

**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,  $\kappa$ ,  $\epsilon_1$  and  $\epsilon_2$ , obtained as functions of N, being represented by the arrows: ↗ and ↘, noting that both  $\eta_n$  and  $E_{gn1}$  increase with increasing N.

N ( $10^{18} \text{ cm}^{-3}$ )	↗	15	26	60	100
<b>x=0</b>					
-----					
For $r_d = r_{Te}$ ,					
$\eta_n \gg 1$	↗	238	344	602	846
$E_{gn1}$ in eV	↗	1.632	1.703	1.910	2.133
n	↘	3.864	3.796	3.591	3.361
$\kappa$	↘	1.822	1.662	1.234	0.844
$\epsilon_1$		11.612	↗ 11.649	↘ 11.371	10.583
$\epsilon_2$	↘	14.082	12.615	8.862	5.676
-----					
For $r_d = r_{Sb}$ ,					
$\eta_n \gg 1$	↗	238	344	602	846
$E_{gn1}$ in eV	↗	1.633	1.704	1.912	2.136
n	↘	3.859	3.791	3.584	3.354
$\kappa$	↘	1.819	1.658	1.229	0.839
$\epsilon_1$		11.584	↗ 11.620	↘ 11.337	10.543
$\epsilon_2$	↘	14.042	12.570	8.813	5.631
-----					
For $r_d = r_{Sn}$ ,					
$\eta_n \gg 1$	↗	238	344	602	846
$E_{gn1}$ in eV	↗	1.637	1.709	1.919	2.145
n	↘	3.844	3.774	3.566	3.332
$\kappa$	↘	1.811	1.647	1.215	0.825
$\epsilon_1$		11.500	↗ 11.533	↘ 11.237	10.425
$\epsilon_2$	↘	13.922	12.436	8.667	5.496

**x=0.5**

For  $r_d = r_{Te}$ ,

$\eta_n \gg 1$	↗	129	187	328	462
$E_{gn1}$ in eV	↗	2.082	2.116	2.220	2.334
n	↘	3.354	3.319	3.210	3.087
$\kappa$	↘	0.926	0.871	0.712	0.556
$\epsilon_1$	↘	10.396	10.260	9.796	9.220
$\epsilon_2$	↘	6.211	5.781	4.575	3.435

For  $r_d = r_{Sb}$ ,

$\eta_n \gg 1$	↗	128.6	186.9	328	462
$E_{gn1}$ in eV	↗	2.083	2.117	2.221	2.336
n	↘	3.350	3.315	3.205	3.081
$\kappa$	↘	0.924	0.869	0.710	0.554
$\epsilon_1$	↘	10.368	10.231	9.765	9.187
$\epsilon_2$	↘	6.194	5.762	4.553	3.413

For  $r_d = r_{Sn}$ ,

$\eta_n \gg 1$	↗	128.5	186.9	328	462
$E_{gn1}$ in eV	↗	2.086	2.120	2.225	2.341
n	↘	3.336	3.300	3.189	3.064
$\kappa$	↘	0.920	0.864	0.704	0.547
$\epsilon_1$	↘	10.285	10.146	9.674	9.090
$\epsilon_2$	↘	6.143	5.705	4.490	3.350

**x=1**

For  $r_d = r_{Te}$ ,

$\eta_n \gg 1$	↗	89	131	233	329
$E_{gn1}$ in eV	↗	2.567	2.592	2.670	2.755
n	↘	2.768	2.739	2.650	2.551

$\kappa$	$\searrow$	0.297	0.274	0.208	0.147
$\varepsilon_1$	$\searrow$	7.571	7.426	6.979	6.489
$\varepsilon_2$	$\searrow$	1.646	1.500	1.104	0.749

For  $r_d = r_{Sb}$ ,

$\eta_n \gg 1$	$\nearrow$	89	131	233	329
$E_{gn1}$ in eV	$\nearrow$	2.567	2.593	2.671	2.756

n	$\searrow$	2.763	2.734	2.645	2.546
$\kappa$	$\searrow$	0.297	0.273	0.207	0.146
$\varepsilon_1$	$\searrow$	7.548	7.402	6.954	6.463
$\varepsilon_2$	$\searrow$	1.640	1.494	1.098	0.743

For  $r_d = r_{Sn}$ ,

$\eta_n \gg 1$	$\nearrow$	89	131	233	329
$E_{gn1}$ in eV	$\nearrow$	2.569	2.595	2.674	2.760

n	$\searrow$	2.750	2.721	2.631	2.531
$\kappa$	$\searrow$	0.295	0.271	0.205	0.143
$\varepsilon_1$	$\searrow$	7.478	7.330	6.879	6.385
$\varepsilon_2$	$\searrow$	1.623	1.475	1.078	0.725

$N (10^{18} \text{ cm}^{-3})$	$\nearrow$	15	26	60	100
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**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,  $\kappa$ ,  $\varepsilon_1$  and  $\varepsilon_2$ , obtained as functions of N, being represented by the arrows:  $\nearrow$  and  $\searrow$ , noting that both  $\eta_p$  and  $E_{gp1}$  increase with increasing N.

$N (10^{20} \text{ cm}^{-3})$	$\nearrow$	1	2	3	4
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**x=0**

For  $r_a = r_{Ga}$ ,

$\eta_p \gg 1$	↗	610	1164	1606	1994
$E_{gp1}$ in eV	↗	1.072	1.217	1.421	1.639
n	↘	4.469	4.343	4.158	3.953
$\kappa$	↘	3.358	2.916	2.356	1.806
$\varepsilon_1$	↗	8.698	10.360	11.790	12.366
$\varepsilon_2$	↘	30.019	25.326	19.510	14.279

For  $r_a = r_{In}$ ,

$\eta_p \gg 1$	↗	517	1098	1551	1944
$E_{gp1}$ in eV	↗	1.155	1.337	1.578	1.827
n	↘	4.305	4.143	3.919	3.676
$\kappa$	↘	3.100	2.573	1.951	1.397
$\varepsilon_1$	↗	8.917	10.540	11.554	11.565
$\varepsilon_2$	↘	26.692	21.323	15.294	10.269

For  $r_a = r_{Cd}$ ,

$\eta_p \gg 1$	↗	513	1096	1548	1942
$E_{gp1}$ in eV	↗	1.157	1.340	1.582	1.833
n	↘	4.299	4.137	3.912	3.669
$\kappa$	↘	3.093	2.564	1.940	1.383
$\varepsilon_1$	↗	8.919	10.538	11.540	11.534
$\varepsilon_2$	↘	26.598	21.214	15.180	10.162

**x=0.5**

For  $r_a = r_{Ga}$ ,

$\eta_p \gg 1$	↗	308	619	863	1077
$E_{gp1}$ in eV		1.542	↘ 1.486	↗ 1.509	1.559
n		3.984	↗ 4.037	↘ 4.014	3.968
$\kappa$		2.038	↗ 2.179	↘ 2.119	1.997
$\varepsilon_1$		11.718	↘ 11.548	↗ 11.626	11.757
$\varepsilon_2$		16.238	↗ 17.591	↘ 17.015	15.849

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For  $r_a = r_{In}$ ,

$\eta_p \gg 1$	↗	245	576	827	1044
$E_{gp1}$ in eV		1.637	↘ 1.590	↗ 1.635	1.705
n		3.804	↗ 3.848	↘ 3.805	3.738
$\kappa$		1.811	↗ 1.921	↘ 1.814	1.657
$\varepsilon_1$		11.188	↘ 11.120	↗ 11.186	11.226
$\varepsilon_2$		13.780	↗ 14.782	↘ 13.807	12.386

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For  $r_a = r_{Cd}$ ,

$\eta_p \gg 1$	↗	243	574	826	1043
$E_{gp1}$ in eV		1.640	↘ 1.593	↗ 1.639	1.709
n		3.798	↗ 3.842	↘ 3.798	3.731
$\kappa$		1.804	↗ 1.913	↘ 1.805	1.647
$\varepsilon_1$		11.169	↘ 11.104	↗ 11.169	11.205
$\varepsilon_2$		13.702	↗ 14.701	↘ 13.716	12.289

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**x=1**

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For  $r_a = r_{Ga}$ ,

$\eta_p \gg 1$	↗	196	426	604	759
$E_{gp1}$ in eV	↗	2.272	2.281	2.335	2.402
n	↘	3.182	3.172	3.113	3.041
$\kappa$	↘	0.638	0.626	0.554	0.472
$\varepsilon_1$	↘	9.718	9.673	9.387	9.024
$\varepsilon_2$	↘	4.061	3.973	3.450	2.873

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For  $r_a = r_{In}$ ,

$\eta_p \gg 1$	↗	138	389	573	731
$E_{gp1}$ in eV	↗	2.336	2.345	2.413	2.492
n	↘	3.026	3.016	2.942	2.854
$\kappa$	↘	0.553	0.542	0.459	0.371

---

$\varepsilon_1$	$\searrow$	8.853	8.805	8.444	8.008
$\varepsilon_2$	$\searrow$	3.350	3.269	2.700	2.120

For  $r_a = r_{Cd}$ ,

$\eta_p \gg 1$	$\nearrow$	135	387	572	730
$E_{gp1}$ in eV	$\nearrow$	2.338	2.347	2.415	2.495
$n$	$\searrow$	3.021	3.011	2.936	2.848
$\kappa$	$\searrow$	0.550	0.539	0.456	0.368
$\varepsilon_1$	$\searrow$	8.824	8.779	8.415	7.977
$\varepsilon_2$	$\searrow$	3.326	3.249	2.679	2.099

$N$ ( $10^{20} \text{ cm}^{-3}$ ) $\nearrow$	<b>1</b>	<b>2</b>	<b>3</b>	<b>4</b>
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**Table 5n:** In the X(x)-system, at  $E=3.2 \text{ eV}$  and  $N = 10^{20} \text{ cm}^{-3}$ , for given  $r_d$  and  $x$ , and from Equations (12, 15, 21, 20, 16), respectively, we can determine the variations of  $\eta_n$  ( $\gg 1$ , degenerate case),  $E_{gn1}$ ,  $n$ ,  $\kappa$ ,  $\varepsilon_1$  and  $\varepsilon_2$ , obtained as functions of  $T$ , being represented by the arrows:  $\nearrow$  and  $\searrow$ , noting that both  $\eta_n$  and  $E_{gn1}$  decrease with increasing  $T$ .

$T$ in K $\nearrow$	20	50	100	300
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$x=0$

For  $r_d = r_{Te}$ ,

$\eta_n \gg 1$	$\searrow$	846	339	169	56
$E_{gn1}$ in eV	$\searrow$	2.133	2.128	2.118	2.063
$n$	$\nearrow$	3.361	3.365	3.376	3.433
$\kappa$	$\nearrow$	0.844	0.851	0.868	0.958
$\varepsilon_1$	$\nearrow$	10.583	10.601	10.647	10.871
$\varepsilon_2$	$\nearrow$	5.676	5.729	5.861	6.576

For  $r_d = r_{Sb}$ ,

$\eta_n \gg 1$	$\searrow$	846	338.6	169	56
$E_{gn1}$ in eV	$\searrow$	2.135	2.131	2.121	2.066

n	↗	3.354	3.358	3.369	3.426
$\kappa$	↗	0.839	0.846	0.863	0.952
$\varepsilon_1$	↗	10.543	10.562	10.608	10.832
$\varepsilon_2$	↗	5.631	5.683	5.815	6.526

For  $r_d = r_{Sn}$ ,

$\eta_n \gg 1$	↘	846	338.6	169	56
$E_{gn1}$ in eV	↘	2.145	2.141	2.130	2.076

n	↗	3.332	3.337	3.348	3.405
$\kappa$	↗	0.825	0.831	0.848	0.936
$\varepsilon_1$	↗	10.425	10.444	10.490	10.717
$\varepsilon_2$	↗	5.496	5.548	5.677	6.378

x=0.5

For  $r_d = r_{Te}$ ,

$\eta_n \gg 1$	↘	462	185	92.4	31
$E_{gn1}$ in eV	↘	2.334	2.329	2.318	2.251

n	↗	3.087	3.092	3.104	3.177
$\kappa$	↗	0.556	0.562	0.577	0.668
$\varepsilon_1$	↗	9.220	9.243	9.303	9.645
$\varepsilon_2$	↗	3.435	3.474	3.581	4.243

For  $r_d = r_{Sb}$ ,

$\eta_n \gg 1$	↘	462	185	92.4	31
$E_{gn1}$ in eV	↘	2.336	2.331	2.320	2.253

n	↗	3.081	3.086	3.098	3.171
$\kappa$	↗	0.554	0.559	0.574	0.665
$\varepsilon_1$	↗	9.187	9.210	9.271	9.612
$\varepsilon_2$	↗	3.413	3.453	3.559	4.219

For  $r_d = r_{Sn}$ ,

$\eta_n \gg 1$	↘	462	185	92.4	31
$E_{gn1}$ in eV	↘	2.341	2.337	2.325	2.258

n	↗	3.064	3.069	3.081	3.154
$\kappa$	↗	0.547	0.552	0.567	0.657
$\varepsilon_1$	↗	9.090	9.112	9.173	9.514
$\varepsilon_2$	↗	3.350	3.389	3.494	4.146

**x=1**

For  $r_d = r_{Te}$ ,

$\eta_n \gg 1$	↘	329	132	66	22
$E_{gn1}$ in eV	↘	2.755	2.750	2.738	2.658

n	↗	2.551	2.557	2.571	2.663
$\kappa$	↗	0.147	0.150	0.158	0.217
$\varepsilon_1$	↗	6.489	6.514	6.586	7.045
$\varepsilon_2$	↗	0.749	0.766	0.814	1.158

For  $r_d = r_{Sb}$ ,

$\eta_n \gg 1$	↘	329	132	66	22
$E_{gn1}$ in eV	↘	2.756	2.752	2.739	2.660

n	↗	2.546	2.551	2.566	2.658
$\kappa$	↗	0.146	0.149	0.157	0.216
$\varepsilon_1$	↗	6.463	6.488	6.560	7.018
$\varepsilon_2$	↗	0.743	0.759	0.807	1.150

For  $r_d = r_{Sn}$ ,

$\eta_n \gg 1$	↘	329	132	66	22
$E_{gn1}$ in eV	↘	2.760	2.756	2.743	2.664

n	↗	2.531	2.536	2.551	2.643
$\kappa$	↗	0.143	0.146	0.154	0.213
$\varepsilon_1$	↗	6.385	6.410	6.482	6.938
$\varepsilon_2$	↗	0.725	0.741	0.788	1.126

T in K	↗	20	50	100	300
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**Table 5p:** In the X(x)-system, at E=3.2 eV and  $N = 10^{20} \text{cm}^{-3}$ , 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,  $\kappa$ ,  $\epsilon_1$  and  $\epsilon_2$ , obtained as functions of T, being represented by the arrows: ↗ and ↘, noting that both  $\eta_p$  and  $E_{gp1}$  decrease with increasing T.

T in K		20	50	100	300
<b>x=0</b>					
-----					
For $r_a = r_{Ga}$ ,					
$\eta_p \gg 1$	↘	610	244	122	41
$E_{gp1}$ in eV	↘	1.072	1.067	1.057	1.002
n	↗	4.469	4.473	4.482	4.528
$\kappa$	↗	3.358	3.372	3.405	3.581
$\epsilon_1$	↘	8.698	8.640	8.495	7.684
$\epsilon_2$	↗	30.019	30.164	30.523	32.433
-----					
For $r_a = r_{In}$ ,					
$\eta_p \gg 1$	↘	517	207	103	34
$E_{gp1}$ in eV	↘	1.155	1.151	1.140	1.085
n	↗	4.305	4.308	4.317	4.365
$\kappa$	↗	3.100	3.113	3.145	3.315
$\epsilon_1$	↘	8.917	8.869	8.747	8.064
$\epsilon_2$	↗	26.692	26.826	27.160	28.938
-----					
For $r_a = r_{Cd}$ ,					
$\eta_p \gg 1$	↘	513	205	102.7	34
$E_{gp1}$ in eV	↘	1.157	1.153	1.142	1.088
n	↗	4.299	4.303	4.312	4.360
$\kappa$	↗	3.093	3.106	3.138	3.307
$\epsilon_1$	↘	8.919	8.871	8.750	8.070
$\epsilon_2$	↗	26.598	26.732	27.065	28.839

**x=0.5**

For  $\mathbf{r}_a = \mathbf{r}_{Ga}$ ,

$\eta_p \gg 1$	↘	308	123	62	20
$E_{gp1}$ in eV	↘	1.542	1.538	1.526	1.459
n	↗	3.984	3.988	3.999	4.062
$\kappa$	↗	2.038	2.049	2.077	2.248
$\varepsilon_1$	↘	11.718	11.707	11.676	11.445
$\varepsilon_2$	↗	16.238	16.339	16.612	18.260

For  $\mathbf{r}_a = \mathbf{r}_{In}$ ,

$\eta_p \gg 1$	↘	245	98	49	16
$E_{gp1}$ in eV	↘	1.637	1.632	1.621	1.553
n	↗	3.804	3.808	3.819	3.883
$\kappa$	↗	1.811	1.821	1.848	2.010
$\varepsilon_1$	↘	11.188	11.183	11.168	11.040
$\varepsilon_2$	↗	13.780	13.872	14.119	15.613

For  $\mathbf{r}_a = \mathbf{r}_{Cd}$ ,

$\eta_p \gg 1$	↘	243	97	48	16
$E_{gp1}$ in eV	↘	1.640	1.636	1.624	1.556
n	↗	3.798	3.802	3.813	3.877
$\kappa$	↗	1.804	1.814	1.841	2.002
$\varepsilon_1$	↘	11.169	11.165	11.151	11.026
$\varepsilon_2$	↗	13.702	13.793	14.039	15.528

**x=1**

For  $\mathbf{r}_a = \mathbf{r}_{Ga}$ ,

$\eta_p \gg 1$	↘	196	78	39	13
$E_{gp1}$ in eV	↘	2.272	2.268	2.255	2.175
n	↗	3.182	3.187	3.200	3.286

$\kappa$	$\nearrow$	0.638	0.644	0.662	0.779
$\varepsilon_1$	$\nearrow$	9.718	9.740	9.804	10.190
$\varepsilon_2$	$\nearrow$	4.061	4.106	4.235	5.118

For  $\Gamma_a = \Gamma_{In}$ ,

$\eta_p \gg 1$	$\searrow$	138	55	27	9.1
$E_{gp1}$ in eV	$\searrow$	2.336	2.331	2.319	2.238

n	$\nearrow$	3.026	3.031	3.045	3.132
$\kappa$	$\nearrow$	0.553	0.559	0.575	0.686
$\varepsilon_1$	$\nearrow$	8.853	8.876	8.941	9.340
$\varepsilon_2$	$\nearrow$	3.350	3.390	3.505	4.297

For  $\Gamma_a = \Gamma_{Cd}$ ,

$\eta_p \gg 1$	$\searrow$	135	54	27	9
$E_{gp1}$ in eV	$\searrow$	2.338	2.334	2.321	2.240

n	$\nearrow$	3.021	3.026	3.040	3.127
$\kappa$	$\nearrow$	0.550	0.556	0.572	0.683
$\varepsilon_1$	$\nearrow$	8.824	8.847	8.912	9.311
$\varepsilon_2$	$\nearrow$	3.326	3.366	3.480	4.270

T in K	$\nearrow$	20	50	100	300
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