wjert, 2024, Vol. 10 Issue 4, 191-220. **Review Article** **ISSN 2454-695X**

World Journal of Engineering Research and Technology
WJERT
www.wjert.org
SJIF Impact Factor: 5.924

CRITICAL DENSITY IN METAL-INSULATOR TRANSITION, OBTAINED IN N(P)- TYPE DEGENERATE [$InSb_{1-x}P_x$ (As_x), $GaSb_{1-x}P_x$(As_x, Te_x), $CdSe_{1-x}S_x$(Te_x)]- CRYSTALLINE ALLOYS, AND EXPLAINED BY THAT OF CARIERS LOCALIZED IN EXPONENTIAL BAND TAILS. (III)

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.

Article Received on 21/02/2024 **Article Revised on 10/03/2024** **Article Accepted on 30/03/2024**

***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.

ABTRACT

By basing on the same physical model and treatment method, as used in our recent works (Van Cong, 2024), for various [$InP_{1-x}As_x$ (Sb_x), $GaAs_{1-x}Te_x$(Sb_x, P_x), $CdS_{1-x}Te_x$(Se_x)]- and- [$InAs_{1-x}P_x$ (Sb_x), $GaTe_{1-x}As_x$(Sb_x, P_x), $CdTe_{1-x}S_x$(Se_x)]- crystalline alloys, referred to as: I and II, we will investigate the critical impurity densities in the metal-insulator transition (MIT), obtained now in n(p)-type degenerate X(x)≡ [$InSb_{1-x}P_x$ (As_x), $GaSb_{1-x}P_x$(As_x, Te_x), $CdSe_{1-x}S_x$(Te_x)]-crystalline alloys, due to the effects of the size of donor (acceptor) d(a)-radius, $r_{d(a)}$ and the x- concentration, assuming that all the impurities are ionized even at T=0 K. In such n(p)-type degenerate X(x)≡-crystalline alloys, we will determine: (i)-the critical impurity density $N_{CDn(CDp)}(r_{d(a)}, x)$ in the MIT, as that given in Eq. (8a), by using an empirical Mott parameter $M_{n(p)} = 0.25$, noting that this one could be explained from the definition of the relative effective Wigner-Seitz (WS) radius in the MIT, being a constant for given $r_{d(a)}$ and x, as that given in Eq. (8b), and *(ii)-the density of electrons (holes) localized in the exponential conduction (valence)-band tails (EBT),* $N^{EBT}_{CDn(CDp)}(r_{d(a)}, x)$*, as that given in Eq. (26), by using our empirical Heisenberg parameter,* $\mathcal{H}_{n(p)} = 0.47137$*, as that given in Eq. (15), suggesting*

also that: for given $r_{d(a)}$ *and x,* $N^{EBT}_{CDn(CDp)}(r_{d(a)}, x) \cong N_{CDn(CDp)}(r_{d(a)}, x)$*, obtained with a precision of the order of* 2.92×10^{-7} *, as observed in Tables 2-8.* In other words, such the critical d(a)-density $N_{CDn(NDp)}(r_{d(a)}), x)$, is just the density of electrons (holes) localized in the EBT, $N^{EBT}_{CDn(CDp)}(r_{d(a)}, x)$. So, if denoting the total impurity density by N, the effective density of free electrons (holes), N^*, given in the parabolic conduction (valence) band of the n(p)-type degenerate $X(x)$- crystalline alloy, can thus be defined, as the compensated ones, by: $N^*(N, r_{d(a)}, x) \equiv N - N_{CDn(NDp)} \cong N - N^{EBT}_{CDn(CDp)}$, needing to determine various optical, electrical, and thermoelectric properties in such n(p)-type degenerate X(x)-crystalline alloys, as those studied in n(p)-type degenerate crystals (Van Cong, 2023).

KEYWORS: $[InSb_{1-x}P_x\,(As_x), GaSb_{1-x}P_x(As_x, Te_x), CdSe_{1-x}S_x(Te_x)]$- crystalline alloys; critical impurity density in the Mott MIT.

INTRODUCTION

By basing on the same energy-band-structure parameters, physical model and treatment method, as used in our recent works for various $[InP_{1-x}As_x\,(Sb_x), GaAs_{1-x}Te_x(Sb_x, P_x), CdS_{1-x}Te_x(Se_x)]$- and- $[InAs_{1-x}P_x\,(Sb_x), GaTe_{1-x}As_x(Sb_x, P_x), CdTe_{1-x}S_x(Se_x)]$- crystalline alloys, referred to as: I and II (Van Cong, 2024), and also other works (Green, 2022; Kittel, 1976; Moon et al., 2016; Van Cong et al., 2014; Van Cong & Debiais, 1993; Van Cong et al., 1984), we will investigate the critical impurity density in the metal-insulator transition (MIT), obtained in X(x)≡ $[InSb_{1-x}P_x\,(As_x), GaSb_{1-x}P_x(As_x, Te_x), CdSe_{1-x}S_x(Te_x)]$- crystalline alloys, being also due to the effects of the size of donor (acceptor) d(a)-radius, $r_{d(a)}$, and the x- concentration, assuming that all the impurities are ionized even at T=0 K. In such n(p)-type degenerate crystalline alloys, we will determine.

(i)- the critical impurity density $N_{CDn(CDp)}(r_{d(a)}, x)$ in the MIT, as that given in Eq. (8a), by using an empirical Mott parameter $M_{n(p)} = 0.25$, noting that this one could be explained from the definition of the relative effective Wigner-Seitz (WS) radius in the MIT, being a constant for given $r_{d(a)}$ and x, as that given in Eq. (8b), and *(ii)-the density of electrons (holes) localized in the exponential conduction(valence)-band tails (EBT),* $N^{EBT}_{CDn(CDp)}(r_{d(a)}, x)$*, as that given in Eq. (26), by using the empirical Heisenberg parameter,* $\mathcal{H}_{n(p)} = 0.47137$*, as that given in Eq. (17), according to: for given* $r_{d(a)}$ *and x,* $N^{EBT}_{CDn(CDp)}(r_{d(a)}, x) \cong N_{CDn(CDp)}(r_{d(a)}, x)$, *with a precision of the order of* 2.92×10^{-7}, *as observed in Tables 2-8. In other words, such the critical d(a)-density* $N_{CDn(NDp)}(r_{d(a)}, x)$, *is just the density of electrons (holes), being localized in the EBT,* $N_{CDn(CDp)}^{EBT}(r_{d(a)}, x)$. In the following, we will determine those functions: $N_{CDn(CDp)}(r_{d(a)}, x)$ and $N_{CDn(CDp)}^{EBT}(r_{d(a)}, x)$.

CRITICAL DENSITY IN THE MOTT MIT

Such the critical impurity density $N_{CDn(CDp)}(r_{d(a)}, x)$, expressed as a function of $r_{d(a)}$ and x, is determined as follows.

Effect of x-concentration

Here, the values of the intrinsic energy-band-structure parameters, such as (Van Cong, 2024): the effective average number of equivalent conduction (valence)-band edges, $g_{c(v)}(x)$, the unperturbed relative effective electron (hole) mass in conduction (valence) bands, $m_{c(v)}(x)/m_o$, m_o being the electron rest mass, the unperturbed relative dielectric static constant, $\varepsilon_o(x)$, and the intrinsic energy gap, $E_{go}(x)$, at $r_{d(a)} = r_{do(ao)}$, are given respectively in Table 1 in Appendix 1.

Table 1 in Appendix 1

Therefore, one gets the effective donor (acceptor)-ionization energy, $E_{do(ao)}(x)$, as:

$$E_{do(ao)}(x) = \frac{13600 \times [m_{c(v)}(x)/m_o]}{[\varepsilon_o(x)]^2} \text{ meV}, \quad (1)$$

and the isothermal bulk modulus, $B_{do(ao)}(x)$, by:

$$B_{do(ao)}(x) \equiv \frac{E_{do(ao)}(x)}{(4\pi/3) \times (r_{do(ao)})^3}. \quad (2)$$

Effects of impurity size, with a given x

Here, one shows that the effects of the size of donor (acceptor) d(a)-radius, $r_{d(a)}$, and the x-concentration, strongly affects the changes in all the energy-band-structure parameters, which can be represented by the effective relative static dielectric constant $\varepsilon(r_{d(a)}, x)$ (Van Cong, 2024; Van Cong et al., 1984), in the following.

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, as: $p_o = 0$, and for the deformation potential energy (or the strain energy) σ, as: $\sigma_o = 0$. Further, the two important equations, 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: $\frac{d}{dV}(\frac{d\sigma}{dV}) = \frac{B}{V}$. Then, by an integration, one gets:

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

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 $E_{gno(gpo)}(r_{d(a)}, x)$, and in the effective donor (acceptor)-ionization energy $E_{d(a)}(r_{d(a)}, x)$ in the absolute values, being obtained from the effective Bohr model, and then such the compression (dilatation) is represented respectively by: $\pm[\Delta\sigma(r_{d(a)}, x)]_{n(p)}$,

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

,

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

$$E_{gno(gpo)}(r_{d(a)}, x) - E_{go}(x) = E_{d(a)}(r_{d(a)}, x) - E_{do(ao)}(x) = E_{do(ao)}(x) \times \left[\left(\frac{\varepsilon_o(x)}{\varepsilon(r_{d(a)})}\right)^2 - 1\right] = -[\Delta\sigma(r_{d(a)}, x)]_{n(p)} \quad . (4)$$

Therefore, from above Equations (3) and (4), one obtains the expressions for relative dielectric constant $\varepsilon(r_{d(a)}, x)$ and energy band gap $E_{gn(gp)}(r_{d(a)}, x)$, as:

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

$$E_{gno(gpo)}(r_{d(a)}, x) - E_{go}(x) = E_{d(a)}(r_{d(a)}, x) - E_{do(ao)}(x) = E_{do(ao)}(x) \times \left[\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 - 1\right] \times \ln\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 \geq 0, \quad (5)$$

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

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

$$E_{gno(gpo)}(r_{d(a)}, x) - E_{go}(x) = E_{d(a)}(r_{d(a)}, x) - E_{do(ao)}(x) = -E_{do(ao)}(x) \times \left[\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 - 1\right] \times \ln\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 \leq 0, \quad (6)$$

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

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

$$a_{Bn(Bp)}(r_{d(a)}, x) \equiv \frac{\varepsilon(r_{d(a)}, x) \times \hbar^2}{m_{c(v)}(x) \times q^2} = 0.53 \times 10^{-8}\ \text{cm} \times \frac{\varepsilon(r_{d(a)}, x)}{m_{c(v)}(x)/m_o}, \quad (7)$$

where $-q$ is the electron charge.

Then, the critical donor (acceptor)-density in the Mott MIT, $N_{CDn(NDp)}(r_{d(a)}, x)$, is determined, using an empirical Mott parameter, $M_{n(p)}$, as:

$$[N_{CDn(NDp)}(r_{d(a)}, x)]^{1/3} \times a_{Bn(Bp)}(r_{d(a)}, x) = M_{n(p)} = 0.25, \qquad (8a)$$

Noting that, in general case, such values of $M_{n(p)}$ could be chosen, such that the obtained numerical $N_{CDn(NDp)}(r_{d(a)}, x)$-results are found to be in good agreement with the corresponding experimental ones.

It should be noted that the above Mott result (8a) could be explained from the definition of the relative effective Wigner-Seitz (WS) radius in the MIT, being a constant for given $r_{d(a)}$ and x, as:

$$r_{s;\,Cn(Cp)}(r_{d(a)}, x) \equiv \frac{\mathcal{C}^{1/3}}{(N_{CDn(NDp)}(r_{d(a)}, x))^{1/3} \times a_{Bn(Bp)}(r_{d(a)}, x)}, \mathcal{C}^{1/3} \equiv \left(\frac{3}{4\pi}\right)^{1/3} = 0.6203505, \text{ or}$$

$$[N_{CDn(NDp)}(r_{d(a)}, x)]^{1/3} \times a_{Bn(Bp)}(r_{d(a)}, x) \equiv \mathcal{C}^{1/3}/r_{s;\,Cn(Cp)}(r_{d(a)}, x) = WS_{n(p)}. \qquad (8b)$$

Here, $WS_{n(p)}$ or $r_{s;\,Cn(Cp)}$ could be chosen, such that the obtained numerical $N_{CDn(NDp)}(r_{d(a)}, x)$-results are found to be in good agreement with the corresponding experimental ones. In particular, if $r_{s;\,Cn(Cp)} = 2.481402$, one gets: $WS_{n(p)} = 0.25 = M_{n(p)}$, as observed in Eq. (8a).

In the following, such numerical $N_{CDn(NDp)}(r_{d(a)}, x)$-results can also be justified by the numerical results of the density of electrons (holes), being localized in exponential conduction (valence)-band (EBT) tails, $N^{EBT}_{CDn(CDp)}(r_{d(a)}, x)$, with a precision of the order of 2.92×10^{-7}, as those observed in Tables 2-8 in Appendix 1.

$N^{EBT}_{CDn(CDp)}(r_{d(a)}, x)$- EXPRESSION

In order to determine $N^{EBT}_{CDn(CDp)}(r_{d(a)}, x)$, we first present our physical model and also our mathematical methods.

Physical model

In n(p)-type degenerate $X(x)$-crystalline alloys, if denoting the Fermi wave number by: $k_{Fn(Fp)}(N, x) \equiv (3\pi^2 N/g_{c(v)}(x))^{1/3}$, N being the total impurity density, the effective reduced Wigner-Seitz radius $r_{sn(sp)}$, characteristic of interactions, is defined by:

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

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

$$R_{sn(sp)}(N, r_{d(a)}, x) \equiv \frac{k_{sn(sp)}}{k_{Fn(Fp)}} = \frac{k_{Fn(Fp)}^{-1}}{k_{sn(sp)}^{-1}} = R_{snWS(spWS)} + \left[R_{snTF(spTF)} - R_{snWS(spWS)}\right] e^{-r_{sn(sp)}} < 1. \quad (10)$$

These ratios, $R_{snTF(spTF)}$ and $R_{snWS(spWS)}$, are determined in the following.

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

$$R_{snTF}(N, r_{d(a)}, x) \equiv \frac{k_{snTF(spTF)}}{k_{Fn(Fp)}} = \frac{k_{Fn(Fp)}^{-1}}{k_{snTF(spTF)}^{-1}} = \sqrt{\frac{4\gamma r_{sn(sp)}(N, r_{d(a)}, x)}{\pi}} \ll 1, \quad (11)$$

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

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

$$R_{snWS(spWS)}(N, r_{d(a)}, x) \equiv \frac{k_{snWS(spWS)}}{k_{Fn(Fp)}} = \left(\frac{3}{2\pi} - \gamma \frac{d\left[r_{sn(sp)}^{2} \times E_{CE}\right]}{dr_{sn(sp)}}\right) \times 0.5 ,$$

(12) where $E_{CE}(N, r_{d(a)}, x)$ is the majority-carrier correlation energy (CE), being determined by:

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

So, n(p)-type degenerate $X(x)$- crystalline alloys, the physical conditions are found to be given by :

$$\frac{k_{Fn(Fp)}^{-1}}{a_{Bn(Bp)}} < \frac{\eta_{n(p)}}{E_{Fno(Fpo)}} \equiv \frac{1}{A_{n(p)}} < \frac{k_{Fn(Fp)}^{-1}}{k_{sn(sp)}^{-1}} \equiv R_{sn(sp)}(N, r_{d(a)}, x) < 1, \quad A_{n(p)}(N, r_{d(a)}, x) \equiv \frac{\pm E_{Fno(Fpo)}}{\eta_{n(p)}}. \quad (13)$$

Here, $\pm E_{Fno(Fpo)}$ is the Fermi energy at 0 K, and $\eta_{n(p)}$ is defined as :$\pm E_{Fno(Fpo)}(N, x) = \frac{\hbar^2 \times k_{Fn(Fp)}(N, x)^2}{2 \times m_{c(v)}(x)} \geq 0, \eta_{n(p)}(N, r_{d(a)}, x) = \frac{\sqrt{2\pi N}}{\varepsilon(r_{d(a)}, x)} \times q^2 k_{sn(sp)}^{-1/2}$.

Then, the total screened Coulomb impurity potential energy due to the attractive interaction between an electron (hole) charge, $-q(+q)$, at position $\vec{r}$, and an ionized donor (ionized acceptor) charge: $+q(-q)$ at position $\overrightarrow{R_j}$, randomly distributed throughout $X(x)$- crystalline alloys, is defined by:

$$V(r) \equiv \sum_{j=1}^{N} v_j(r) + V_o, \quad (14)$$

where $\mathbb{N}$ is the total number of ionized donors (acceptors), V_o is a constant potential energy, and the screened Coulomb potential energy $v_j(r)$ is defined as:

$$v_j(r) \equiv -\frac{q^2 \times \exp(-k_{sn(sp)} \times |\vec{r}-\vec{R_j}|)}{\varepsilon(r_{d(a)}) \times |\vec{r}-\vec{R_j}|},$$

where $k_{sn(sp)}$ is the inverse screening length determined in Eq. (11).

Further, using a Fourier transform, the v_j-representation in wave vector $\vec{k}$-espace is given by

$$v_j(\vec{k}) = -\frac{q^2}{\varepsilon(r_{d(a)})} \times \frac{4\pi}{\Omega} \times \frac{1}{k^2 + k_{sn(sp)}^2},$$

where Ω is the total $X(x)$- crystalline alloy volume.

Then, the effective auto-correlation function for potential fluctuations, $W_{n(p)}(\nu_{n(p)}, N, r_{d(a)}) \equiv \langle V(r)V(r') \rangle$, was determined, [4, 5] as :

$$W_{n(p)}(\nu_{n(p)}, N, r_{d(a)}, x) \equiv \eta_{n(p)}^2 \times \exp\left(\frac{-\mathcal{H}_{n(p)} \times R_{sn(sp)}(N, r_{d(a)}, x)}{2\sqrt{|\nu_{n(p)}|}}\right), \quad \eta_{n(p)}(N, r_{d(a)}, x) \equiv \frac{\sqrt{2\pi N}}{\varepsilon(r_{d(a)})} \times q^2 k_{sn(sp)}^{-1/2},$$

$$\nu_{n(p)}(E, N, x) \equiv \frac{\mp E}{\pm E_{Fno(Fpo)}(N, x)}, \quad \mathcal{H}_{n(p)} = 0.47137 . \qquad (15)$$

Here, E is the total electron energy, and the empirical Heisenberg parameter $\mathcal{H}_{n(p)} = 0.47137$ was chosen above such that the determination of the density of electrons localized in the conduction(valence)-band tails will be accurate, noting that as $E \to \pm\infty$, $|\nu_{n(p)}| \to \infty$, and therefore, $W_{n(p)} \to \eta_{n(p)}^2$.

In the following, we will calculate the ensemble average of the function: $(E - V)^{a-\frac{1}{2}} \equiv E_k^{a-\frac{1}{2}}$, for $a \geq 1$, $E_k \equiv \frac{\hbar^2 \times k^2}{2 \times m_{c(v)}(x)}$ being the kinetic energy of the electron (hole), and $V(r)$ determined in Eq. (16), by using the two following integration methods, which strongly depend on $W_{n(p)}(\nu_{n(p)}, N, r_{d(a)}, x)$.

Mathematical Methods

Kane integration method (KIM)

Here, the effective Gaussian distribution probability is defined by:

$$P(V) \equiv \frac{1}{\sqrt{2\pi W_{n(p)}}} \times \exp\left[\frac{-V^2}{2W_{n(p)}}\right]. \qquad (16)$$

So, in the Kane integration method, the Gaussian average of $(E - V)^{a-\frac{1}{2}} \equiv E_k^{a-\frac{1}{2}}$ is defined by

$$\langle (E - V)^{a-\frac{1}{2}} \rangle_{KIM} \equiv \langle E_k^{a-\frac{1}{2}} \rangle_{KIM} = \int_{-\infty}^{E} (E - V)^{a-\frac{1}{2}} \times P(V) dV, \quad \text{for } a \geq 1.$$

Then, by variable changes: $s = (E - V)/\sqrt{W_{n(p)}}$ and $y = \mp E/\sqrt{W_{n(p)}} \equiv \frac{\pm E_{Fno(Fpo)}}{\eta_{n(p)}} \times v_{n(p)} \times \exp\left(\frac{\mathcal{H}_{n(p)} \times R_{sn(sp)}}{4 \times \sqrt{|v_{n(p)}|}}\right)$, and using an identity:

$\int_0^{\infty} s^{a-\frac{1}{2}} \times \exp(-ys - \frac{s^2}{2}) ds \equiv \Gamma(a + \frac{1}{2}) \times \exp(y^2/4) \times D_{-a-\frac{1}{2}}(y)$,

where $D_{-a-\frac{1}{2}}(y)$ is the parabolic cylinder function and $\Gamma(a + \frac{1}{2})$ is the Gamma function, one thus has:

$$\langle E_k^{a-\frac{1}{2}} \rangle_{KIM} = \frac{\exp(-y^2/4) \times W_{n(p)}^{\frac{2a-1}{4}}}{\sqrt{2\pi}} \times \Gamma(a + \tfrac{1}{2}) \times D_{-a-\frac{1}{2}}(y) = \frac{\exp(-y^2/4) \times \eta_{n(p)}^{a-\frac{1}{2}}}{\sqrt{2\pi}} \times \exp\left(-\frac{\mathcal{H}_{n(p)} \times R_{sn(sp)} \times (2a-1)}{8 \times \sqrt{|v_{n(p)}|}}\right) \times \Gamma(a + \tfrac{1}{2}) \times D_{-a-\frac{1}{2}}(y) \quad . \ (16)$$

Feynman path-integral method (FPIM)

Here, the ensemble average of $(E - V)^{a-\frac{1}{2}} \equiv E_k^{a-\frac{1}{2}}$ is defined by

$\langle (E - V)^{a-\frac{1}{2}} \rangle_{FPIM} \equiv \langle E_k^{a-\frac{1}{2}} \rangle_{FPIM} \equiv \frac{\hbar^{a-\frac{1}{2}}}{2^{3/2} \times \sqrt{2\pi}} \times \frac{\Gamma(a+\frac{1}{2})}{\Gamma(\frac{3}{2})} \times \int_{-\infty}^{\infty} (it)^{-a-\frac{1}{2}} \times \exp\left\{\frac{iEt}{\hbar} - \frac{(t\sqrt{W_{n(p)}})^2}{2\hbar^2}\right\} dt$,

$i^2 = -1$,

Noting that as a=1, $(it)^{-\frac{3}{2}} \times \exp\left\{-\frac{(t\sqrt{W_p})^2}{2\hbar^2}\right\}$ is found to be proportional to the averaged Feynman propagator given the dense donors (acceptors). Then, by variable changes: $t = \frac{\hbar}{\sqrt{W_{n(p)}}}$ and $y = \mp E/\sqrt{W_{n(p)}} \equiv \frac{\pm E_{Fno(Fpo)}}{\eta_{n(p)}} \times v_{n(p)} \times \exp\left(\frac{\mathcal{H}_{n(p)} \times R_{sn(sp)}}{4 \times \sqrt{|v_{n(p)}|}}\right)$, for n(p)-type respectively, and then using an identity

$\int_{-\infty}^{\infty} (is)^{-a-\frac{1}{2}} \times \exp\left\{iys - \frac{s^2}{2}\right\} ds \equiv 2^{3/2} \times \Gamma(3/2) \times \exp(-y^2/4) \times D_{-a-\frac{1}{2}}(y)$,

one finally obtains: $\langle E_k^{a-\frac{1}{2}} \rangle_{FPIM} \equiv \langle E_k^{a-\frac{1}{2}} \rangle_{KIM}$, $\langle E_k^{a-\frac{1}{2}} \rangle_{KIM}$ being determined in Eq. (16).

In the following, with the use of asymptotic forms for $D_{-a-\frac{1}{2}}(y)$, those given for $\langle (E - V)^{a-\frac{1}{2}} \rangle_{KIM}$ can be obtained in the two following cases.

First case: n-type ($E \geq 0$) and p-type ($E \leq 0$)

As $E \to \pm\infty$, one has: $v_{n(p)} \to \mp\infty$ and $y \to \mp\infty$. In this case, one gets: $D_{-a-\frac{1}{2}}(y \to \mp\infty) \approx \frac{\sqrt{2\pi}}{\Gamma(a+\frac{1}{2})} \times e^{\frac{y^2}{4}} \times (\mp y)^{a-\frac{1}{2}}$, and therefore from Eq. (16), one gets:

$$\langle E_k^{a-\frac{1}{2}} \rangle_{KIM} \approx E^{a-\frac{1}{2}}. \quad (17)$$

Further, as $E \to \pm 0$, one has: $v_{n(p)} \to \mp 0$ and $y \to \mp 0$. So, one obtains:

$$D_{-a-\frac{1}{2}}(y \to \mp 0) \simeq \beta(a) \times \exp\left(\left(\sqrt{a} + \frac{1}{16a^{\frac{3}{2}}}\right) y - \frac{y^2}{16a} + \frac{y^3}{24\sqrt{a}}\right) \to \beta(a), \quad \beta(a) = \frac{\sqrt{\pi}}{2^{\frac{2a+1}{4}}\Gamma(\frac{a}{2}+\frac{3}{4})}. \quad (18)$$

Therefore, as $E \to \pm 0$, from Eq. (16), one gets: $\langle E_k^{a-\frac{1}{2}} \rangle_{KIM} \to 0$.

Thus, in this case, one gets:

$$\langle E_k^{a-\frac{1}{2}} \rangle_{KIM} \cong E^{a-\frac{1}{2}}. \quad (19)$$

Second case: n-type-case ($E \le 0$) and p-type-case ($E \ge 0$)

As $E \to \mp 0$, one has: $(y, v_{n(p)}) \to \pm 0$, and by putting $f(a) \equiv \frac{\eta_{n(p)}^{a-\frac{1}{2}}}{\sqrt{2\pi}} \times \Gamma(a + \frac{1}{2}) \times \beta(a)$, Eq. (18) yields:

$$H_{n(p)}(v_{n(p)} \to \pm 0, N, r_{d(a)}, x, a) = \frac{\langle E_k^{a-\frac{1}{2}} \rangle_{KIM}}{f(a)} = \exp\left[-\frac{\mathcal{H}_{n(p)} \times R_{sn(sp)} \times (2a-1)}{8 \times \sqrt{|v_{n(p)}|}} - \left(\sqrt{a} + \frac{1}{16a^{\frac{3}{2}}}\right) y - \left(\frac{1}{4} + \frac{1}{16a}\right) y^2 - \frac{y^3}{24\sqrt{a}}\right] \to 0. \quad (20)$$

Further, as $E \to \mp\infty$, one has: $(y, v_{n(p)}) \to \pm\infty$. Thus, one gets: $D_{-a-\frac{1}{2}}(y \to \pm\infty) \approx y^{-a-\frac{1}{2}} \times e^{-\frac{y^2}{4}} \to 0$.

Therefore, from Eq. (16), one gets

$$K_{n(p)}(v_{n(p)} \to \pm\infty, N, r_{d(a)}, x, a) \equiv \frac{\langle E_k^{a-\frac{1}{2}} \rangle_{KIM}}{f(a)} \simeq \frac{1}{\beta(a)} \times \exp\left(-\frac{(A_{n(p)} \times v_{n(p)})^2}{2}\right) \times (A_{n(p)} \times v_{n(p)})^{-a-\frac{1}{2}} \to 0. \quad (21)$$

Noting that $\beta(a) = \frac{\sqrt{\pi}}{2^{\frac{2a+1}{4}}\Gamma(\frac{a}{2}+\frac{3}{4})}$, being equal to: $\frac{\sqrt{\pi}}{2^{\frac{3}{4}} \times \Gamma(5/4)}$ for a=1, and $\frac{\sqrt{\pi}}{2^{3/2}}$ for $a = 5/2$.

It should be noted that those ratios: $\frac{\langle E_k^{a-\frac{1}{2}} \rangle_{KIM}}{f(a)}$, obtained in Equations (20) and (21), can be taken in an approximate form as

$$F_{n(p)}(v_{n(p)}, N, r_{d(a)}, x, a) = K_{n(p)}(v_{n(p)}, N, r_{d(a)}, x, a) + [H_{n(p)}(v_{n(p)}, N, r_{d(a)}, x, a) - K_{n(p)}(v_{n(p)}, N, r_{d(a)}, x, a)] \times \exp\left[-c_1 \times (A_{n(p)} v_{n(p)})^{c_2}\right],$$

so that: $F_{n(p)}(v_{n(p)}, N, r_{d(a)}, x, a) \to H_{n(p)}(v_{n(p)}, N, r_{d(a)}, x, a)$ for $0 \le v_n \le 16$, and $F_{n(p)}(v_{n(p)}, N, r_{d(a)}, x, a) \to K_{n(p)}(v_{n(p)}, N, r_{d(a)}, x, a)$ for $v_{n(p)} \ge 16$. Here, the constants c_1 and c_2 may be respectively chosen as: $c_1 = 10^{-40}$ and $c_2 = 80$, as $a = 1$, being used to determine the critical density of electrons (holes) localized in the exponential conduction(valence) band-tails (EBT), $N_{CDn(CDp)}^{EBT}(N, r_{d(a)}, x)$, given in the following.

Here, by using Eq. (18) for a=1, the density of states $\mathcal{D}(E)$ is defined by

$$\langle \mathcal{D}(E_k)\rangle_{KIM} \equiv \frac{g_{c(v)}}{2\pi^2}\left(\frac{2m_{c(v)}}{\hbar^2}\right)^{\frac{3}{2}} \times \langle E_k^{\frac{1}{2}}\rangle_{KIM} = \frac{g_{c(v)}}{2\pi^2}\left(\frac{2m_{c(v)}}{\hbar^2}\right)^{\frac{3}{2}} \times \frac{\exp\left(-\frac{y^2}{4}\right)\times W_n^{\frac{1}{4}}}{\sqrt{2\pi}} \times \Gamma\left(\frac{3}{2}\right) \times D_{-\frac{3}{2}}(y) = \mathcal{D}(E). \quad (23)$$

Going back to the functions: H_n, K_n and F_n, given respectively in Equations (20-22), in which the factor $\frac{\langle E_k^{\frac{1}{2}}\rangle_{KIM}}{f(a=1)}$ is now replaced by

$$\frac{\langle E_k^{\frac{1}{2}}\rangle_{KIM}}{f(a=1)} = \frac{\mathcal{D}(E\le 0)}{\mathcal{D}_o} = F_{n(p)}\left(\nu_{n(p)}, N, r_{d(a)}, x, a=1\right),$$

$$\mathcal{D}_o(N, r_{d(a)}, x, a=1) = \frac{g_{c(v)}\times\left(m_{c(v)}\times m_o\right)^{3/2}\times\sqrt{\eta_{n(p)}}}{2\pi^2\hbar^3} \times \beta(a), \beta(a=1) = \frac{\sqrt{\pi}}{2^{\frac{5}{4}}\times\Gamma(5/4)}. \quad (24)$$

Therefore, $N^{EBT}_{CDn(CDp)}(N, r_{d(a)}, x)$ can be defined by: $N^{EBT}_{CDn(CDp)}(N, r_{d(a)}, x) = \int_{-\infty}^{0} \mathcal{D}(E \le 0)\, dE$,

$$N^{EBT}_{CDn(CDp)}(N, r_{d(a)}, x) = \frac{g_{c(v)}\times\left(m_{c(v)}\right)^{3/2}\sqrt{\eta_{n(p)}}\times\left(\pm E_{Fno(Fpo)}\right)}{2\pi^2\hbar^3} \times \left\{\int_0^{16} \beta(a=1) \times F_{n(p)}\left(\nu_{n(p)}, N, r_{d(a)}, x, a=1\right) d\nu_{n(p)} + I_{n(p)}\right\},$$

(25) where

$$I_{n(p)} \equiv \int_{16}^{\infty} \beta(a=1) \times K_{n(p)}\left(\nu_{n(p)}, N, r_{d(a)}, x, a=1\right) d\nu_{n(p)} = \int_{16}^{\infty} e^{\frac{-\left(A_{n(p)}\times\nu_{n(p)}\right)^2}{2}} \times \left(A_{n(p)}\nu_{n(p)}\right)^{-3/2} d\nu_{n(p)}.$$

Then, by another variable change: $t = \left[A_{n(p)}\nu_{n(p)}/\sqrt{2}\right]^2$, the integral $I_{n(p)}$ yields:

$I_{n(p)} = \frac{1}{2^{5/4}A_{n(p)}} \times \int_{z_{n(p)}}^{\infty} t^{b-1}e^{-t}dt \equiv \frac{\Gamma(b, z_{n(p)})}{2^{5/4}\times A_{n(p)}}$, where $b = -1/4$, $z_{n(p)} = \left[16A_{n(p)}/\sqrt{2}\right]^2$, and $\Gamma(b, z_{n(p)})$ is the incomplete Gamma function, defined by: $\Gamma(b, z_{n(p)}) \simeq z_{n(p)}^{b-1} \times e^{-z_{n(p)}}\left[1 + \sum_{j=1}^{16}\frac{(b-1)(b-2)\dots(b-j)}{z_{n(p)}^{j}}\right]$.

Finally, Eq. (25) now yields:

$$N^{EBT}_{CDn(CDp)}[N = N_{CDn(NDp)}(r_{d(a)}, x), r_{d(a)}, x] = \frac{g_{c(v)}\times\left(m_{c(v)}\right)^{3/2}\sqrt{\eta_{n(p)}}\times\left(\pm E_{Fno(Fpo)}\right)}{2\pi^2\hbar^3} \times \left\{\int_0^{16} \beta(a=1) \times F_{n(p)}\left(\nu_{n(p)}, N, r_{d(a)}, x, a=1\right) d\nu_{n(p)} + \frac{\Gamma(b, z_{n(p)})}{2^{5/4}\times A_{n(p)}}\right\}, \quad (26)$$

Being the density of electrons (holes) localized in the EBT, respectively.

In n(p)-type degenerate X(x)≡ $[InSb_{1-x}P_x\,(As_x), GaSb_{1-x}P_x(As_x, Te_x), CdSe_{1-x}S_x(Te_x)]$-crystalline alloys, the numerical results of $N^{EBT}_{CDn(CDp)}[N = N_{CDn(NDp)}(r_{d(a)}, x), r_{d(a)}, x] \equiv N^{EBT}_{CDn(CDp)}(r_{d(a)}, x)$, for a simplicity of presentation, evaluated using Eq. (26), are given in Tables 2-8 in Appendix 1, in which those of other functions such as: $B_{do(ao)}$, ε, $E_{gno(gpo)}$, and $N_{CDn(CDp)}$ are computed, using Equations (2), (5), (6), and (8), respectively, noting that the relative deviations in absolute values are defined by: $|RD| \equiv \left|1 - \frac{N^{EBT}_{CDn(CDp)}}{N_{CDn(CDp)}}\right|$.

Tables 2-8 in Appendix 1

CONCLUSION

In those Tables 2-8, some concluding remarks are given and discussed in the following.

(1)-For a given x, while $\varepsilon(r_{d(a)},x)$ decreases (↘), the functions: $E_{gno(gpo)}(r_{d(a)},x)$, $N_{CDn(CDp)}(r_{d(a)},x)$ and $N^{EBT}_{CDn(CDp)}(r_{d(a)},x)$ increase (↗), with increasing (↗) $r_{d(a)}$, due to the impurity size effect.

(2)-Further, for a given $r_{d(a)}$, while $\varepsilon(r_{d(a)},x)$ also decreases (↘), the functions: $E_{gno(gpo)}(r_{d(a)},x)$, $N_{CDn(CDp)}(r_{d(a)},x)$ and $N^{EBT}_{CDn(CDp)}(r_{d(a)},x)$ also increase (↗), with increasing (↗) x.

(3)- In those Tables 2-8, one notes that the maximal value of $|RD|$ is found to be given by: 2.91×10^{-7}, meaning that $N^{EBT}_{CDn}\cong N_{CDn}$. In other words, such the critical d(a)-density $N_{CDn(NDp)}(r_{d(a)}),x)$, is just the density of electrons (holes), being localized in the EBT, $N^{EBT}_{CDn(CDp)}(r_{d(a)},x)$, respectively.

(4) Finally, once $N_{CDn(CDp)}$ is determined, the effective density of free electrons (holes), N^*, given in the parabolic conduction (valence) band of the n(p)-type degenerate X(x)≡ $[InSb_{1-x}P_x\,(As_x), GaSb_{1-x}P_x(As_x, Te_x), CdSe_{1-x}S_x(Te_x)]$- crystalline alloy, can thus be defined now as the compensated ones, by:

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

Needing to determine the optical, electrical, and thermoelectric properties in such n(p)-type degenerate X(x)-crystalline alloys, as those studied in n(p)-type degenerate crystals (Van Cong, 2023; Van Cong et al., 2014; Van Cong & Debiais, 1993; Van Cong et al., 1984).

REFERENCES

1. Green, M.A. et al. Solar cell efficiency tables (version 60). *Prog. Photovolt. Res. & Appl.*, 2022; 30: 687-701.
2. Kittel, C. Introduction to Solid State Physics, Wiley, New York, 1976; 84-100.
3. Moon S. et al. Highly efficient single GaAs thin-film solar cell on flexible substrate. *Sci. Rep.*, 2016; 6: 30107.
4. Van Cong, H. New Critical Impurity Density in the Metal-Insulator Transition, obtained in various n(p)-Type Degenerate Crystalline Alloys, being just That of Carriers Localized in Exponential Band Tails. (I), being accepted for publication in *World Journal of Engineering Research and Technology*, 2024; 10: 4.

5. Van Cong, H. New Critical Impurity Density in the Metal-Insulator Transition, obtained in various n(p)-Type Degenerate Crystalline Alloys, being just That of Carriers Localized in Exponential Band Tails. (II), being accepted for publication in *World Journal of Engineering Research and Technology*, 2024; 10(4).
6. Van Cong, H. Accurate expressions of the optical coefficients, given in n(p)-type degenerate GaAs-crystals, due to the impurity-size effect, and obtained by an improved Forouhi-Bloomer parameterization model (FB-PM). *SCIREA J. Phys.*, 2023; 8: 172-197. Same maximum figure of merit ZT(=1), due to effects of impurity size and heavy doping, obtained in n(p)-type degenerate InP-crystal, at same reduced Fermi energy and same minimum (maximum) Seebeck coefficient , at which same Mott ZT (=1). *SCIREA J. Phys.*, 2023; 8: 91-114; Same maximum figure of merit ZT(=1), due to effects of impurity size and heavy doping, obtained in n(p)-type degenerate GaAs-crystal, at same reduced Fermi energy and same minimum (maximum) Seebeck coefficient , at which same Mott ZT (=1). *SCIREA J. Phys.*, 2023; 8: 133-157; Same maximum figure of merit ZT(=1), due to effects of impurity size and heavy doping, obtained in n(p)-type degenerate InSb-crystal, at same reduced Fermi energy and same minimum (maximum) Seebeck coefficient , at which same Mott ZT (=1). *SCIREA J. Phys.*, 2023; 8: 383-406. Same maximum figure of merit ZT(=1), due to effects of impurity size and heavy doping, obtained in n(p)-type degenerate InAs-crystal, at same reduced Fermi energy and same minimum (maximum) Seebeck coefficient , at which same Mott ZT (=1). *SCIREA J. Phys.*, 2023; 8: 431-455.
7. Van Cong, H. et al. Optical bandgap in various impurity-Si systems from the metal-insulator transition study. *Physica B*, 2014; 436: 130-139.
8. Van Cong, H. & Debiais, G. A simple accurate expression of the reduced Fermi energy for any reduced carrier density. J. Appl. Phys., 1993; 73: 1545-1546.
9. Van Cong, H. et al. Size effect on different impurity levels in semiconductors. *Solid State Communications*, 1984; 49: 697-699.
10. Critical Impurity Densities in the Mott Metal-Insulator Transition, Obtained in Three n(p)- Type Degenerate Ga$As_{1-x}Te_x(Sb_x, P_x)$-Crystalline Alloys.

APPENDIX 1

Table 1. The values of various energy-band-structure parameters are given in various crystalline alloys as follows.

In $InSb_{1-x}P_x$**-alloys**, in which $r_{do(ao)}$=$r_{Sb(In)}$=0.136 nm (0.144 nm), we have: $g_{c(v)}(x) = 1 \times x + 1 \times (1-x)$, $m_{c(v)}(x)/m_o = 0.077\ (0.5) \times x + 0.1\ (0.4) \times (1-x)$, $\varepsilon_o(x) = 12.5 \times x + 16.8 \times (1-x)$, $E_{go}(x) = 1.424 \times x + 0.23 \times (1-x)$, and

In $InSb_{1-x}As_x$**-alloys**, in which $r_{do(ao)}$=$r_{Sb(In)}$=0.136 nm (0.144 nm), we have: $g_{c(v)}(x) = 1 \times x + 1 \times (1-x)$, $m_{c(v)}(x)/m_o = 0.09\ (0.3) \times x + 0.1\ (0.4) \times (1-x)$, $\varepsilon_o(x) = 14.55 \times x + 16.8 \times (1-x)$, $E_{go}(x) = 0.43 \times x + 0.23 \times (1-x)$.

In $GaSb_{1-x}P_x$**-alloys**, in which $r_{do(ao)}$=$r_{Sb(Ga)}$=0.136 nm (0.126 nm), we have: $g_{c(v)}(x) = 1 \times x + 1 \times (1-x)$, $m_{c(v)}(x)/m_o = 0.13(0.5) \times x + 0.047(0.3) \times (1-x)$, $\varepsilon_o(x) = 11.1 \times x + 15.69 \times (1-x)$, $E_{go}(x) = 1.796 \times x + 0.81 \times (1-x)$,

In $GaSb_{1-x}As_x$**-alloys**, in which $r_{do(ao)}$=$r_{Sb(Ga)}$=0.136 nm (0.126 nm), we have: $g_{c(v)}(x) = 1 \times x + 1 \times (1-x)$, $m_{c(v)}(x)/m_o = 0.066\ (0.291) \times x + 0.047(0.3) \times (1-x)$, $\varepsilon_o(x) = 13.13 \times x + 15.69 \times (1-x)$, $E_{go}(x) = 1.52 \times x + 0.81 \times (1-x)$, and

In $GaSb_{1-x}Te_x$**-alloys**, in which $r_{do(ao)}$=$r_{Sb(Ga)}$=0.136 nm (0.126 nm), we have: $g_{c(v)}(x) = 1 \times x + 1 \times (1-x)$, $m_{c(v)}(x)/m_o = 0.209(0.4) \times x + 0.047(0.3) \times (1-x)$, $\varepsilon_o(x) = 12.3 \times x + 15.69 \times (1-x)$, $E_{go}(x) = 1.796 \times x + 0.81 \times (1-x)$.

In $CdSe_{1-x}S_x$**-alloys**, in which $r_{do(ao)}$=$r_{Se(Cd)}$=0.114 nm (0.148 nm), we have: $g_{c(v)}(x) = 1 \times x + 1 \times (1-x)$, $m_{c(v)}(x)/m_o = 0.197\ (0.801) \times x + 0.11\ (0.45) \times (1-x)$, $\varepsilon_o(x) = 9 \times x + 10.2 \times (1-x)$, $E_{go}(x) = 2.58 \times x + 1.84 \times (1-x)$, and

In $CdSe_{1-x}Te_x$**-alloys**, in which $r_{do(ao)}$=$r_{Se(Cd)}$=0.114 nm (0.148 nm), we have: $g_{c(v)}(x) = 1 \times x + 1 \times (1-x)$, $m_{c(v)}(x)/m_o = 0.095(0.82) \times x + 0.11\ (0.45) \times (1-x)$, $\varepsilon_o(x) = 10.31 \times x + 10.2 \times (1-x)$, $E_{go}(x) = 1.62 \times x + 1.84 \times (1-x)$.

Table 2. In the $InSb_{1-x}P_x$-alloy the numerical results of $B_{do(ao)}$, ε, $E_{gno(gpo)}$, $N_{CDn(CDp)}$, and $N^{EBT}_{CDn(CDp)}$ are computed, using Equations (2), (5), (6), and (8a), and (26), respectively, noting that the relative deviations in absolute values are defined by: $|RD| \equiv \left|1 - \frac{N^{EBT}_{CDn(CDp)}}{N_{CDn(Cdp)}}\right|$, giving rise to their maximal value equal to $\mathbf{2.86 \times 10^{-7}}$, meaning that such the critical d(a)-density $N_{CDn(NDp)}(r_{d(a)}, x)$, determined in Eq. (8a), is just the density of electrons (holes) localized in the EBT, $N^{EBT}_{CDn(CDp)}(r_{d(a)}, x)$, determined in Eq. (26), respectively. Here, on notes that in the limiting conditions: x=0, 1, these results are reduced to those given in InSb-and-InP crystals, respectively, as observed in Table 1.

Donor	P	As
r_d (nm) ↗	0.110	0.118
x ↗	0, 0.5, 1	0, 0.5, 1
$\varepsilon(r_d, x)$ ↘	20.07583, 17.50661, 14.93738	18.19773, 15.8689, 13.53998
$E_{gno}(r_d, x)$ eV ↗	0.2285558, 0.825319, 1.4219912	0.229288, 0.8261716, 1.42301
$N_{CDn}(r_d, x)$ in 10^{16} cm^{-3} ↗	1.2971031, 1.3558738, 1.4376212	1.7415804, 1.8204900, 1.9302497
$N^{EBT}_{CDn}(r_d, x)$ in 10^{16} cm^{-3} ↗	1.2971027, 1.3558734, 1.4376208	1.7415799, 1.8204895, 1.9302492

$\lvert RD \rvert$ in 10^{-7}	2.71, 2.59, 2.56	**2.86,** 2.60, 2.59

Donor	$\mathbf{r_{do}}$=Sb	Sn
r_d (nm) ↗	0.136	0.140
x ↗	0, 0.5, 1	0, 0.5, 1
$B_{do}(x)$ in 10^7 (N/m^2) ↗	7.3261789, 8.5263687,10.189826	
$\varepsilon(r_d, x)$ ↘	**16.8**, 14.65, **12.5**	16.734022, 14.592465, 12.450909
$E_{gno}(r_d, x)$ eV ↗	**0.23**, 0.827, **1.424**	0.230038, 0.8270443, 1.424053
$N_{CDn}(r_d, x)$ in 10^{16} cm^{-3} ↗	2.2134389, 2.3137281, 2.4532257	2.2397234, 2.3412035, 2.4823577
$N_{CDn}^{EBT}(r_d, x)$ in 10^{16} cm^{-3} ↗	2.2134383, 2.3137275, 2.4532251	2.2397228, 2.3412029, 2.4823570
$\lvert RD \rvert$ in 10^{-7}	2.81, 2.80, 2.62	2.75, 2.62, 2.68

Acceptor	Ga	Mg
r_a (nm) ↗	0.126	0.140
x ↗	0, 0.5, 1	0, 0.5, 1
$\varepsilon(r_a, x)$ ↘	18.0345915, 15.726593, 13.4185948	16.857828, 14.7004274, 12.5430268
$E_{gpo}(r_a, x)$ eV ↗	0.2274514, 0.8232295, 1.4182455	0.229868, 0.8268047, 1.4237019
$N_{CDp}(r_a, x)$ in 10^{18} cm^{-3} ↗	1.1451343, 2.4588326, 5.4298054	1.4020726, 3.0105305, 6.6481122
$N_{CDp}^{EBT}(r_a, x)$ in 10^{18} cm^{-3} ↗	1.1451340, 2.4588319, 5.4298040	1.4020722, 3.0105297, 6.6481104
$\lvert RD \rvert$ in 10^{-7}	2.74, **2.76**, 2.60	2.81, 2.69, 2.74

Acceptor	In	Cd
r_a (nm) ↗	$\mathbf{r_{ao}}$**=0.144**	0.148
x ↗	0, 0.5, 1	0, 0.5, 1
$B_{ao}(x)$ in 10^8 (N/m^2) ↗	2.4686912, 3.6522677, 5.5741072	
$\varepsilon(r_a, x)$ ↘	**16.8**, 14.65, **12.5**	16.7411597, 14.598690, 12.45622
$E_{gpo}(r_a, x)$ eV ↗	**0.23**, 0.827, **1.424**	0.2301357, 0.8272008, 1.4243065
$N_{CDp}(r_a, x)$ in 10^{18} cm^{-3} ↗	1.4166009, 3.0417257, 6.717	1.4315903, 3.0739109, 6.7880742
$N_{CDp}^{EBT}(r_a, x)$ in 10^{18} cm^{-3} ↗	1.4166005, 3.0417249, 6.7169982	1.4315899, 3.0739101, 6.7880723
$\lvert RD \rvert$ in 10^{-7}	2.82, 2.76, 2.69	2.91, 2.70, 2.74

Table 3. In the $InSb_{1-x}As_x$-alloy the numerical results of $B_{do(ao)}$, ε, $E_{gno(gpo)}$, $N_{CDn(CDp)}$, and $N_{CDn(CDp)}^{EBT}$ are computed, using Equations (2), (5), (6), and (8a), and (26), respectively, noting that the relative deviations in absolute values are defined by: $|RD| \equiv \left|1 - \frac{N_{CDn(CDp)}^{EBT}}{N_{CDn(Cdp)}}\right|$, giving rise to their maximal value equal to **2.86**$\times 10^{-7}$, meaning that such the critical d(a)-density $N_{CDn(NDp)}(r_{d(a)}, x)$, determined in Eq. (8a), is just the density of electrons (holes) localized in the EBT, $N_{CDn(CDp)}^{EBT}(r_{d(a)}, x)$, determined in Eq. (26), respectively. Here, on notes that in the limiting conditions: x=0, 1, these results are reduced to those given in InSb-and-InAs crystals, respectively, as observed in Table 1.

Donor	P	As
r_d (nm) ↗	0.110	**0.118**
x ↗	0, 0.5, 1	0, 0.5, 1
$\varepsilon(r_d, x)$ ↘	20.0758, 18.73147, 17.387107	18.1977329, 16.97913, 15.7605365

$E_{gno}(r_d, x)$ eV ↗	0.228556, 0.328424, 0.4282671	0.2292882, 0.329223, 0.4291459
$N_{CDn}(r_d, x)$ in 10^{16} cm^{-3} ↗	1.2971031, 1.3691483, 1.4555961	1.7415804, 1.8383133, 1.9543841
$N_{CDn}^{EBT}(r_d, x)$ in 10^{16} cm^{-3} ↗	1.2971027, 1.3691480, 1.4555957	1.7415799, 1.8383128, 1.9543835
$\lvert RD \rvert$ in 10^{-7}	2.71, 2.54, 2.67	**2.86,** 2.69, 2.81
Donor	r_{do}=Sb	Sn
r_d (nm) ↗	0.136	0.140
x ↗	0, 0.5, 1	0, 0.5, 1
$B_{do}(x)$ in 10^7 (N/m^2) ↗	7.3261789, 7.994745, 8.7904804	
$\varepsilon(r_d, x)$ ↘	**16.8,** 15.675, **14.55**	16.73402, 15.61344, 14.49286
$E_{gno}(r_d, x)$ eV ↗	**0.23,** 0.33, **0.43**	0.2300381, 0.330041, 0.4300457
$N_{CDn}(r_d, x)$ in 10^{16} cm^{-3} ↗	2.2134389, 2.3363803, 2.4838989	2.2397234, 2.3641248, 2.5133952
$N_{CDn}^{EBT}(r_d, x)$ in 10^{16} cm^{-3} ↗	2.2134383, 2.3363797, 2.4838983	2.2397228, 2.3641241, 2.5133945
$\lvert RD \rvert$ in 10^{-7}	2.81, 2.61, 2.58	2.75, 2.75, 2.67

Acceptor	Ga	Mg
r_a (nm) ↗	0.126	0.140
x ↗	0, 0.5, 1	0, 0.5, 1
$\varepsilon(r_a, x)$ ↘	18.035915, 16.8269179, 15.619244	16.857828, 15.72896, 14.6000832
$E_{gpo}(r_a, x)$ eV ↗	0.2274514, 0.3274384, 0.4274517	0.229868, 0.3298673, 0.429868
$N_{CDp}(r_a, x)$ in 10^{18} cm^{-3} ↗	1.1451343, 0.9444648, 0.74366797	1.4020726, 1.1563781, 0.91052768
$N_{CDp}^{EBT}(r_a, x)$ in 10^{18} cm^{-3} ↗	1.1451340, 0.94446455, 0.74366777	1.4020722, 1.1563778, 0.91052743
$\lvert RD \rvert$ in 10^{-7}	2.68, 2.64, 2.68	2.81, **2.83**, 2.77
Acceptor	In	Cd
r_a (nm) ↗	r_{ao}**=0.144**	0.148
x ↗	0, 0.5, 1	0, 0.5, 1
$B_{ao}(x)$ in 10^8 (N/m^2)	2.468691, 2.4812943, 2.4684288	
$\varepsilon(r_a, x)$ ↘	**16.8,** 15.675, **14.55**	16.741160, 15.6201, 14.499040
$E_{gpo}(r_a, x)$ eV ↗	**0.23,** 0.33, **0.43**	0.2301357, 0.3301364, 0.430136
$N_{CDp}(r_a, x)$ in 10^{18} cm^{-3} ↗	1.4166009, 1.1683605, 0.91996257	1.4315903, 1.1807232, 0.92969691
$N_{CDp}^{EBT}(r_a, x)$ in 10^{18} cm^{-3} ↗	1.4166005, 1.1683602, 0.91996232	1.4315899, 1.1807229, 0.92969666
$\lvert RD \rvert$ in 10^{-7}	2.82, 2.78, 2.68	2.91, 2.83, 2.71

Table 4. In the $GaSb_{1-x}P_x$-alloy the numerical results of $B_{do(ao)}$, ε, $E_{gno(gpo)}$, $N_{CDn(CDp)}$, and $N_{CDn(CDp)}^{EBT}$ are computed, using Equations (2), (5), (6), and (8a), and (26), respectively, noting that the relative deviations in absolute values are defined by: $|RD| \equiv \left|1 - \frac{N_{CDn(CDp)}^{EBT}}{N_{CDn(Cdp)}}\right|$, giving rise to their maximal value equal to $\mathbf{2.92 \times 10^{-7}}$, meaning that such the critical d(a)-density $N_{CDn(NDp)}(r_{d(a)}), x)$, *determined in Eq.* (8a), is just the density of electrons (holes) localized in the EBT, $N_{CDn(CDp)}^{EBT}(r_{d(a)}, x)$, determined in Eq. (26), respectively. Here, on notes that in the limiting conditions: x=0, 1, these results are reduced to those given in GaSb-and-GaP crystals, respectively, as observed in Table 1.

Donor	P	As

r_d (nm) ↗	0.110	0.118
x ↗	0, 0.5, 1	0, 0.5, 1
$\varepsilon(r_d, x)$ ↘	18.749396, 16.006894, 13.26439	16.99538, 14.509442, 12.023502
$E_{gno}(r_d, x)$ eV ↗	0.8092218, 1.300989, 1.7916992	0.809616, 1.3020091, 1.7938803
$N_{CDn}(r_d, x)$ in 10^{16} cm^{-3} ↗	0.16532064, 1.7737973, 9.8801482	0.22197093, 2.381623, 13.265771
$N_{CDn}^{EBT}(r_d, x)$ in 10^{16} cm^{-3} ↗	0.16532060, 1.7737968, 9.8801455	0.22197087, 2.3816224, 13.265767
$\|RD\|$ in 10^{-7}	2.63, 2.60, 2.72	2.67, **2.83**, 2.90

Donor	Sb	Sn
r_d (nm) ↗	$\mathbf{r_{do}}$ =0.136	0.140
x ↗	0, 0.5, 1	0, 0.5, 1
$B_{do}(x)$ in 10^7 (N/m^2) ↗	3.947736, 10.198914, 21.81692	
$\varepsilon(r_d, x)$ ↘	**15.69**, 13.395, **11.1**	15.628381, 13.3424, 11.056407
$E_{gno}(r_d, x)$ eV ↗	**0.81**, 1.303, **1.796**	0.810020, 1.303053, 1.7961134
$N_{CDn}(r_d, x)$ in 10^{16} cm^{-3} ↗	0.28211106, 3.0268927, 16.859958	0.28546113, 3.062837, 17.06017
$N_{CDn}^{EBT}(r_d, x)$ in 10^{16} cm^{-3} ↗	0.28211099, 3.0268919, 16.859954	0.28546105, 3.0628362, 17.060165
$\|RD\|$ in 10^{-7}	2.62, 2.59, 2.60	2.73, 2.57, 2.70

Acceptor	Ga	Mg
r_a (nm) ↗	$\mathbf{r_{ao}}$**=0.126**	0.140
x ↗	0, 0.5, 1	0, 0.5, 1
$B_{ao}(x)$ in 10^8 (N/m^2) ↘	3.1686666, 5.796632, 10.551768	
$\varepsilon(r_a, x)$ ↘	**15.6**, 13.395, **11.1**	14.84222, 12.67123, 10.50023
$E_{gpo}(r_a, x)$ eV ↗	**0.81**, 1.303, **1.796**	0.8119, 1.3065625, 1.802485
$N_{CDp}(r_a, x)$ in 10^{18} cm^{-3} ↗	0.73365234, 2.7947772, 9.5926026	0.86668661, 3.3015583, 11.332043
$N_{CDp}^{EBT}(r_a, x)$ in 10^{18} cm^{-3} ↗	0.73365214, 2.7947765, 9.5926000	0.86668638,3.3015574, 11.332040
$\|RD\|$ in 10^{-7}	2.68, 2.65, 2.71	2.67, 2.63, 2.45

Acceptor	In	Cd
r_a (nm) ↗	0.144	0.148
x ↗	0, 0.5, 1	0, 0.5, 1
$\varepsilon(r_a, x)$ ↘	14.33862, 12.24129, 10.143959	13.76307, 11.74993, 9.736782
$E_{gpo}(r_a, x)$ eV ↗	0.813271, 1.308984, 1.8068933	0.814966, 1.312084, 1.8125359
$N_{CDp}(r_a, x)$ in 10^{18} cm^{-3} ↗	0.96125108, 3.6617925, 12.568487	1.0869583, 4.1406617, 14.212125
$N_{CDp}^{EBT}(r_a, x)$ in 10^{18} cm^{-3} ↗	0.96125083, 3.6617915, 12.568483	1.0869580, 4.1406606, 14.212121
$\|RD\|$ in 10^{-7}	2.62, 2.77, **2.92**	2.87, 2.62, 2.84

Table 5. In the $GaSb_{1-x}As_x$-alloy the numerical results of $B_{do(ao)}$, ε, $E_{gno(gpo)}$, $N_{CDn(CDp)}$, and $N_{CDn(CDp)}^{EBT}$ are computed, using Equations (2), (5), (6), and (8a), and (26), respectively, noting that the relative deviations in absolute values are defined by: $|RD| \equiv \left|1 - \frac{N_{CDn(CDp)}^{EBT}}{N_{CDn(Cdp)}}\right|$, giving rise to their maximal value equal to $\mathbf{2.90 \times 10^{-7}}$, meaning that such the critical d(a)-density

$N_{CDn(NDp)}(r_{d(a)}), x)$, *determined in Eq.* (8a), is just the density of electrons (holes) localized in the EBT, $N^{EBT}_{CDn(CDp)}(r_{d(a)}, x)$, determined in Eq. (26), respectively. Here, on notes that in the limiting conditions: x=0, 1, these results are reduced to those given in GaSb- and-GaAs crystals, respectively, as observed in Table 1.

Donor	P	As
r_d (nm) ↗	0.110	0.118
x ↗	0, 0.5, 1	0, 0.5, 1
$\varepsilon(r_d, x)$ ↘	18.7494, 17.21981, 15.690221	16.995383, 15.60889, 14.22239
$E_{gno}(r_d, x)$ eV ↗	0.80922, 1.163891, 1.5184395	0.809616, 1.164453, 1.5192309
$N_{CDn}(r_d, x)$ in 10^{16} cm^{-3} ↗	0.16532064, 0.3707283, 0.78115995	0.22197093, 0.49776547, 1.0488394
$N^{EBT}_{CDn}(r_d, x)$ in 10^{16} cm^{-3} ↗	0.16532060, 0.3707282, 0.78115974	0.22197087, 0.49776534, 1.0488391
$\lvert RD \rvert$ in 10^{-7}	2.63, 2.64, 2.73	2.67, 2.69, 2.72
Donor	Sb	Sn
r_d (nm) ↗	r_{do}=0.136	0.140
x ↗	0, 0.5, 1	0, 0.5, 1
$B_{do}(x)$ in 10^7 (N/m^2) ↘	3.9477356, 5.626218, 7.9160872	
$\varepsilon(r_d, x)$ ↘	**15.69**, 14.41, **13.13**	15.628381, 14.35341, 13.078435
$E_{gno}(r_d, x)$ eV ↗	**0.81**, 1.165, **1.52**	0.8100205, 1.165029, 1.5200411
$N_{CDn}(r_d, x)$ in 10^{16} cm^{-3} ↗	0.28211106, 0.63262853, 1.3330088	0.28546113, 0.64014098, 1.3488382
$N^{EBT}_{CDn}(r_d, x)$ in 10^{16} cm^{-3} ↗	0.28211099, 0.63262836, 1.3330084	0.28546105, 0.64014081, 1.3488378
$\lvert RD \rvert$ in 10^{-7}	2.62, 2.66, **2.87**	2.73, 2.72, 2.70

Acceptor	Ga	Mg
r_a (nm) ↗	**r_{ao}=0.126**	0.140
x ↗	0, 0.5, 1	0, 0.5, 1
$B_{ao}(x)$ in 10^8 (N/m^2) ↘	3.1686666, 3.700247, 4.388991	
$\varepsilon(r_a, x)$ ↘	**15.69**, 14.41, **13.13**	14.84222, 13.63139, 12.420549
$E_{gpo}(r_a, x)$ eV ↗	**0.81**, 1.165, **1.52**	0.811947, 1.1672741, 1.5226974
$N_{CDp}(r_a, x)$ in 10^{18} cm^{-3} ↗	0.73365234, 0.90505691, 1.1425630	0.86668661, 1.0691722, 1.3497457
$N^{EBT}_{CDp}(r_a, x)$ in 10^{18} cm^{-3} ↗	0.73365214, 0.90505667, 1.1425627	0.86668638, 1.0691719, 1.3497453
$\lvert RD \rvert$ in 10^{-7}	2.68, 2.70, 2.59	2.67, 2.55, 2.82

Acceptor	In	Cd
r_a (nm) ↗	0.144	0.148
x ↗	0, 0.5, 1	0, 0.5, 1
$\varepsilon(r_a, x)$ ↘	14.338622, 13.168869, 11.99911	13.76307, 12.64027, 11.517473
$E_{gpo}(r_a, x)$ eV ↗	0.8132712, 1.16882, 1.5245311	0.8149657, 1.170799, 1.5268781
$N_{CDp}(r_a, x)$ in 10^{18} cm^{-3} ↗	0.96125108, 1.1858300, 1.4970169	1.0869583, 1.3409063, 1.6927886
$N^{EBT}_{CDp}(r_a, x)$ in 10^{18} cm^{-3} ↗	0.96125083, 1.1858297, 1.4970165	1.0869580, 1.3409060, 1.6927881
$\lvert RD \rvert$ in 10^{-7}	2.62, **2.90**, 2.80	2.87, 2.46, 2.74

Table 6. In the $GaSb_{1-x}Te_x$-alloy the numerical results of $B_{do(ao)}$, ε, $E_{gno(gpo)}$, $N_{CDn(CDp)}$, and $N^{EBT}_{CDn(CDp)}$ are computed, using Equations (2), (5), (6), and (8a), and (26), respectively, noting that the relative deviations in absolute values are defined by:

$|RD| \equiv \left|1 - \frac{N^{EBT}_{CDn(CDp)}}{N_{CDn(Cdp)}}\right|$, giving rise to their maximal value equal to $\mathbf{2.87 \times 10^{-7}}$, meaning that such the critical d(a)-density $N_{CDn(NDp)}(r_{d(a)}, x)$, *determined in Eq.* (8a), is just the density of electrons (holes) localized in the EBT, $N^{EBT}_{CDn(CDp)}(r_{d(a)}, x)$, determined in Eq. (26), respectively. Here, on notes that in the limiting conditions: x=0, 1, these results are reduced to those given in GaSb-and-GaTe crystals, respectively, as observed in Table 1.

Donor	P	As
r_d (nm) ↗	0.110	0.118
x ↗	0, 0.5, 1	0, 0.5, 1
$\varepsilon(r_d, x)$ ↘	18.7494, 16.72389, 14.698379	16.995383, 15.15936, 13.3233401
$E_{gno}(r_d, x)$ eV ↗	0.80922, 1.300336, 1.7903689	0.809616, 1.3016871, 1.7932247
$N_{CDn}(r_d, x)$ in 10^{16} cm^{-3} ↗	0.16532064, 4.7055841, 0.30173512	0.22197093, 6.3180428, 40.513045
$N^{EBT}_{CDn}(r_d, x)$ in 10^{16} cm^{-3} ↗	0.16532060, 4.7055828, 0.30173509	0.22197087, 6.3180411, 40.513034
|RD| in 10^{-7}	2.63, 2.69, 2.67	2.67, 2.69, 2.63
Donor	**Sb**	Sn
r_d (nm) ↗	$\mathbf{r_{do}=0.136}$	0.140
x ↗	0, 0.5, 1	0, 0.5, 1
$B_{do}(x)$ in 10^7 (N/m^2) ↘	3.9477356, 13.51326, 28.564863	
$\varepsilon(r_d, x)$ ↘	**15.69**, 13.995, **12.3**	15.628381, 13.940038, 12.251694
$E_{gno}(r_d, x)$ eV ↗	**0.81**, 1.303, **1.796**	0.8100205, 1.303070, 1.7961484
$N_{CDn}(r_d, x)$ in 10^{16} cm^{-3} ↗	0.28211106, 8.0298341, 51.489527	0.28546113, 8.1251882, 0.52100964
$N^{EBT}_{CDn}(r_d, x)$ in 10^{16} cm^{-3} ↗	0.28211099, 8.0298330, 51.489513	0.28546105, 8.1251870, 0.52100955
|RD| in 10^{-7}	2.62, 2.66, **2.74**	2.73, 2.69, 2.73

Acceptor	Ga	Mg
r_a (nm) ↗	$\mathbf{r_{ao}=0.126}$	0.140
x ↗	0, 0.5, 1	0, 0.5, 1
$B_{ao}(x)$ in 10^8 (N/m^2) ↘	3.1686666, 4.646473, 6.8746556	
$\varepsilon(r_a, x)$ ↘	**15.69**, 13.995, **12.3**	14.84222, 13.23881, 11.63539
$E_{gpo}(r_a, x)$ eV ↗	**0.81**, 1.303, **1.796**	0.811947, 1.305855, 1.800225
$N_{CDp}(r_a, x)$ in 10^{18} cm^{-3} ↗	0.73365234, 1.6416509, 3.6096078	0.86668661, 1.9393338, 4.2641433
$N^{EBT}_{CDp}(r_a, x)$ in 10^{18} cm^{-3} ↗	0.73365214, 1.6416504, 3.6096068	0.86668638, 1.9393333, 4.2641421
|RD| in 10^{-7}	2.68, 2.82, 2.72	2.67, 2.50, 2.75

Acceptor	In	Cd
r_a (nm) ↗	0.144	0.148
x ↗	0, 0.5, 1	0, 0.5, 1
$\varepsilon(r_a, x)$ ↘	14.338622, 12.78961, 11.240603	13.76307, 12.27624, 10.78941
$E_{gpo}(r_a, x)$ eV ↗	0.8132712, 1.307797, 1.8030972	0.8149657, 1.31028, 1.8067734
$N_{CDp}(r_a, x)$ in 10^{18} cm^{-3} ↗	0.96125108, 2.1509352, 4.7294055	1.0869583, 2.4322228, 5.3478913
$N^{EBT}_{CDp}(r_a, x)$ in 10^{18} cm^{-3} ↗	0.96125083, 2.1509347, 4.7294042	1.0869580, 2.4322221, 5.3478899
|RD| in 10^{-7}	2.62, 2.53, 2.81	**2.87**, 2.70, 2.67

Table 7. In the $CdSe_{1-x}S_x$-alloy the numerical results of $B_{do(ao)}$, ε, $E_{gno(gpo)}$, $N_{CDn(CDp)}$, and $N^{EBT}_{CDn(CDp)}$ are computed, using Equations (2), (5), (6), and (8a), and (26), respectively, noting that the relative deviations in absolute values are defined by:

$|RD| \equiv \left|1-\frac{N^{EBT}_{CDn(CDp)}}{N_{CDn(Cdp)}}\right|$, giving rise to their maximal value equal to 2.88×10^{-7}, meaning that such the critical d(a)-density $N_{CDn(NDp)}(r_{d(a)}, x)$, *determined in Eq.* (8*a*), is just the density of electrons (holes) localized in the EBT, $N^{EBT}_{CDn(CDp)}(r_{d(a)}, x)$, determined in Eq. (26), respectively. Here, on notes that in the limiting conditions: x=0, 1, these results are reduced to those given in CdSe-and-CdS crystals, respectively, as observed in Table 1.

Donor	S	r_{do}=Se
r_d (nm) ↗	0.104	0.114
x ↗	0, 0.5, 1	0, 0.5, 1
$B_{do}(x)$ in 10^8 (N/m^2) ↗		3.7118515, 5.847418, 8.538458
$\varepsilon(r_d, x)$ ↘	10.55597, 9.93503, 9.314094	**10.2**, 9.6, **9**
$E_{gno}(r_d, x)$ eV ↗	1.839047, 2.20849, 2.577807	**1.84**, 2.21, **2.58**
$N_{CDn}(r_d, x)$ in 10^{16} cm^{-3} ↗	11.876230,38.709048, 99.305248	13.163547, 42.904892, 110.06938
$N^{EBT}_{CDn}(r_d, x)$ in 10^{16} cm^{-3} ↗	11.876227**,** 38.709038**,** 99.305222	13.163543**,** 42.904881**,** 110.06935
$\lvert RD\rvert$ in 10^{-7}	2.78**,** 2.65**,** 2.65	**2.88,** 2.67, 2.63
Donor	Te	Sn
r_d (nm) ↗	0.132	0.140
x ↗	0, 0.5, 1	0, 0.5, 1
$\varepsilon(r_d, x)$ ↘	9.148968, 8.61079, 8.0726192	8.2592044, 7.773369, 7.2875333
$E_{gno}(r_d, x)$ eV ↗	1.843493, 2.21550, 2.5880362	1.8475518, 2.221897, 2.5973715
$N_{CDn}(r_d, x)$ in 10^{16} cm^{-3} ↗	18.241353, 59.455350, 152.52838	24.794696, 80.815133, 207.32535
$N^{EBT}_{CDn}(r_d, x)$ in 10^{16} cm^{-3} ↗	18.241348**,** 59.455334**,** 152.52834	24.794689**,** 80.815112**,** 207.32529
$\lvert RD\rvert$ in 10^{-7}	2.70**,** 2.61, 2.75	2.70, 2.64, 2.84

Acceptor	Ga	Mg
r_a (nm) ↗	0.126	0.140
x ↗	0, 0.5, 1	0, 0.5, 1
$\varepsilon(r_a, x)$ ↘	11.29769, 10.63312, 9.9685481	10.333116, 9.72529, 9.1174555
$E_{gpo}(r_a, x)$ eV ↗	1.8291247, 2.1929346, 2.5551356	1.838494, 2.207637, 2.5765572
$N_{CDp}(r_a, x)$ in 10^{18} cm^{-3} ↗	6.6323007, 21.364632, 54.449915	8.6684006, 27.923522, 71.165903
$N^{EBT}_{CDp}(r_a, \mathbf{x})$ in 10^{18} cm^{-3} ↗	6.6322989**,** 21.364627**,** 54.449900	8.6683983**,** 27.923514**,** 71.165884
$\lvert RD\rvert$ in 10^{-7}	2.69, 2.53, **2.82**	2.65, 2.83, 2.67
Acceptor	In	Cd
r_a (nm) ↗	0.144	**r_{ao}=0.148**
x ↗	0, 0.5, 1	0, 0.5, 1
$B_{ao}(x)$ in 10^8 (N/m^2) ↗		6.9396862, 10.88961, 1.5866282
$\varepsilon(r_a, x)$ ↘	10.23324, 9.631286, 9.0293303	**10.2**, 9.6, **9**
$E_{gpo}(r_a, x)$ eV ↗	1.839618, 2.209401, 2.5791277	**1.84**, 2.21, **2.58**
$N_{CDp}(r_a, x)$ in 10^{18} cm^{-3} ↗	8.9246936, 28.749118, 73.270019	9.0122328, 29.031108, 73.98870
$N^{EBT}_{CDp}(r_a, \mathbf{x})$ in 10^{18} cm^{-3} ↗	8.9246911**,** 28.749111**,** 73.269999	9.0122304**,** 29.031100**,** 73.98868
$\lvert RD\rvert$ in 10^{-7}	2.77, 2.59, 2.71	2.70, 2.61, 2.72

Table 8. In the $CdSe_{1-x}Te_x$-alloy the numerical results of $B_{do(ao)}$, ε, $E_{gno(gpo)}$, $N_{CDn(CDp)}$, and $N^{EBT}_{CDn(CDp)}$ are computed, using Equations (2), (5), (6), and (8a), and (26), respectively, noting that the relative deviations in absolute values are defined by: $|RD| \equiv \left|1-\frac{N^{EBT}_{CDn(CDp)}}{N_{CDn(Cdp)}}\right|$, giving rise to their maximal value equal to 2.88×10^{-7}, meaning that such the critical d(a)-density $N_{CDn(NDp)}(r_{d(a)}),x)$, *determined in Eq.* (8a), is just the density of electrons (holes) localized in the EBT, $N^{EBT}_{CDn(CDp)}(r_{d(a)},x)$, determined in Eq. (26), respectively. Here, on notes that in the limiting conditions: x=0, 1, these results are reduced to those given in CdSe-and-CdTe crystals, respectively, as observed in Table 1.

Donor	S	r_{do}=Se
r_d (nm) ↗	0.104	0.114
x ↗	0, 0.5, 1	0, 0.5, 1
$B_{do}(x)$ in 10^8 (N/m^2) ↘		3.71185, 3.4217698, 3.1376502
$\varepsilon(r_d,x)$ ↘	10.555973, 10.612893, 10.66981	**10.2**, 10.255, **10.31**
$E_{gno}(r_d,x)$ eV ↗	1.8390466, 1.7291211, 1.619194	**1.84**, 1.73, **1.62**
$N_{CDn}(r_d,x)$ in 10^{16} cm^{-3} ↗	11.876230, 9.4550897, 7.407913	13.163547, 10.479968, 8.2108893
$N^{EBT}_{CDn}(r_d,x)$ in 10^{16} cm^{-3} ↗	11.876227, 9.4550871, 7.407911	13.163543, 10.479965, 8.2108871
$\lvert RD\rvert$ in 10^{-7}	2.78, 2.73, 2.65	**2.88,** 2.42, 2.72
Donor	Te	Sn
r_d (nm) ↗	0.132	0.140
x ↗	0, 0.5, 1	0, 0.5, 1
$\varepsilon(r_d,x)$ ↘	9.148968, 9.198301, 9.2476338	8.2592044, 8.303739, 8.3482742
$E_{gno}(r_d,x)$ eV ↗	1.8434935, 1.733220, 1.6229531	1.8475518, 1.736962, 1.6263835
$N_{CDn}(r_d,x)$ in 10^{16} cm^{-3} ↗	18.241353, 14.522591, 11.378220	24.794696, 19.739941, 15.465931
$N^{EBT}_{CDn}(r_d,x)$ in 10^{16} cm^{-3} ↗	18.241348, 14.522587, 11.378217	24.794689, 19.739936, 15.465927
$\lvert RD\rvert$ in 10^{-7}	2.70, 2.71, 2.79	2.70, 2.65, 2.60

Acceptor	Ga	Mg
r_a (nm) ↗	0.126	0.140
x ↗	0, 0.5, 1	0, 0.5, 1
$\varepsilon(r_a,x)$ ↘	11.297688, 11.358607, 11.419526	10.333116, 10.3888, 10.444552
$E_{gpo}(r_a,x)$ eV ↗	1.8291247, 1.7148179, 1.6006033	1.8384942, 1.72790, 1.6173143
$N_{CDp}(r_a,x)$ in 10^{19} cm^{-3} ↗	0.66323007, 1.8337552, 3.8859101	0.86684006, 2.3967135, 5.0788748
$N^{EBT}_{CDp}(r_a,x)$ in 10^{19} cm^{-3} ↗	0.66322989, 1.8337547, 3.8859090	0.86683983, 2.3967129, 5.0788734
$\lvert RD\rvert$ in 10^{-7}	2.69, 2.61, 2.72	2.65, 2.58, 2.69
Acceptor	In	Cd
r_a (nm) ↗	0.144	r_{ao}=**0.148**
x ↗	0, 0.5, 1	0, 0.5, 1
$B_{ao}(x)$ in 10^8 (N/m^2) ↘		6.939686, 9.687909, 12.377251
$\varepsilon(r_a,x)$ ↘	10.23324, 10.288420, 10.343599	**10.2**, 10.225, **10.31**
$E_{gpo}(r_a,x)$ eV ↗	1.839618, 1.7294674, 1.6193195	**1.84**, 1.73, **1.62**
$N_{CDp}(r_a,x)$ in 10^{19} cm^{-3} ↗	0.89246936, 2.4675756, 5.2290386	0.90122328, 2.4917792, 5.2803284

$N_{CDp}^{EBT}(r_a, \mathbf{x})$ in 10^{19} cm^{-3} $\nearrow$	0.89246911, 2.4675749, 5.2290372	0.90122304, 2.4917785, 5.2803270
$\lvert RD \rvert$ in 10^{-7}	2.77, 2.65, **2.76**	2.70, 2.69, 2.66