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NEW CRITICAL DENSITY IN METAL-INSULATOR TRANSITION, OBTAINED IN VARIOUS N(P)- TYPE DEGENERATE CRYSTALLINE ALLOYS, BEING JUST THAT OF CARIERS LOCALIZED IN EXPONENTIAL BAND TAILS. (II)

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ABTRACT

By basing on the same physical model and treatment method, as used in our recent work (Van Cong, 2024), for $[\mathrm{InP_{1-x}As_x}\ (\mathrm{Sb_x}), \mathrm{GaAs_{1-x}Te_x}(\mathrm{Sb_x}, \mathrm{P_x}), \mathrm{CdS_{1-x}Te_x}(\mathrm{Se_x})]$- crystalline alloys, $0 \leq x \leq 1$, referred to as (I), we will investigate the critical impurity densities in the metal-insulator transition (MIT), obtained now in n(p)-type degenerate $\mathrm{X(x)} \equiv [\mathrm{InAs_{1-x}P_x}\ (\mathrm{Sb_x}), \mathrm{GaTe_{1-x}As_x}(\mathrm{Sb_x}, \mathrm{P_x}), \mathrm{CdTe_{1-x}S_x}(\mathrm{Se_x})]$- crystalline alloys, being due to the effects of the size of donor (acceptor) d(a)-radius, $\mathrm{r_{d(a)}}$ 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. (8), by using an empirical Mott parameter $M_{n(p)} = 0.2$, and (ii)-the density of electrons (holes) localized in the exponential conduction (valence)-band tails (EBT), $N^{EBT}_{CDn(CDp)}\left(r_{d(a)}, x\right)$, as that given in Eq. (26), by using our empirical Heisenberg parameter, $\mathcal{H}_{n(p)} = 0.47137$, as given in Eq. (15), suggesting that: for given $r_{d(a)}$ and x, $N^{EBT}_{CDn(CDp)}\left(r_{d(a)}, x\right) \cong N_{CDn(CDp)}(r_{d(a)}, x)$, obtained with a precision of the order of 2.91×10^{-7}, as observed in Tables 2-8. In other words, such the critical d(a)-density $\mathrm{N_{CDn(NDp)}(r_{d(a)}), x)}$, 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: $[InAs_{1-x}P_x\ (Sb_x), GaTe_{1-x}As_x(Sb_x, P_x), CdTe_{1-x}S_x(Se_x)]$- crystalline alloys; 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 (Van Cong, 2024), for $[InP_{1-x}As_x\ (Sb_x), GaAs_{1-x}Te_x(Sb_x, P_x), CdS_{1-x}Te_x(Se_x)]$- crystalline alloys, $0 \leq x \leq 1$, 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 n(p)-type degenerate $X(x) \equiv [InAs_{1-x}P_x\ (Sb_x), GaTe_{1-x}As_x(Sb_x, P_x), CdTe_{1-x}S_x(Se_x)] -$ crystalline alloys, 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 densities $N_{CDn(CDp)}(r_{d(a)}, x)$ in the MIT, as that given in Eq. (10), by using an empirical Mott parameter $M_{n(p)} = 0.25$, 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 2.91×10^{-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, $N^{EBT}_{CDn(CDp)}(r_{d(a)}, x)$.

In the following, we will determine those functions: $N_{CDn(CDp)}(r_{d(a)}, x)$ and $N^{EBT}_{CDn(CDp)}(r_{d(a)}, x)$.

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:

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

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

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

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

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

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:

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

(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:

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

(8)

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, being found to be in good agreement with the corresponding experimental ones.

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 2.91×10^{-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:

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

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

$$R_{sn(sp)}(N, r_{d(a)}, x) \equiv \frac{k_{sn(sp)}}{k_{Fn(Fp)}} = \frac{k^{-1}_{Fn(Fp)}}{k^{-1}_{sn(sp)}} =$$

$$R_{snWS(spWS)} + [R_{snTF(spTF)} - R_{snWS(spWS)}]e^{-r_{sn(sp)}} < 1. \quad (10)$$

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:

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

(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 :

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

(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 $\vec{R_j}$, randomly distributed throughout X(x)- crystalline alloys, is defined by:

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

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 :

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

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

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

(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

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

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

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

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:

$$\langle E_k^{a-\frac{1}{2}} \rangle_{KIM} = \frac{\exp(-y^2/4) \times W_{n(p)}^{\frac{2a-1}{4}}}{\sqrt{2\pi}} \times \Gamma(a + \tfrac{1}{2}) \times D_{-a-\frac{1}{2}}(y) =$$

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

(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 $y = \mp E/\sqrt{W_{n(p)}} \equiv \frac{\pm E_{Fno(Fpo)}}{\eta_{n(p)}} \times \nu_{n(p)} \times \exp\left(\frac{\mathcal{H}_{n(p)} \times R_{sn(sp)}}{4 \times \sqrt{|\nu_{n(p)}|}}\right)$, 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: $\nu_{n(p)} \to \mp\infty$ 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:

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

(17)

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

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

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

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

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

As $E \to \mp 0$, one has: $(y, \nu_{n(p)}) \to \pm 0$, 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:

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

Further, as $E \to \mp\infty$, one has: $(y, \nu_{n(p)}) \to \pm\infty$. 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:

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

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:

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

(22)

so that: $F_{n(p)}(\nu_{n(p)}, N, r_{d(a)}, x, a) \to H_{n(p)}(\nu_{n(p)}, N, r_{d(a)}, x, a)$ for $0 \le \nu_n \le 16$, and $F_{n(p)}(\nu_{n(p)}, N, r_{d(a)}, x, a) \to K_{n(p)}(\nu_{n(p)}, N, r_{d(a)}, x, a)$ for $\nu_{n(p)} \ge 16$. 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), $N^{EBT}_{CDn(CDp)}(N, r_{d(a)}, x)$, 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:

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

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

(24)

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

$$N^{EBT}_{CDn(CDp)}(N, r_{d(a)}, x) = \frac{g_{c(v)}\times(m_{c(v)})^{3/2}\sqrt{\eta_{n(p)}}\times(\pm E_{Fno(Fpo)})}{2\pi^2\hbar^3} \times \left\{\int_0^{16}\beta(a = 1) \times F_{n(p)}\big(\nu_{n(p)}, N, r_{d(a)}, x, a = 1\big)\, d\nu_{n(p)} + I_{n(p)}\right\}, \quad (25)$$

where

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

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: $\Gamma(b, z_{n(p)}) \simeq z_{n(p)}^{b-1} \times e^{-z_{n(p)}}\left[1 + \sum_{j=1}^{16} \frac{(b-1)(b-2)\ldots(b-j)}{z_{n(p)}^{j}}\right]$.

Finally, Eq. (25) now yields:

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

(26)

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

In n(p)-type degenerate X(x)- crystalline alloys, the numerical results of $N_{CDn(CDp)}^{EBT}[N = N_{CDn(NDp)}(r_{d(a)}, x), r_{d(a)}, x] \equiv N_{CDn(CDp)}^{EBT}(r_{d(a)}, x)$, 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: $|RD| \equiv \left|1 - \frac{N_{CDn(CDp)}^{EBT}}{N_{CDn(CDp)}}\right|$.

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 $N_{CDn(CDp)}^{EBT}(r_{d(a)}, x)$ 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 $N_{CDn(CDp)}^{EBT}(r_{d(a)}, x)$ 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 $N_{CDn}^{EBT} \cong N_{CDn}$. 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)- 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 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).

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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.

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10. Critical Impurity Densities in the Mott Metal-Insulator Transition, Obtained in Three n(p)- Type Degenerate $\mathrm{GaAs_{1-x}Te_x(Sb_x, P_x)}$-Crystalline Alloys

APPENDIX 1

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

In $\boldsymbol{InAs_{1-x}P_x}$**-alloys**, in which $r_{do(ao)} = r_{As(In)}$ =0.118 nm (0.144 nm), we have: $g_{c(v)}(x) = 1 \times x + 1 \times (1-x)$, $m_{c(v)}(x)/m_o = 0.077\ (0.5) \times x + 0.09(0.3) \times (1-x)$, $\varepsilon_o(x) = 12.5 \times x + 14.55 \times (1-x)$, $E_{go}(x) = 1.424 \times x + 0.43 \times (1-x)$, and

In $\boldsymbol{InAs_{1-x}Sb_x}$**-alloys**, in which $r_{do(ao)} = r_{As(In)}$ =0.118 nm (0.144 nm), we have: $g_{c(v)}(x) = 1 \times x + 1 \times (1-x)$, $m_{c(v)}(x)/m_o = 0.1\ (0.4) \times x + 0.09\ (0.3) \times (1-x)$, $\varepsilon_o(x) = 16.8 \times x + 14.55 \times (1-x)$, $E_{go}(x) = 0.23 \times x + 0.43 \times (1-x)$.

In $\boldsymbol{GaTe_{1-x}As_x}$**-alloys**, in which $r_{do(ao)} = r_{Te(Ga)}$ =0.132 nm (0.126 nm), we have: $g_{c(v)}(x) = 1 \times x + 1 \times (1-x)$, $m_{c(v)}(x)/m_o = 0.066\ (0.291) \times x + 0.209(0.4) \times (1-x)$, $\varepsilon_o(x) = 13.13 \times x + 12.3 \times (1-x)$, $E_{go}(x) = 1.52 \times x + 1.796 \times (1-x)$,

In $\boldsymbol{GaTe_{1-x}Sb_x}$**-alloys**, in which $r_{do(ao)} = r_{Te(Ga)}$ =0.132 nm (0.126 nm), we have: $g_{c(v)}(x) = 1 \times x + 1 \times (1-x)$, $m_{c(v)}(x)/m_o = 0.047(0.3) \times x + 0.209(0.4) \times (1-x)$, $\varepsilon_o(x) = 15.69 \times x + 12.3 \times (1-x)$, $E_{go}(x) = 0.81 \times x + 1.796 \times (1-x)$, and

In $\boldsymbol{GaTe_{1-x}P_x}$**-alloys**, in which $r_{do(ao)} = r_{Te(Ga)}$ =0.132 nm (0.126 nm), we have: $g_{c(v)}(x) = 1 \times x + 1 \times (1-x)$, $m_{c(v)}(x)/m_o = 0.13(0.5) \times x + 0.209(0.4) \times (1-x)$, $\varepsilon_o(x) = 11.1 \times x + 12.3 \times (1-x)$, $E_{go}(x) = 1.796 \times x + 1.796 \times (1-x)$.

In $\boldsymbol{CdTe_{1-x}S_x}$**-alloys**, in which $r_{do(ao)} = r_{S(Cd)}$ =0.104 nm (0.148 nm), we have: $g_{c(v)}(x) = 1 \times x + 1 \times (1-x)$, $m_{c(v)}(x)/m_o = 0.197\ (0.801) \times x + 0.095(0.82) \times (1-x)$, $\varepsilon_o(x) = 9 \times x + 10.31 \times (1-x)$, $E_{go}(x) = 2.58 \times x + 1.62 \times (1-x)$, and

In $\boldsymbol{CdTe_{1-x}Se_x}$**-alloys**, in which $r_{do(ao)} = r_{S(Cd)}$ =0.104 nm (0.148 nm), we have: $g_{c(v)}(x) = 1 \times x + 1 \times (1-x)$, $m_{c(v)}(x)/m_o = 0.11\ (0.45) \times x + 0.095(0.82) \times (1-x)$, $\varepsilon_o(x) = 10.2 \times x + 10.31 \times (1-x)$, $E_{go}(x) = 1.84 \times x + 1.62 \times (1-x)$.

Table 2: In the $\mathrm{InAs_{1-x}P_x}$-alloy the numerical results of $\mathrm{B_{do(ao)}}$, ε, $\mathrm{E_{gno(gpo)}}$, $\mathrm{N_{CDn(CDp)}}$, and $\mathrm{N^{EBT}_{CDn(CDp)}}$ are computed, using Equations (2), (5), (6), and (8), and (26), respectively, noting that the relative deviations in absolute values are defined by: $|\mathrm{RD}| \equiv \left|1 - \frac{\mathrm{N^{EBT}_{CDn(CDp)}}}{\mathrm{N_{CDn(Cdp)}}}\right|$, giving rise to their maximal value equal to 2.76×10^{-7} , meaning that such the critical d(a)-density

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

Donor	P	As
r_d (nm) ↗	0.110	$\mathbf{r_{do}}$**=0.118**
x ↗	0, 0.5, 1	0, 0.5, 1
$B_{do}(x)$ in 10^8 (N/m^2) ↗		1.3458086, 1.4450362,1.5600463
$\varepsilon(r_d, x)$ ↘	14.85002, 13.8039, 12.75774	**14.55**, 13.525, **12.5**
$E_{gno}(r_d, x)$ eV ↗	0.4297687, 0.926752, 1.42373	**0.43**, 0.927, **1.424**
$N_{CDn}(r_d, x)$ in 10^{16} cm^{-3} ↗	2.3363729, 2.3230107, 2.3075214	2.4838989, 2.469693, 2.4532257
$N^{EBT}_{CDn}(r_d, x)$ in 10^{16} cm^{-3} ↗	2.3363723, 2.3230101, 2.3075208	2.4838983, 2.4696924, 2.4532251
$\lvert RD \rvert$ in 10^{-7}	**2.75,** 2.57, 2.56	2.57, 2.57, 2.62
Donor	Sb	Sn
r_d (nm) ↗	0.136	0.140
x ↗	0, 0.5, 1	0, 0.5, 1
$\varepsilon(r_d, x)$ ↘	13.139864, 12.214203, 11.28854	12.552119, 11.667863, 10.78361
$E_{gno}(r_d, x)$ eV ↗	0.431307, 0.9284039, 1.4255157	0.431987, 0.9291335, 1.4263033
$N_{CDn}(r_d, x)$ in 10^{16} cm^{-3} ↗	3.3724874, 3.3531995, 3.3308411	3.868760, 3.8466338, 3.8209854
$N^{EBT}_{CDn}(r_d, x)$ in 10^{16} cm^{-3} ↗	3.3724865, 3.3531986, 3.3308402	3.868759, 3.8466328, 3.8209844
$\lvert RD \rvert$ in 10^{-7}	2.74, 2.74, 2.60	2.67, 2.62, 2.64
Acceptor	Ga	Mg
r_a (nm) ↗	0.126	0.140
x ↗	0, 0.5, 1	0, 0.5, 1
$\varepsilon(r_a, x)$ ↘	15.6192444, 14.5189196, 13.4185948	14.6000832, 13.571555, 12.5430268
$E_{gpo}(r_a, x)$ eV ↗	0.4274517, 0.9230677, 1.4182455	0.429868, 0.9267963, 1.4237019
$N_{CDp}(r_a, x)$ in 10^{18} cm^{-3} ↗	0.74366797, 2.1946863, 5.4298054	0.91052768, 2.6871166, 6.6481122
$N^{EBT}_{CDp}(r_a, \mathbf{x})$ in 10^{18} cm^{-3} ↗	0.74366777, 2.1946857, 5.4298040	0.91052743, 2.6871159, 6.6481104
$\lvert RD \rvert$ in 10^{-7}	2.68, **2.76**, 2.68	2.77, 2.62, 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) ↗	2.4684288, 3.808998, 5.5741072	
$\varepsilon(r_a, x)$ ↘	**14.55**, 13.525, **12.5**	14.4990401, 13.47763, 12.45622
$E_{gpo}(r_a, x)$ eV ↗	**0.43**, 0.927, **1.424**	0.4301357, 0.9272094, 1.4243065
$N_{CDp}(r_a, x)$ in 10^{18} cm^{-3} ↗	0.91996257, 2.7149606, 6.717	0.92969691, 2.7436882, 6.7880742
$N^{EBT}_{CDp}(r_a, \mathbf{x})$ in 10^{18} cm^{-3} ↗	0.91996232, 2.7149599, 6.7169982	0.92969666, 2.7436875, 6.7880723
$\lvert RD \rvert$ in 10^{-7}	2.68, 2.75, 2.69	2.71, 2.63, 2.74

Table 3. In the $\mathbf{InAs_{1-x}Sb_x}$-alloy the numerical results of $\mathbf{B_{do(ao)}}$, $\boldsymbol{\varepsilon}$, $\mathbf{E_{gno(gpo)}}$, $\mathbf{N_{CDn(CDp)}}$, and $\mathbf{N^{EBT}_{CDn(CDp)}}$ are computed, using Equations (2), (5), (6), and (8), and (26), respectively, noting that the relative deviations in absolute values are defined by: $\lvert RD \rvert \equiv \left| 1 - \frac{N^{EBT}_{CDn(CDp)}}{N_{CDn(Cdp)}} \right|$, giving rise to their maximal value equal to 2.91×10^{-7}, meaning that such the critical d(a)-density

$N_{CDn(NDp)}(r_{d(a)}, x)$, determined in Eq. (8), 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 GaAs-and-GaTe crystals, respectively, as observed in Table 1.

Donor	P	As
r_d (nm) ↗	0.110	**r_{do}=0.118**
x ↗	0, 0.5, 1	0, 0.5, 1
$B_{do}(x)$ in 10^8 (N/m^2) ↘		1.3458086, 1.2239827, 1.1216264
$\varepsilon(r_d, x)$ ↘	14.85001, 15.998213, 17.14641	**14.55**, 15.675, **16.8**
$E_{gno}(r_d, x)$ eV ↗	0.4297687, 0.32979, 0.2298073	**0.43**, 0.33, **0.23**
$N_{CDn}(r_d, x)$ in 10^{16} cm^{-3} ↗	2.3363729, 2.1976158, 2.0819762	2.4838989, 2.3363803, 2.2134389
$N^{EBT}_{CDn}(r_d, x)$ in 10^{16} cm^{-3} ↗	2.3363723, 2.1976152, 2.0819756	2.4838983, 2.3363797, 2.2134383
$\lvert RD\rvert$ in 10^{-7}	2.75, 2.61, 2.67	2.58, 2.61, **2.81**
Donor	Sb	Sn
r_d (nm) ↗	0.136	0.140
x ↗	0, 0.5, 1	0, 0.5, 1
$\varepsilon(r_d, x)$ ↘	13.139864, 14.15583, 15.171801	12.552119, 13.52264, 14.49317
$E_{gno}(r_d, x)$ eV ↗	0.4313075, 0.33119, 0.2310897	0.431987, 0.3318071, 0.231656
$N_{CDn}(r_d, x)$ in 10^{16} cm^{-3} ↗	3.3724874, 3.1721955, 3.0052730	3.868760, 3.6389946, 3.4475089
$N^{EBT}_{CDn}(r_d, x)$ in 10^{16} cm^{-3} ↗	3.3724865, 3.1721946, 3.0052722	3.868759, 3.6389936, 3.4475080
$\lvert RD\rvert$ in 10^{-7}	2.74, 2.69, 2.61	2.67, 2.79, 2.70
Acceptor	Ga	Mg
r_a (nm) ↗	0.126	0.140
x ↗	0, 0.5, 1	0, 0.5, 1
$\varepsilon(r_a, x)$ ↘	15.6192444, 16.8269179, 18.0345915	14.600083, 15.72896, 16.857828
$E_{gpo}(r_a, x)$ eV ↗	0.4274517, 0.3274384, 0.2274514	0.429868, 0.3298673, 0.229868
$N_{CDp}(r_a, x)$ in 10^{18} cm^{-3} ↗	0.74366797, 0.9444648, 1.1451343	0.91052768, 1.1563781, 1.4020726
$N^{EBT}_{CDp}(r_a, x)$ in 10^{18} cm^{-3} ↗	0.74366777, 0.9444646, 1.1451340	0.91052743, 1.1563778, 1.4020722
$\lvert RD\rvert$ in 10^{-7}	2.68, 2.64, 2.74	2.77, 2.83, 2.81
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) ↘	5.5741072, 3.6522677, 2.4686912	
$\varepsilon(r_a, x)$ ↘	**14.55**, 15.675, **16.8**	14.499040, 15.6201, 16.7411597
$E_{gpo}(r_a, x)$ eV ↗	**0.43**, 0.33, **0.23**	0.4301357, 0.3301364, 0.2301357
$N_{CDp}(r_a, x)$ in 10^{18} cm^{-3} ↗	0.91996257, 1.1683605, 1.4166009	0.92969691, 1.1807232, 1.4315903
$N^{EBT}_{CDp}(r_a, x)$ in 10^{18} cm^{-3} ↗	0.91996232, 1.1683602, 1.4166005	0.92969666, 1.1807229, 1.4315899
$\lvert RD\rvert$ in 10^{-7}	2.68, 2.78, 2.82	2.71, 2.83, **2.91**

Table 4: In the $GaTe_{1-x}As_x$-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 (8), 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 2.91×10^{-7}, meaning that such the critical d(a)-density

$N_{CDn(NDp)}(r_{d(a)}, x)$, **determined in Eq. (8), 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 GaAs-and-GaTe crystals, respectively, as observed in Table 1.**

Donor	P	As	Te
r_d (nm) ↗	0.110	0.118	**r_{do}=0.132**
x ↗	0, 0.5, 1	0, 0.5, 1	0, 0.5, 1
$B_{do}(x)$ in 10^8 (N/m^2) ↘			3.1241155, 1.923362, 0.8657759
$\varepsilon(r_d, x)$ ↘	14.021105, 14.494174, 14.967244	12.937135, 13.3736, 13.81013	**12.3**, 12.715, **13.13**
$E_{gno}(r_d, x)$ eV ↗	1.7916707, 1.6553346, 1.5188002	1.794195, 1.656889, 1.51950	**1.796**, 1.658, **1.52**
$N_{CDn}(r_d, x)$ in 10^{16} cm^{-3} ↗	34.760623, 8.9603097, 0.89991533	44.250678, 11.406579, 1.1456027	51.489527, 13.27255, 1.3330088
$N^{EBT}_{CDn}(r_d, x)$ in 10^{16} cm^{-3} ↗	34.760613, 8.9603073, 0.899915083	44.250666, 11.406576, 1.1456024	51.489513, 13.272547, 1.3330084
$\lvert RD \rvert$ in 10^{-7}	2.78, 2.45, 2.72	2.78, 2.83, 2.74	2.74, 2.62, 2.87

Donor	Sb	Sn
r_d (nm) ↗	0.136	0.140
x ↗	0, 0.5, 1	0, 0.5, 1
$\varepsilon(r_d, x)$ ↘	12.248718, 12.66199, 13.0752578	12.095622, 12.50373, 12.9118304
$E_{gno}(r_d, x)$ eV ↗	1.7961576, 1.6580971, 1.5200437	1.7966403, 1.658394, 1.5201774
$N_{CDn}(r_d, x)$ in 10^{16} cm^{-3} ↗	52.138951, 13.439954, 1.3498217	54.143913, 13.956776, 1.4017280
$N^{EBT}_{CDn}(r_d, x)$ in 10^{16} cm^{-3} ↗	52.138937, 13.439950, 1.3498213	54.143898, 13.956772, 1.4017276
$\lvert RD \rvert$ in 10^{-7}	2.64, **2.91**, 2.77	2.74, 2.61, 2.77

Acceptor	B	Ga	Mg
r_a (nm) ↗	0.088	**r_{ao}=0.126**	0.140
x ↗	0, 0.5, 1	0, 0.5, 1	0, 0.5, 1
$B_{ao}(x)$ in 10^8 (N/m^2) ↘		6.8746556, 5.556694, 4.388991	
$\varepsilon(r_a, x)$ ↘	22.8400, 23.61066, 24.3812808	**12.3**, 12.715, **13.13**	11.635396, 12.0279, 12.42055
$E_{gpo}(r_a, x)$ eV ↗	1.77047, 1.637365, 1.5037013	**1.796**, 1.658, **1.52**	1.800225, 1.66141, 1.522697
$N_{CDp}(r_a, x)$ in 10^{18} cm^{-3} ↗	0.56374752, 0.3288630, 0.17844517	3.6096078, 2.105671, 1.142563	4.2641433, 2.487495, 1.3497457
$N^{EBT}_{CDp}(r_a, \mathbf{x})$ in 10^{18} cm^{-3} ↗	0.56374737, 0.3288629, 0.17844512	3.6096068, 2.105670, 1.1425627	4.2641421, 2.487494, 1.3497453
$\lvert RD \rvert$ in 10^{-7}	2.71, 2.72, 2.71	2.72, 2.65, 2.59	2.75, 2.67, **2.82**

Acceptor	In	Cd
r_a (nm) ↗	0.144	0.148
x ↗	0, 0.5, 1	0, 0.5, 1
$\varepsilon(r_a, x)$ ↘	11.240603, 11.6198, 11.9991	10.789407, 11.15344, 11.51747

$E_{gpo}(r_a, x)$ eV ↗	1.803097, 1.66374, 1.5245311	1.806773, 1.666708, 1.5268781
$N_{CDp}(r_a, x)$ in 10^{18} cm^{-3} ↗	4.7294055, 2.7589064, 1.4970169	5.3478913, 3.1197012, 1.6927886
$N_{CDp}^{EBT}(r_a, \mathbf{x})$ in 10^{18} cm^{-3} ↗	4.7294042, 2.7589057, 1.4970165	5.3478899, 3.1197004, 1.6927881
$\|RD\|$ in 10^{-7}	2.81, 2.69, 2.81	2.67, 2.68, 2.74

Table 5: In the $GaTe_{1-x}Sb_x$-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 (8), 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 2.87×10^{-7}, meaning that such the critical d(a)-density $N_{CDn(NDp)}(r_{d(a)}), x), determined\ in\ Eq. (8)$, 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 GaAs-and-GaP crystals, respectively, as observed in Table 1.

Donor	P	As	Te
r_d (nm) ↗	0.110	0.118	**r_{do}=0.132**
x ↗	0, 0.5, 1	0, 0.5, 1	0, 0.5, 1
$B_{do}(x)$ in 10^8 (N/m^2) ↘			3.1241155, 1.477934, 0.4317606
$\varepsilon(r_d, x)$ ↘	14.02110, 15.95328, 17.885458	12.937135, 14.71993, 16.50273	**12.3**, 13.995, **15.69**
$E_{gno}(r_d, x)$ eV ↗	1.791671, 1.300952, 0.8094017	1.794195, 1.302146, 0.80975	**1.796**, 1.303, **0.81**
$N_{CDn}(r_d, x)$ in 10^{16} cm^{-3} ↗	34.760623, 5.4209478,0.19045342	44.250678, 6.9009297, 0.2424494	51.489527, 8.0298341, 0.28211106
$N_{CDn}^{EBT}(r_d, x)$ in 10^{16} cm^{-3} ↗	34.760613, 5.4209463, 0.19045337	44.250666, 6.9009279, 0.2424493	51.489513, 8.0298320, 0.28211099
$\|RD\|$ in 10^{-7}	2.78, 2.73, **2.83**	2.78, 2.64, 2.72	2.74, 2.66, 2.62
Donor	Sb	Sn	
r_d (nm) ↗	0.136	0.140	
x ↗	0, 0.5, 1	0, 0.5, 1	
$\varepsilon(r_d, x)$ ↘	12.248718, 13.93665, 15.624585	12.095622, 13.76246, 15.429293	
$E_{gno}(r_d, x)$ eV ↗	1.7961576, 1.303075, 0.8100218	1.7966403, 1.303303, 0.8100885	
$N_{CDn}(r_d, x)$ in 10^{16} cm^{-3} ↗	52.138951, 8.1311125, 0.28566926	54.143913, 8.4437878, 0.29665444	
$N_{CDn}^{EBT}(r_d, x)$ in 10^{16} cm^{-3} ↗	52.138937, 8.1311103, 0.28566918	54.143898, 8.4437855, 0.29665436	
$\|RD\|$ in 10^{-7}	2.64, 2.66, 2.70	2.51, 2.68, 2.69	

Acceptor	B	Ga	Mg
r_a (nm) ↗	0.088	**r_{ao}=0.126**	0.140
x ↗	0, 0.5, 1	0, 0.5, 1	0, 0.5, 1
$B_{ao}(x)$ in 10^8 (N/m^2) ↘		6.8746556, 4.646473, 3.1686666	
$\varepsilon(r_a, x)$ ↘	22.8400, 25.987511, 29.134981	**12.3**, 13.995, **15.69**	11.63540, 13.2388, 14.842225
$E_{gpo}(r_a, x)$ eV ↗	1.77047, 1.2857451, 0.798233	**1.796**, 1.303, **0.81**	1.800225, 1.305856, 0.8119474
$N_{CDp}(r_a, x)$ in 10^{18} cm^{-3} ↗	0.56374752, 0.25639256, 0.11458161	3.6096078, 1.6416509, 0.73365234	4.2641433, 1.9393338, 0.86668661

$N^{EBT}_{CDp}(r_a, \mathbf{x})$ in 10^{18} cm^{-3} ↗	0.56374737, 0.25639249, 0.11458158	3.6096068, 1.6416504, 0.73365214	4.2641421, 1.9393333, 0.86668638
$\lvert RD \rvert$ in 10^{-7}	2.71, 2.62, 2.50	2.72, 2.82, 2.68	2.75, 2.50, 2.67

Acceptor	In	Cd
r_a (nm) ↗	0.144	0.148
x ↗	0, 0.5, 1	0, 0.5, 1
$\varepsilon(r_a, x)$ ↘	11.240603, 12.78961, 14.3386225	10.78941, 12.27624, 13.763073
$E_{gpo}(r_a, x)$ eV ↗	1.8030972, 1.3077969, 0.8132712	1.806773, 1.310282, 0.8149657
$N_{CDp}(r_a, x)$ in 10^{18} cm^{-3} ↗	4.7294055, 2.1509352, 0.96125108	5.3478913, 2.4322228, 1.0869583
$N^{EBT}_{CDp}(r_a, \mathbf{x})$ in 10^{18} cm^{-3} ↗	4.7294042, 2.1509347, 0.96125083	5.3478899, 2.4322221, 1.0869580
$\lvert RD \rvert$ in 10^{-7}	2.81, 2.53, 2.62	2.67, 2.70, **2.87**

Table 6: In the $GaTe_{1-x}P_x$-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 (8), 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 2.91×10^{-7}, meaning that such the critical d(a)-density $N_{CDn(NDp)}(r_{d(a)}), x), determined\ in\ Eq. (8)$, 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 GaAs-and-GaSb crystals, respectively, as observed in Table 1.

Donor	P	As	Te
r_d (nm) ↗	0.110	0.118	**r_{do}=0.132**
x ↗	0, 0.5, 1	0, 0.5, 1	0, 0.5, 1
$B_{do}(x)$ in 10^8 (N/m^2) ↘			3.1241155, 2.8002, 2.386099
$\varepsilon(r_d, x)$ ↘	14.02111, 13.337148, 12.653192	12.9371348, 12.30605, 11.67497	**12.3**, 11.7, **11.1**
$E_{gno}(r_d, x)$ eV ↗	1.791671, 1.7921195, 1.7926934	1.794195, 1.794382, 1.7946214	**1.796**, 1.796, **1.796**
$N_{CDn}(r_d, x)$ in 10^{17} cm^{-3} ↗	3.4760623, 2.1543464, 1.1382172	4.4250678, 2.7425081, 1.4489638	5.1489527, 3.1911476, 1.6859958
$N^{EBT}_{CDn}(r_d, x)$ in 10^{17} cm^{-3} ↗	3.47606213, 2.1543458, 1.1382169	4.4250666, 2.7425074, 1.44896384	5.1489513, 3.1911468, 1.6859954
$\lvert RD \rvert$ in 10^{-7}	2.78, 2.61, 2.64	2.78, 2.66, **2.90**	2.74, 2.62, 2.60

Donor	Sb	Sn
r_d (nm) ↗	0.136	0.140
x ↗	0, 0.5, 1	0, 0.5, 1
$\varepsilon(r_d, x)$ ↘	12.248718, 11.65122, 11.053721	12.095622, 11.50559, 10.9155611
$E_{gno}(r_d, x)$ eV ↗	1.7961576, 1.796141, 1.7961204	1.7966403, 1.796574, 1.7964890
$N_{CDn}(r_d, x)$ in 10^{17} cm^{-3} ↗	5.2138951, 3.2313968, 1.7072609	5.4143913, 3.3556576, 1.7729122
$N^{EBT}_{CDn}(r_d, x)$ in 10^{17} cm^{-3} ↗	5.2138937, 3.2313960, 1.7072604	5.4143898, 3.3556567, 1.7729117
$\lvert RD \rvert$ in 10^{-7}	2.64, 2.65, 2.77	2.74, 2.83, 2.58

Acceptor	B	Ga	Mg
r_a (nm) ↗	0.088	$\mathbf{r_{ao}=0.126}$	0.140
x ↗	0, 0.5, 1	0, 0.5, 1	0, 0.5, 1
$B_{ao}(x)$ in 10^8 (N/m^2) ↗		6.8746556, 8.547556, 10.55177	
$\varepsilon(r_a, x)$ ↘	22.8400, 21.72589, 20.611745	**12.3**, 11.7, **11.1**	11.635396, 11.06782, 10.500236
$E_{gpo}(r_a, x)$ eV ↗	1.77047, 1.764258, 1.7568155	**1.796**, 1.796, **1.796**	1.800225, 1.801253, 1.8024849
$N_{CDp}(r_a, x)$ in 10^{18} cm^{-3} ↗	0.56374752, 0.93260976, 1.4981699	3.6096078, 5.9713885, 9.592602	4.2641433, 7.0541893, 11.332043
$N_{CDp}^{EBT}(r_a, \mathbf{x})$ in 10^{18} cm^{-3} ↗	0.56374737**,** 0.93260951**,** 1.4981695	3.6096068**,** 5.9713869**,** 9.592600	4.2641421**,** 7.0541874**,** 11.332040
$\lvert RD\rvert$ in 10^{-7}	2.71, 2.65, 2.52	2.72, 2.64, 2.71	2.75, 2.65, 2.45

Acceptor	In	Cd
r_a (nm) ↗	0.144	0.148
x ↗	0, 0.5, 1	0, 0.5, 1
$\varepsilon(r_a, x)$ ↘	11.240603, 10.6923, 10.14396	10.789407, 10.26309, 9.7367823
$E_{gpo}(r_a, x)$ eV ↗	1.8030972, 1.80482, 1.8068933	1.8067734, 1.8093951, 1.812559
$N_{CDp}(r_a, x)$ in 10^{18} cm^{-3} ↗	4.7294055, 7.8238743, 12.568487	5.3478913, 8.8470379, 14.212125
$N_{CDp}^{EBT}(r_a, \mathbf{x})$ in 10^{18} cm^{-3} ↗	4.7294042**,** 7.8238722, 12.568483	5.3478899**,** 8.8470356**,** 14.212121
$\lvert RD\rvert$ in 10^{-7}	2.81, 2.73, **2.91**	2.67, 2.60, 2.84

Table 7: In the $CdTe_{1-x}S_x$-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 (8), 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 2.82×10^{-7}, meaning that such the critical d(a)-density $N_{CDn(NDp)}(r_{d(a)}, x)$, *determined in Eq.* (8), 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 GaAs-and-GaTe crystals, respectively, as observed in Table 1.

Donor	S	Se
r_d (nm) ↗	0.104	0.114
x ↗	0, 0.5, 1	0, 0.5, 1
$\varepsilon(r_d, x)$ ↘	12.942503, 12.1202, 11.298015	11.2257881, 10.51261, 9.799427
$E_{gno}(r_d, x)$ eV ↗	1.6155583, 2.09222, 2.567913	1.6180978, 2.096666, 2.5748234
$N_{CDn}(r_d, x)$ in 10^{16} cm^{-3} ↗	4.1506041,18.345022, 55.640067	6.3608576, 28.113996, 85.269163
$N_{CDn}^{EBT}(r_d, x)$ in 10^{16} cm^{-3} ↗	4.1506030**,** 18.345017, 55.640052	6.3608559, 28.113988**,** 85.269141
$\lvert RD\rvert$ in 10^{-7}	2.6**,** 2.79, 2.66	2.73**,** 2.67, 2.59

Donor	Te	Sn
r_d (nm) ↗	$\mathbf{r_{do}=0.132}$	0.140
x ↗	0, 0.5, 1	0, 0.5, 1
$B_{do}(x)$ in 10^8 (N/m^2) ↗	2.0211442, 3.541925, 5.5001208	
$\varepsilon(r_d, x)$ ↘	**10.31**, 9.655, **9**	10.138688, 9.494571, 8.850455
$E_{gno}(r_d, x)$ eV ↗	**1.62**, 2.1, **2.58**	1.6204142, 2.100726, 2.5811272
$N_{CDn}(r_d, x)$ in 10^{16} cm^{-3} ↗	8.2108893, 36.290847, 110.06938	8.6341767, 38.161712, 115.74367

$N^{EBT}_{CDn}(r_d, x)$ in 10^{16} cm^{-3} ↗	8.2108871**,** 36.290837**,** 110.06935	8.6341743, 38.161702, 115.74364
$\|RD\|$ in 10^{-7}	2.72**,** 2.65, 2.63	2.76, 2.72, 2.56

Acceptor	Ga	Mg
r_a (nm) ↗	0.126	0.140
x ↗	0, 0.5, 1	0, 0.5, 1
$\varepsilon(r_a, x)$ ↘	11.41926, 10.69404, 9.9685481	10.444552, 9.781004, 9.1174555
$E_{gpo}(r_a, x)$ eV ↗	1.6006033, 2.078139, 2.5551356	1.6173143, 2.09697, 2.5765572
$N_{CDp}(r_a, x)$ in 10^{19} cm^{-3} ↗	3.8859101, 4.5690868, 5.4449915	5.0788748, 5.9717851, 7.1165903
$N^{EBT}_{CDp}(r_a, \mathbf{x})$ in 10^{19} cm^{-3} ↗	3.8859090, 4.5690856**,** 5.4449900	5.0788734**,** 5.9717835**,** 7.1165884
$\|RD\|$ in 10^{-7}	2.75, 2.68, **2.82**	2.679, 2.62, 2.67
Acceptor	In	Cd
r_a (nm) ↗	0.144	$\mathbf{r_{ao}=0.148}$
x ↗	0, 0.5, 1	0, 0.5, 1
$B_{ao}(x)$ in 10^9 (N/m^2) ↗		1.2377251, 1.3950062, 1.5866282
$\varepsilon(r_a, x)$ ↘	10.343599, 9.686465, 9.0293303	**10.31**, 9.655, **9**
$E_{gpo}(r_a, x)$ eV ↗	1.6193195, 2.099233, 2.5791277	**1.62**, 2.1, **2.58**
$N_{CDp}(r_a, x)$ in 10^{19} cm^{-3} ↗	5.2290386, 6.148349, 7.3270019	5.2803284, 6.208656, 7.398870
$N^{EBT}_{CDp}(r_a, \mathbf{x})$ in 10^{19} cm^{-3} ↗	5.2290372**,** 6.1483473**,** 7.3270000	5.2803270**,** 6.2086543**,** 7.398868
$\|RD\|$ in 10^{-7}	2.76, 2.78, 2.71	2.66, 2.68, 2.72

Table 8: In the $CdTe_{1-x}Se_x$-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 (8), 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 $N_{CDn(NDp)}(r_{d(a)}), x), determined\ in\ Eq. (8)$, 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 GaAs-and-GaTe crystals, respectively, as observed in Table 1.

Donor	S	Se
r_d (nm) ↗	0.104	0.114
x ↗	0, 0.5, 1	0, 0.5, 1
$\varepsilon(r_d, x)$ ↘	12.9425036, 12.87346, 12.804417	11.225788, 11.165903, 11.1060173
$E_{gno}(r_d, x)$ eV ↗	1.6155583, 1.7251561, 1.834745	1.6180978, 1.7279255, 1.8377496
$N_{CDn}(r_d, x)$ in 10^{16} cm^{-3} ↗	4.1506041, 5.2976236, 6.6541722	6.3608576, 8.1186805, 10.197610
$N^{EBT}_{CDn}(r_d, x)$ in 10^{16} cm^{-3} ↗	4.1506030**,** 5.2976222, 6.6541704	6.3608559**,** 8.1186783, 10.197607
$\|RD\|$ in 10^{-7}	2.60**,** 2.71, 2.73	2.73**,** 2.65, 2.77
Donor	Te	Sn
r_d (nm) ↗	$\mathbf{r_{do}=0.132}$	0.140
x ↗	0, 0.5, 1	0, 0.5, 1
$B_{do}(x)$ in 10^8 (N/m^2) ↗	2.0211442, 2.204162, 2.3910208	
$\varepsilon(r_d, x)$ ↘	**10.31**, 10.255, **10.2**	10.1386879, 10.084602, 10.030516
$E_{gno}(r_d, x)$ eV ↗	**1.62**, 1.73, **1.84**	1.6204142, 1.730452, 1.84049
$N_{CDn}(r_d, x)$ in 10^{16} cm^{-3} ↗	8.2108893, 10.479968, 13.163547	8.6341767, 11.020231, 13.842153

$N_{CDn}^{EBT}(r_d, x)$ in 10^{16} cm^{-3} ↗	8.2108871**,** 10.479965**,** 13.163543	8.6341743**,** 11.020228**,** 13.842149
$\lvert RD\rvert$ in 10^{-7}	2.72**,** 2.42, **2.88**	2.76, 2.38, 2.53

Acceptor	Ga	Mg
r_a (nm) ↗	0.126	0.140
x ↗	0, 0.5, 1	0, 0.5, 1
$\varepsilon(r_a, x)$ ↘	11.419526, 11.358607, 11.2976878	10.44455, 10.3888, 10.3331162
$E_{gpo}(r_a, x)$ eV ↗	1.6006033, 1.7148179, 1.8291247	1.617314, 1.72790, 1.8384942
$N_{CDp}(r_a, x)$ in 10^{19} cm^{-3} ↗	3.8859101, 1.8337552, 0.66323007	5.0788748, 2.3967135, 0.86684006
$N_{CDp}^{EBT}(r_a, \mathbf{x})$ in 10^{19} cm^{-3} ↗	3.8859090**,** 1.8337547, 0.66322989	5.0788734**,** 2.3967129, 0.86683983
$\lvert RD\rvert$ in 10^{-7}	2.75, 2.61, 2.69	2.69, 2.58, 2.65
Acceptor	In	Cd
r_a (nm) ↗	0.144	$\mathbf{r_{ao}=0.148}$
x ↗	0, 0.5, 1	0, 0.5, 1
$B_{ao}(x)$ in 10^9 (N/m^2) ↘		1.2377251**,** 0.9687909, 0.69396862
$\varepsilon(r_a, x)$ ↘	10.343599, 10.288420, 10.233241	**10.31**, 10.225, **10.2**
$E_{gpo}(r_a, x)$ eV ↗	1.6193195, 1.7294674, 1.8396185	**1.62**, 1.73, **1.84**
$N_{CDp}(r_a, x)$ in 10^{19} cm^{-3} ↗	5.2290386, 2.4675756, 0.89246936	5.2803284, 2.4917792, 0.90122328
$N_{CDp}^{EBT}(r_a, \mathbf{x})$ in 10^{19} cm^{-3} ↗	5.2290372**,** 2.4675749, 0.89246911	5.2803327**,** 2.4917785, 0.90122304
$\lvert RD\rvert$ in 10^{-7}	2.76, 2.65, **2.77**	2.66, 2.69, 2.70