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

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ABTRACT

By basing on the same physical model and treatment method, as used in our recent works (Van Cong, 2023; 2023; 2023), we will investigate the critical impurity densities in the metal-insulator transition (MIT), obtained in two n(p)-type degenerate $[InP_{1-x}As_x(Sb_x), GaAs_{1-x}Te_x(Sb_x, P_x), CdS_{1-x}Te_x(Se_x)]$-crystalline alloys, $0 \leq x \leq 1$, being due to the effects of the size of donor (acceptor) d(a)-radius, $r_{d(a)}$, the x- concentration, and finally the high d(a)-density, N, 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. (8), 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),* $N_{CDn(CDp)}^{EBT}(r_{d(a)}, x)$, *as that given in Eq. (26), by using our empirical Heisenberg parameter,* $\mathcal{H}_{n(p)} = 0.47137$, *as given in Eq. (15), according to: for given* $r_{d(a)}$ *and x,* $N_{CDn(CDp)}^{EBT}(r_{d(a)}, x) \cong N_{CDn(CDp)}(r_{d(a)}, x)$, *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) localized in the EBT, $N_{CDn(CDp)}^{EBT}(r_{d(a)}, x)$, respectively.

KEYWORS: $[\text{InP}_{1-x}\text{As}_x(\text{Sb}_x), \text{GaAs}_{1-x}\text{Te}_x(\text{Sb}_x, \text{P}_x), \text{CdS}_{1-x}\text{Te}_x(\text{Se}_x)]$- crystalline alloys; critical impurity density in the Mott MIT.

INTRODUCTION

By basing on the same intrinsic energy-band-structure parameters, physical model and treatment method, as used in our recent works (Van Cong, 2023; 2023; 2023), and also other works (Green, 2022; Kitell, 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 three n(p)-type degenerate $X(x)$- crystalline alloys, $X(x) \equiv [\text{InP}_{1-x}\text{As}_x(\text{Sb}_x), \text{GaAs}_{1-x}\text{Te}_x(\text{Sb}_x, \text{P}_x), \text{CdS}_{1-x}\text{Te}_x(\text{Se}_x)] - \text{crystalline alloys}, 0 \leq x \leq 1$, being due to the effects of the size of donor (acceptor) d(a)-radius, $r_{d(a)}$, the x- concentration, and finally the high d(a)-density, N, 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), $N_{CDn(CDp)}^{EBT}(r_{d(a)}, x)$, 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, $N_{CDn(CDp)}^{EBT}(r_{d(a)}, x) \cong N_{CDn(CDp)}(r_{d(a)}, x)$, 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) localized in the EBT, $N_{CDn(CDp)}^{EBT}(r_{d(a)}, x)$, respectively.

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, 2023; 2023; 2023): 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 reduced effective mass $m_r(x)/m_c$, the unperturbed relative dielectric static constant $\varepsilon_o(x)$, the effective donor (acceptor)-ionization

energy $E_{do(ao)}(x)$, and the isothermal bulk modulus $B_{do(ao)}(x) \equiv \frac{E_{do(ao)}(x)}{(4\pi/3)\times(r_{do(ao)})^3}$, at $r_{d(a)} = r_{do(ao)}$, are given respectively in Table 1 in Appendix 1.

Table 1

Therefore, one gets.

$$E_{do(ao)}(x) = \frac{13600 \times [m_{c(v)}(x)/m_0]}{[\varepsilon_0(x)]^2} \text{ meV, and} \quad (1)$$

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

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, 2023; 2023; 2023; 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: $\pm [\Delta\sigma(r_{d(a)},x)]_{n(p)}$,

$$E_{gno(gpo)}(r_{d(a)},x) - E_{go}(x) = E_{d(a)}(r_{d(a)},x) - E_{do(ao)}(x) = E_{do(ao)}(x) \times \left[\left(\frac{\varepsilon_0(x)}{\varepsilon(r_{d(a)})}\right)^2 - 1\right] = +[\Delta\sigma(r_{d(a)},x)]_{n(p)},$$

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

$$E_{gno(gpo)}(r_{d(a)},x) - E_{go}(x) = E_{d(a)}(r_{d(a)},x) - E_{do(ao)}(x) = E_{do(ao)}(x) \times \left[\left(\frac{\varepsilon_0(x)}{\varepsilon(r_{d(a)})}\right)^2 - 1\right] = -[\Delta\sigma(r_{d(a)},x)]_{n(p)}. \quad (4)$$

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 $\varepsilon(r_{d(a)}, x) = \dfrac{\varepsilon_0(x)}{\sqrt{1 + \left[\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 - 1\right] \times \ln\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3}} \leq \varepsilon_0(x),$

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

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 $\varepsilon(r_{d(a)}, x) = \dfrac{\varepsilon_0(x)}{\sqrt{1 - \left[\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 - 1\right] \times \ln\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3}} \geq \varepsilon_0(x),$ with a condition,

given by: $\left[\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 - 1\right] \times \ln\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 < 1,$

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

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.

$$a_{Bn(Bp)}(r_{d(a)}, x) \equiv \frac{\varepsilon(r_{d(a)}, x) \times \hbar^2}{m_{c(v)}(x) \times q^2} = 0.53 \times 10^{-8}\ cm \times \frac{\varepsilon(r_{d(a)}, x)}{m_{c(v)}(x)/m_0}, (7)$$

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, $M_{n(p)} = 0.25$, for each the conduction (valence) band, as:

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

noting that $M_{n(p)}$ could be chosen in general case so 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, these obtained numerical results can also be justified by calculating the numerical results of the density of electrons (holes) localized in exponential conduction (valence)-band (EBT) tails, $N_{CDn(CDp)}^{EBT}(r_{d(a)}, x)$.

$N_{CDn(CDp)}^{EBT}(r_{d(a)}, x)$ EXPRESSION

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

Physical model

In n(p)-type degenerate $X(x)$-crystalline alloys, $X(x) \equiv [CdS_{1-x}Te_x, CdS_{1-x}Se_x]$, if denoting the Fermi wave number by: $k_{Fn(Fp)}(N,x) \equiv \left(3\pi^2 N / g_{c(v)}(x)\right)^{1/3}$, N being the total impurity density, assuming that all the impurities are ionized even at 0 K, the effective reduced Wigner-Seitz radius $r_{sn(sp)}$, characteristic of interactions, is defined by.

$$r_{sn(sp)}\left(N, r_{d(a)}, x\right) \equiv \left(\frac{3g_{c(v)}(x)}{4\pi N}\right)^{1/3} \times \frac{1}{a_{Bn(Bp)}(r_{d(a)}, x)} = 1.1723 \times 10^8 \times \left(\frac{g_{c(v)}(x)}{N}\right)^{1/3} \times \frac{m_{c(v)}(x)/m_0}{\varepsilon(r_{d(a)}, x)}. \quad (9)$$

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

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

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 $R_{snTF}\left(N, r_{d(a)}, x\right) \equiv \frac{k_{snTF(spTF)}}{k_{Fn(Fp)}} = \frac{k_{Fn(Fp)}^{-1}}{k_{snTF(spTF)}^{-1}} = \sqrt{\frac{4\gamma r_{sn(sp)}\left(N, r_{d(a)}, x\right)}{\pi}} \ll 1, \quad (11)$ being proportional to $N^{-1/6}$.

Secondly, $N < N_{CDn(NDp)}(r_{d(a)})$, according to the Wigner-Seitz (WS)-approximation, the ratio $R_{snWS(spWS)}$ is reduced to.[3]

$$R_{snWS(spWS)}\left(N, r_{d(a)}, x\right) \equiv \frac{k_{snWS(spWS)}}{k_{Fn(Fp)}} = \left(\frac{s}{2\pi} - \gamma \frac{d\left[r_{sn(sp)}^2 \times E_{CE}\right]}{dr_{sn(sp)}}\right) \times 0.5, \quad (12)$$

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

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

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

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

Here, $\pm E_{Fno(Fpo)}$ is the Fermi energy at 0 K, and $\eta_{n(p)}$ is defined in next Eq. (15),

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

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.

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

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, $W_{n(p)}\big(v_{n(p)}, N, r_{d(a)}\big) \equiv \langle V(r)V(r')\rangle$, was determined, [4, 5] as.

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

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

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 $E \to \pm\infty$, $|v_{n(p)}| \to \infty$, 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 $W_{n(p)}\left(v_{n(p)}, N, r_{d(a)}, x\right)$.

MATHEMATICAL AND METHODS

Kane integration method (KIM)

Here, the effective Gaussian distribution probability is defined by:

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

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

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

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

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

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

$$\Gamma\left(a + \frac{1}{2}\right) \times D_{-a-\frac{1}{2}}(y) \qquad\qquad . \quad (16)$$

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

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

noting that as a=1, $(it)^{-\frac{3}{2}} \times \exp\left\{-\frac{\left(t\sqrt{W_p}\right)^2}{2\hbar^2}\right\}$ is found to be proportional to the averaged Feynman propagator given the dense donors (acceptors). Then, by variable changes:

$$t = \frac{\hbar}{\sqrt{W_{n(p)}}} \quad \text{and} \quad y = \mp E/\sqrt{W_{n(p)}} \equiv \frac{\pm E_{Fno(Fpo)}}{\eta_{n(p)}} \times v_{n(p)} \times \exp\left(\frac{\mathcal{H}_{n(p)} \times R_{sn(sp)}}{4 \times \sqrt{|v_{n(p)}|}}\right), \quad \text{for} \quad \text{n(p)-type}$$

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.

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

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

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

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

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.

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

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.

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

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.

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

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.

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

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.

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

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

$$\beta(a = 1) = \frac{\sqrt{\pi}}{2^{\frac{3}{4}} \times \Gamma(5/4)}. \quad (24)$$

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

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

where

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

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

$$I_{n(p)} = \frac{1}{2^{5/4}A_{n(p)}} \times \int_{z_{n(p)}}^{\infty} t^{b-1}e^{-t}dt \equiv \frac{\Gamma(b, z_{n(p)})}{2^{5/4} \times A_{n(p)}}, \text{ where } b = -1/4, \; z_{n(p)} = [16 A_{n(p)}/\sqrt{2}]^2, \text{ and}$$

$\Gamma(b, z_{n(p)})$ is the incomplete Gamma function, defined by.

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

Finally, Eq. (25) now yields.

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

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

In n(p)-type degenerate X(x)- 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 following Tables 2-8, 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:

$$|RD| \equiv \left| 1 - \frac{N_{CDn(CDp)}^{EBT}}{N_{CDn(CDp)}} \right|.$$

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: 2.92×10^{-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, $N_{CDn(CDp)}^{EBT}(r_{d(a)}, x)$, 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.

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

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; 2023; 2023; Van Cong et al., 2014; Van Cong & Debiais, 1993; Van Cong et al., 1984).

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APPENDIX 1

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

In $InP_{1-x}As_x$-alloys, in which $r_{do(ao)} = r_{P(In)} = 0.110$ nm (0.144 nm), we have: $g_{c(v)}(x) = 1 \times x + 1 \times (1-x)$, $m_{c(v)}(x)/m_0 = 0.09(0.3) \times x + 0.077(0.5) \times (1-x)$, $\varepsilon_0(x) = 14.55 \times x + 12.5 \times (1-x)$, $E_{g0}(x) = 0.43 \times x + 1.424 \times (1-x)$, and

In $InP_{1-x}Sb_x$-alloys, in which $r_{do(ao)} = r_{P(In)} = 0.110$ nm (0.144 nm), we have: $g_{c(v)}(x) = 1 \times x + 1 \times (1-x)$, $m_{c(v)}(x)/m_0 = 0.1(0.4) \times x + 0.077(0.5) \times (1-x)$, $\varepsilon_0(x) = 16.8 \times x + 12.5 \times (1-x)$, $E_{g0}(x) = 0.23 \times x + 1.424 \times (1-x)$.

In $GaAs_{1-x}Te_x$-alloys, in which $r_{do(ao)} = r_{As(Ga)} = 0.118$ nm (0.126 nm), we have: $g_{c(v)}(x) = 1 \times x + 1 \times (1-x)$, $m_{c(v)}(x)/m_0 = 0.209(0.4) \times x + 0.066(0.291) \times (1-x)$, $\varepsilon_0(x) = 12.3 \times x + 13.13 \times (1-x)$, $E_{g0}(x) = 1.796 \times x + 1.52 \times (1-x)$,

In $GaAs_{1-x}Sb_x$-alloys, in which $r_{do(ao)} = r_{As(Ga)} = 0.118$ nm (0.126 nm), we have. $g_{c(v)}(x) = 1 \times x + 1 \times (1-x)$, $m_{c(v)}(x)/m_0 = 0.047(0.3) \times x + 0.066(0.291) \times (1-x)$, $\varepsilon_0(x) = 15.69 \times x + 13.13 \times (1-x)$, $E_{g0}(x) = 0.81 \times x + 1.52 \times (1-x)$, and

In $GaAs_{1-x}P_x$-alloys, in which $r_{do(ao)} = r_{As(Ga)} = 0.118$ nm (0.126 nm), we have: $g_{c(v)}(x) = 1 \times x + 1 \times (1-x)$, $m_{c(v)}(x)/m_0 = 0.13(0.5) \times x + 0.066(0.291) \times (1-x)$, $\varepsilon_0(x) = 11.1 \times x + 13.13 \times (1-x)$, $E_{g0}(x) = 1.796 \times x + 1.52 \times (1-x)$,

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In $CdS_{1-x}Te_x$-alloys, in which $r_{do(ao)} = r_{S(Cd)} = 0.104$ nm (0.148 nm), we have: $g_{c(v)}(x) = 1 \times x + 1 \times (1-x)$, $m_{c(v)}(x)/m_0 = 0.095(0.82) \times x + 0.197(0.801) \times (1-x)$, $\varepsilon_0(x) = 10.31 \times x + 9 \times (1-x)$, $E_{g0}(x) = 1.62 \times x + 2.58 \times (1-x)$, and

In $CdS_{1-x}Se_x$-alloys, in which $r_{do(ao)} = r_{S(Cd)} = 0.104$ nm (0.148 nm), we have: $g_{c(v)}(x) = 1 \times x + 1 \times (1-x)$, $m_{c(v)}(x)/m_0 = 0.11(0.45) \times x + 0.197(0.801) \times (1-x)$, $\varepsilon_0(x) = 10.2 \times x + 9 \times (1-x)$, $E_{g0}(x) = 1.84 \times x + 2.58 \times (1-x)$.

Table 2: In the $InP_{1-x}As_x$**-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 (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** 2.77×10^{-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	P	As
r_d (nm) ↗	r_{do}=0.110	0.118
x ↗	0, 0.5, 1	0, 0.5, 1
$B_{do}(x)$ in 10^5 (N/m²) ↘	1.925775, 1.783802, 1.6613123	
$\varepsilon(r_d, x)$ ↘	**12.5**, 13.255, **14.55**	12.202384, 13.20298, 14.203575
$E_{gno}(r_d, x)$ eV ↗	**1.424**, 0.927, **0.43**	1.4243309, 0.927306, 0.4302855
$N_{CDn}(r_d, x)$ in 10^{18} cm⁻³ ↗	2.4532257, 2.469693, 2.4838989	2.6371418, 2.6548437, 2.6701146
$N_{CDn}^{EBT}(r_d, x)$ in 10^{18} cm⁻³ ↗	2.4532251, 2.4696924, 2.4838983	2.6371411, 2.6548430, 2.6701139
$|RD|$ in 10^{-7}	2.62, 2.57, 2.58	2.63, 2.74, 2.76
Donor	Sb	Sn
r_d (nm) ↗	0.136	0.140
x ↗	0, 0.5, 1	0, 0.5, 1
$\varepsilon(r_d, x)$ ↘	9.9874098, 10.80638, 11.625345	4.4007324, 10.171592, 10.9424525
$E_{gno}(r_d, x)$ eV ↗	1.4277963, 0.930516, 0.4332750	1.4291476, 0.9317681, 0.4344407
$N_{CDn}(r_d, x)$ in 10^{18} cm⁻³ ↗	4.8095998, 4.8418843, 4.8697353	5.767432, 5.806146, 5.8395435
$N_{CDn}^{EBT}(r_d, x)$ in 10^{18} cm⁻³ ↗	4.8095985, 4.8418830, 4.8697340	5.7674304, 5.8061445, 5.8395419
$|RD|$ in 10^{-7}	2.70, 2.67, 2.73	2.74, 2.65, 2.76

Acceptor	Ga	Mg	
r_a (nm) ↗	0.126	0.140	
x ↗	0, 0.5, 1	0, 0.5, 1	$\varepsilon(r_a, x)$ ↘
13.4185948, 14.5189196, 15.619244	12.5430268, 13.571555, 14.6000832		
$E_{gpo}(r_a, x)$ eV ↗	1.4182455, 0.9230677, 0.4274517	1.4237019, 0.9267963, 0.429868	
$N_{CDp}(r_a, x)$ in 10^{18} cm⁻³ ↗	5.4298054, 2.1946863, 0.74366797	6.6481122, 2.6871166, 0.91052768	
$N_{CDp}^{EBT}(r_a, x)$ in 10^{18} cm⁻³ ↗	5.4298040, 2.1946857, 0.74366777	6.6481104, 2.6871159, 0.91052743	
$|RD|$ in 10^{-7}	2.60, 2.76, 2.68	2.74, 2.624, **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 10^5 (N/m²) ↘	5.5741072, 3.808998,2.4684288		
$\varepsilon(r_a, x)$ ↘	**12.5**, 13.525, **14.55**	12.45622, 13.47763, 14.4990401	
$E_{gpo}(r_a, x)$ eV ↗	**1.424**, 0.927, **0.43**	1.4243065, 0.9272094, 0.4301357	
$N_{CDp}(r_a, x)$ in 10^{18} cm⁻³ ↗	6.717, 2.7149606, 0.91996257	6.7880742, 2.7436882, 0.92969691	
$N_{CDp}^{EBT}(r_a, x)$ in 10^{18} cm⁻³ ↗	6.7169982, 2.7149599, 0.91996232	6.7880723, 2.7436875, 0.92969666	
$|RD|$ in 10^{-7}	2.69, 2.75, 2.68	2.74, 2.63, 2.71	

Table 3: In the $InP_{1-x}Sb_x$-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 2.91×10^{-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, $N_{CDn(CDp)}^{EBT}(r_{d(a)}, x)$, 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	**P**	**As**
r_d (nm) ↗	r_{do}=0.110	0.118
x ↗	0, 0.5, 1	0, 0.5, 1
$B_{do}(x)$ in 10^5 (N/m²) ↘	1.925775, 1.611398, 1.3845741	
$\varepsilon(r_d, x)$ ↘	**12.5**, 14.65, **16.8**	12.202384, 14.301194, 16.4000041
$E_{gno}(r_d, x)$ eV ↗	**1.424**, 0.827, **0.23**	1.4243309, 0.8272769, 0.2302379
$N_{CDn}(r_d, x)$ in 10^{16} cm⁻³ ↗	2.4532257, 2.3137281, 2.2134389	2.6371418, 2.4871861, 2.3793784
$N_{CDn}^{EBT}(r_d, x)$ in 10^{16} cm⁻³ ↗	2.4532251, 2.3137275, 2.2134383	2.6371411, 2.4871855, 2.3793777
$|RD|$ in 10^{-7}	2.62, 2.81, 2.81	2.63, 2.55, 2.83
Donor	**Sb**	**Sn**
r_d (nm) ↗	0.136	0.140
x ↗	0, 0.5, 1	0, 0.5, 1
$\varepsilon(r_d, x)$ ↘	9.9874098, 11.70524, 13.423079	4.4007324, 11.0176583, 12.6345843
$E_{gno}(r_d, x)$ eV ↗	1.4277963, 0.830177, 0.2327295	1.4291476, 0.8313073, 0.233701
$N_{CDn}(r_d, x)$ in 10^{16} cm⁻³ ↗	4.8095998, 4.5361117, 4.3394927	5.767432, 5.4394787, 5.2037030
$N_{CDn}^{EBT}(r_d, x)$ in 10^{16} cm⁻³ ↗	4.8095985, 4.5361105, 4.3394915	5.7674304, 5.4394773, 5.2037016
$|RD|$ in 10^{-7}	2.70, 2.70, 2.65	2.74, 2.57, 2.68
Acceptor	**Ga**	**Mg**
r_a (nm) ↗	0.126	0.140
x ↗	0, 0.5, 1	0, 0.5, 1
$\varepsilon(r_a, x)$ ↘	13.4185948, 15.726593, 18.0345915	12.5430268, 14.700427, 16.857828
$E_{gpo}(r_a, x)$ eV ↗	1.4182455, 0.8232295, 0.2274514	1.4237019, 0.8268047, 0.229868
$N_{CDp}(r_a, x)$ in 10^{18} cm⁻³ ↗	5.4298054, 2.4588326, 1.1451343	6.6481122, 3.0105305, 1.4020726
$|RD|$ in 10^{-7}	2.60, 2.77, 2.74	2.74, 2.69, 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 10^5 (N/m²) ↘	5.5741072, 3.6522677, 2.4686912	
$\varepsilon(r_a, x)$ ↘	**12.5**, 14.65, **16.8**	12.45622, 14.5986898, 16.7411597
$E_{gpo}(r_a, x)$ eV ↗	**1.424**, 0.827, **0.23**	1.4243065, 0.8272008, 0.2301357
$N_{CDp}(r_a, x)$ in 10^{18} cm⁻³ ↗	6.717, 3.0417257, 1.4166009	6.7880742, 3.0739109, 1.4315903
$N_{CDp}^{EBT}(r_a, x)$ in 10^{18} cm⁻³ ↗	6.7169982, 3.0417249, 1.4166005	6.7880723, 3.0739101, 1.4315899
$|RD|$ in 10^{-7}	2.69, 2.76, 2.82	2.74, 2.70, **2.91**

Table 4: In the $GaAs_{1-x}Te_x$-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 2.89×10^{-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	P		As		Te	
r_d (nm) ↗	**0.110**		r_{do}=**0.118**		**0.132**	
x ↗	0, 0.5, 1		0, 0.5, 1		0, 0.5, 1	
$B_{do}(x)$ in 10^5 (N/m²) ↗		1.211940, 2.692382, 4.3732354				
$\varepsilon(r_d, x)$ ↘	13.40073, 12.97718, 12.553622		**13.13**, 12.715, **12.3**		12.327231, 11.93760, 11.547977	
$E_{gno}(r_d, x)$ eV ↗	1.519792, 1.657537, 1.7952485		**1.52**, 1.658, **1.796**		1.5207002, 1.659555, 1.7985267	
$N_{CDn}(r_d, x)$ in 10^{16} cm⁻³ ↗	1.253837, 12.484254, 48.431412		1.3330088, 13.27255, 51.489527		1.6107592, 16.03807, 62.218067	
$N_{CDn}^{EBT}(r_d, x)$ in 10^{16} cm⁻³ ↗	1.2538371, 12.484251, 48.431399		1.3330084, 13.272547, 51.489513		1.6107588, 16.038061, 62.218050	
$|RD|$ in 10^{-7}	**2.89**, 2.45, 2.68		2.87, 2.62, 2.74		2.69, 2.83, 2.70	

Donor	Sb		Sn	
r_d (nm) ↗	**0.136**		**0.140**	
x ↗	0, 0.5, 1		0, 0.5, 1	
$\varepsilon(r_d, x)$ ↘	11.857485, 11.48270, 11.107926		11.327101, 10.96908, 10.611069	
$E_{gno}(r_d, x)$ eV ↗	1.5211775, 1.660616, 1.8002489		1.5217893, 1.661975, 1.8024567	
$N_{CDn}(r_d, x)$ in 10^{16} cm⁻³ ↗	1.8098785, 18.02066, 69.909357		2.0762080, 20.67246, 80.196749	
$N_{CDn}^{EBT}(r_d, x)$ in 10^{16} cm⁻³ ↗	1.8098780, 18.020659, 69.909340		2.0762075, 20.672458, 80.196728	
$|RD|$ in 10^{-7}	2.87, 2.84, 2.64		2.51, 2.75, 2.63	

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 10^5 (N/m²) ↗		4.388991, 5.556694, 6.874656				
$\varepsilon(r_a, x)$ ↘	24.3813, 23.61066, 22.8400		**13.13**, 12.715, **12.3**		12.42055, 12.0279, 11.6354	
$E_{gpo}(r_a, x)$ eV ↗	1.50370, 1.637365, 1.77047		**1.52**, 1.658, **1.796**		1.5226974, 1.66111, 1.80022	
$N_{CDp}(r_a, x)$ in 10^{18} cm⁻³ ↗	0.178445, 0.3288630, 0.5637475		1.142563, 2.105671, 3.6096078		1.3497457, 2.487495, 4.264143	
$N_{CDp}^{EBT}(r_a, x)$ in 10^{18} cm⁻³ ↗	0.1784451, 0.3288629, 0.5637474		1.1425627, 2.105670, 3.6096068		1.3497453, 2.4874943, 4.264142	
$|RD|$ in 10^{-7}	2.75, 2.72, 2.71		2.59, 2.65, 2.72		2.82, 2.67, 2.75	

Acceptor	In		Cd	
r_a (nm) ↗	**0.144**		**0.148**	
x ↗	0, 0.5, 1		0, 0.5, 1	
$\varepsilon(r_a, x)$ ↘	11.999115, 11.6198, 11.24060		11.51747, 11.15344, 10.78941	
$E_{gpo}(r_a, x)$ eV ↗	1.5245311, 1.66374, 1.803097		1.526878, 1.666708, 1.806773	
$N_{CDp}(r_a, x)$ in 10^{18} cm⁻³ ↗	1.4970169, 2.7589064, 4.7294055		1.6927886, 3.1197012, 5.3478913	
$N_{CDp}^{EBT}(r_a, x)$ in 10^{18} cm⁻³ ↗	1.4970165, 2.7589057, 4.7294042		1.6927881, 3.1197004, 5.3478899	
$|RD|$ in 10^{-7}	2.81, 2.69, 2.81		2.74, 2.68, 2.67	

Table 5: In the $GaAs_{1-x}Sb_x$-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 2.90×10^{-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-GaSb crystals, respectively, as observed in Table 1.

Donor	P			As			Te		
r_d (nm) ↗	**0.110**			r_{do}=**0.118**			**0.132**		
x ↗	0,	0.5,	1	0,	0.5,	1	0,	0.5,	1
$B_{do}(x)$ in 10^5 (N/m²) ↘				1.211940,	0.861365,	0.6043921			
$\varepsilon(r_d, x)$ ↘	13.40073,	14.707129,	16.013522	**13.13**,	14.41,	**15.69**	12.32723,	13.52897,	14.730712
$E_{gno}(r_d, x)$ eV ↗	1.519792,	1.164852,	0.8098961	**1.52**,	1.165,	**0.81**	1.520700,	1.165498,	0.8103492
$N_{CDn}(r_d, x)$ in 10^{16} cm⁻³ ↗	1.253837,	0.5950549,	0.2653557	1.3330088,	0.6326285,	0.2821111	1.6107592,	0.764445,	0.3408927
$N_{CDn}^{EBT}(r_d, x)$ in 10^{16} cm⁻³ ↗	1.2538371,	0.5950547,	0.2653556	1.3330084,	0.6326284,	0.2821110	1.6107588,	0.7644451,	0.3408926
$|RD|$ in 10^{-7}	2.89,	2.70,	2.77	2.87,	2.66,	2.62	2.69,	2.70,	2.80

Donor	Sb			Sn		
r_d (nm) ↗	**0.136**			**0.140**		
x ↗	0,	0.5,	1	0,	0.5,	1
$\varepsilon(r_d, x)$ ↘	11.857485,	13.01343,	14.169379	11.327101,	12.43134,	13.535584
$E_{gno}(r_d, x)$ eV ↗	1.5211775,	1.165837,	0.8105872	1.5217893,	1.166272,	0.8108923
$N_{CDn}(r_d, x)$ in 10^{16} cm⁻³ ↗	1.8098785,	0.858945,	0.3830333	2.0762080,	0.9853412,	0.4393979
$N_{CDn}^{EBT}(r_d, x)$ in 10^{16} cm⁻³ ↗	1.8098780,	0.8589444,	0.3830332	2.0762075,	0.98534094,	0.4393978
$|RD|$ in 10^{-7}	2.87,	2.65,	2.63	2.51,	2.68,	2.75

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 10^5 (N/m²) ↘				4.388991,	3.7002469,	3.1686667			
$\varepsilon(r_a, x)$ ↘	24.3813,	26.75813,	29.13498	**13.13**,	14.41,	**15.69**	12.42055,	13.63139,	14.84222
$E_{gpo}(r_a, x)$ eV ↗	1.50370,	1.151259,	0.798233	**1.52**,	1.165,	**0.81**	1.5226974,	1.167274,	0.8119474
$N_{CDp}(r_a, x)$ in 10^{18} cm⁻³ ↗	0.178445,	0.1413515,	0.1145816	1.142563,	0.90505691,	0.7336523	1.3497457,	1.069172,	0.86668661
$N_{CDp}^{EBT}(r_a, x)$ in 10^{18} cm⁻³ ↗	0.1784451,	0.14135149,	0.1145816	1.1425627,	0.9050567,	0.7336521	1.3497453,	1.0691719,	0.86668638
$|RD|$ in 10^{-7}	2.75,	2.70,	2.49	2.59,	2.70,	2.72	2.82,	2.55,	2.67

Acceptor	In			Cd		
r_a (nm) ↗	**0.144**			**0.148**		
x ↗	0,	0.5,	1	0,	0.5,	1
$\varepsilon(r_a, x)$ ↘	11.999115,	13.1689,	14.33862	11.51747,	12.64027,	13.763073
$E_{gpo}(r_a, x)$ eV ↗	1.5245311,	1.16882,	0.813271	1.526878,	1.170799,	0.8149657
$N_{CDp}(r_a, x)$ in 10^{18} cm⁻³ ↗	1.4970169,	1.1858300,	0.96125108	1.6927886,	1.3409063,	1.0869583
$N_{CDp}^{EBT}(r_a, x)$ in 10^{18} cm⁻³ ↗	1.4970165,	1.1858297,	0.96125083	1.6927881,	1.3409060,	1.0869580
$|RD|$ in 10^{-7}	2.81,	**2.90**,	2.81	2.74,	2.46,	2.87

Table 6: In the $GaAs_{1-x}P_x$-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 (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 2.92×10^{-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**		r_{do}=**0.118**		**0.132**	
x ↗	0,	0.5, 1	0,	0.5, 1	0,	0.5, 1
$B_{do}(x)$ in 10^5 (N/m²) ↗			1.211940, 2.113713, 3.340137			
$\varepsilon(r_d, x)$ ↘	13.40073, 12.36481, 11.328878		**13.13**, 12.115, **11.1**		12.32723, 11.374288, 10.421345	
$E_{gno}(r_d, x)$ eV ↗	1.519792, 1.65574, 1.7954260		**1.52**, 1.658, **1.796**		1.520700, 1.659221, 1.797930	
$N_{CDn}(r_d, x)$ in 10^{16} cm⁻³ ↗	1.253837, 5.2253042, 15.858596		1.3330088, 5.5552466, 16.859958		1.6107592, 6.7127576, 20.372959	
$N_{CDn}^{EBT}(r_d, x)$ in 10^{16} cm⁻³ ↗	1.2538371, 5.2253028, 15.858592		1.3330084, 5.5552451, 16.859954		1.6107588, 6.7127558, 20.372954	
$|RD|$ in 10^{-7}	2.89,	2.73, 2.74	2.87,	2.64, 2.60	2.69,	2.72, 2.69

Donor	Sb		Sn	
r_d (nm) ↗	**0.136**		**0.140**	
x ↗	0,	0.5, 1	0,	0.5, 1
$\varepsilon(r_d, x)$ ↘	11.857485, 10.94085, 10.024226		11.327101, 10.45147, 9.5758431	
$E_{gno}(r_d, x)$ eV ↗	1.5211775, 1.660054, 1.7992452		1.5217893, 1.661121, 1.8009315	
$N_{CDn}(r_d, x)$ in 10^{16} cm⁻³ ↗	1.8098785, 7.542577, 22.891429		2.0762080, 8.6524921, 26.259978	
$N_{CDn}^{EBT}(r_d, x)$ in 10^{16} cm⁻³ ↗	1.8098780, 7.542575, 22.891423		2.0762075, 8.6524898, 26.259971	
$|RD|$ in 10^{-7}	2.87,	2.65, 2.80	2.51,	2.61, 2.57

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 10^5 (N/m²) ↗			4.388991, 7.0064952, 10.55177			
$\varepsilon(r_a, x)$ ↘	24.3813, 22.496513, 20.61174		**13.13**, 12.115, **11.1**		12.42055, 11.46039, 10.500236	
$E_{gpo}(r_a, x)$ eV ↗	1.50370, 1.1631981, 0.756815		**1.52**, 1.658, **1.796**		1.5226974, 1.662306, 1.802485	
$N_{CDp}(r_a, x)$ in 10^{18} cm⁻³ ↗	0.178445, 0.5702814, 1.4981699		1.142563, 3.6514435, 9.592603		1.3497457, 4.3135651, 11.332043	
$N_{CDp}^{EBT}(r_a, x)$ in 10^{18} cm⁻³ ↗	0.1784451, 0.5702813, 1.4981695		1.1425627, 3.6514425, 9.592600		1.3497453, 4.3135640, 11.332040	
$|RD|$ in 10^{-7}	2.75,	2.63, 2.52	2.59,	2.702, 2.71	2.82,	2.61, 2.44

Acceptor	In		Cd	
r_a (nm) ↗	**0.144**		**0.148**	
x ↗	0,	0.5, 1	0,	0.5, 1
$\varepsilon(r_a, x)$ ↘	11.999115, 11.07154, 10.14396		11.51747, 10.62713, 9.7367823	
$E_{gpo}(r_a, x)$ eV ↗	1.5245311, 1.665233, 1.806893		1.526878, 1.668980, 1.8125359	
$N_{CDp}(r_a, x)$ in 10^{18} cm⁻³ ↗	1.4970169, 4.7842197, 12.5684870		1.6927886, 5.4098739, 14.2121250	
$N_{CDp}^{EBT}(r_a, x)$ in 10^{18} cm⁻³ ↗	1.4970165, 4.7842184, 12.5684830		1.6927881, 5.4098724, 14.2121210	
$|RD|$ in 10^{-7}	2.81,	2.70, **2.92**	2.74,	2.71, 2.84

Table 7: In the $CdS_{1-x}Te_x$-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 2.84×10^{-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) ↗	r_{do}=0.104			0.114		
x ↗	0,	0.5, 1		0,	0.5, 1	
$B_{do}(x)$ in 10^8 (N/m²) ↘	11.24589, 7.242043, 4.132559					
$\varepsilon(r_d, x)$ ↘	9,	9.655, **10.31**		8.631002,	9.259147, 9.8872925	
$E_{gno}(r_d, x)$ eV ↗	**2.58**,	2.1, **1.62**		2.5828887,	2.101860, 1.6210615	
$N_{CDn}(r_d, x)$ in 10^{18} cm⁻³ ↗	1.1006938, 0.3629085, 0.08210889			1.2479879,	0.41147264, 0.09309665	
$N_{CDn}^{EBT}(r_d, x)$ in 10^{18} cm⁻³ ↗	1.1006935, 0.3629084, 0.082108871			1.2479876,	0.41147253, 0.093096623	
$|RD|$ in 10^{-7}	2.63,	2.65, 2.72		2.53,	2.70, 2.76	
Donor	**Te**			**Sn**		
r_d (nm) ↗	**0.132**			**0.140**		
x ↗	0,	0.5, 1		0,	0.5, 1	
$\varepsilon(r_d, x)$ ↘	6.8088533, 7.304386, 7.7999197			5.9556997, 6.389142, 6.8225848		
$E_{gno}(r_d, x)$ eV ↗	2.6047141, 2.115915, 1.6290817			2.6224569, 2.1273411, 1.6356018		
$N_{CDn}(r_d, x)$ in 10^{18} cm⁻³ ↗	2.5419800, 0.8381132, 0.18962509			3.7983562, 1.2523516, 0.28334748		
$N_{CDn}^{EBT}(r_d, x)$ in 10^{18} cm⁻³ ↗	2.5419793, 0.83811302, 0.18962504			3.7983551, 1.2523513, 0.28334741		
$|RD|$ in 10^{-7}	2.80,	2.69, 2.75		**2.84**,	2.63, 2.5	
Acceptor	**Ga**			**Mg**		
r_a (nm) ↗	**0.126**			**0.140**		
x ↗	0,	0.5, 1		0,	0.5, 1	
$\varepsilon(r_a, x)$ ↘	9.968548, 10.69404, 11.419526			9.117455, 9.781004, 10.444552		
$E_{gpo}(r_a, x)$ eV ↗	2.5551356, 2.078139, 1.6006033			2.5765572, 2.09697, 1.6173143		
$N_{CDp}(r_a, x)$ in 10^{19} cm⁻³ ↗	5.4449915, 4.5690868, 3.8859101			7.1165903, 5.9717851, 5.0788748		
$N_{CDp}^{EBT}(r_a, x)$ in 10^{19} cm⁻³ ↗	5.4449900, 4.5690856, 3.8859090			7.1165884, 5.9717835, 5.0788734		
$|RD|$ in 10^{-7}	2.82,	2.68, 2.75		2.67,	2.62, 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 10^9 (N/m²) ↘				1.5866282, 1.3950062, 1.2377251		
$\varepsilon(r_a, x)$ ↘	9.0293303, 9.686465, 10.343599			9,	9.655, **10.31**	
$E_{gpo}(r_a, x)$ eV ↗	2.5791277, 2.099233, 1.6193195			**2.58**,	2.1, **1.62**	
$N_{CDp}(r_a, x)$ in 10^{19} cm⁻³ ↗	7.3270019, 6.148349, 5.2290386			7.39887, 6.208656, 5.2803284		
$N_{CDp}^{EBT}(r_a, x)$ in 10^{19} cm⁻³ ↗	7.3269999, 6.1483473, 5.2290372			7.398868, 6.2086543, 5.2803270		
$|RD|$ in 10^{-7}	2.71,	2.78, 2.76		2.72,	2.68, 2.66	

Table 8: In the $CdS_{1-x}Se_x$-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) ↗	r_{do}=0.104	0.114
x ↗	0, 0.5, 1	0, 0.5, 1
$B_{do}(x)$ in 10^8 (N/m²) ↘	11.24589, 7.70156, 4.8888322	
$\varepsilon(r_d, x)$ ↘	**9**, 9.6, **10.2**	8.631002, 9.2064023, 9.7818024
$E_{gno}(r_d, x)$ eV ↗	**2.58**, 2.21, **1.84**	2.5828887, 2.2119783, 1.8412558
$N_{CDn}(r_d, x)$ in 10^{18} cm^{-3} ↗	1.1006938, 0.4290489, 0.13163547	1.2479879, 0.48646396, 0.14925083
$N^{EBT}_{CDn}(r_d, x)$ in 10^{18} cm^{-3} ↗	1.1006935, 0.42904881, 0.13163543	1.2479876, 0.48646383, 0.14925079
$|RD|$ in 10^{-7}	2.63, 2.67, **2.88**	2.53, 2.73, 2.44
Donor	**Te**	**Sn**
r_d (nm) ↗	0.132	0.140
x ↗	0, 0.5, 1	0, 0.5, 1
$\varepsilon(r_d, x)$ ↘	6.8088533, 7.262777, 7.7167004	5.9556997, 6.3527463, 6.7497929
$E_{gno}(r_d, x)$ eV ↗	2.6047141, 2.226925, 1.8507437	2.6224569, 2.2390759, 1.8584569
$N_{CDn}(r_d, x)$ in 10^{18} cm^{-3} ↗	2.5419800, 0.99086027, 0.30400345	3.7983562, 1.480594, 0.45425747
$N^{EBT}_{CDn}(r_d, x)$ in 10^{18} cm^{-3} ↗	2.5419793, 0.99086001, 0.30400337	3.7983551, 1.4805936, 0.45425735
$|RD|$ in 10^{-7}	2.80, 2.61, 2.75	2.84, 2.78, 2.57
Acceptor	**Ga**	**Mg**
r_a (nm) ↗	0.126	0.140
x ↗	0, 0.5, 1	0, 0.5, 1
$\varepsilon(r_a, x)$ ↘	9.968548, 10.633118, 11.2976878	9.117455, 9.725286, 10.3331162
$E_{gpo}(r_a, x)$ eV ↗	2.5551356, 2.1929346, 1.8291247	2.5765572, 2.207637, 1.8384942
$N_{CDp}(r_a, x)$ in 10^{19} cm^{-3} ↗	5.4449915, 2.1364632, 0.66323007	7.1165903, 2.7923522, 0.86684006
$N^{EBT}_{CDp}(r_a, x)$ in 10^{19} cm^{-3} ↗	5.4449900, 2.1364627, 0.66322989	7.1165884, 2.7923514, 0.86683983
$|RD|$ in 10^{-7}	2.82, 2.53, 2.69	2.67, 2.83, 2.65
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 10^9 (N/m²) ↘		1.586628, 1.0889615, 0.69396862
$\varepsilon(r_a, x)$ ↘	9.0293303, 9.6312856, 10.233241	**9**, 9.6, **10.2**
$E_{gpo}(r_a, x)$ eV ↗	2.5791277, 2.2094013, 1.8396185	**2.58**, 2.21, **1.84**
$N_{CDp}(r_a, x)$ in 10^{19} cm^{-3} ↗	7.3270019, 2.8749118, 0.89246936	7.39887, 2.9031108, 0.90122328
$N^{EBT}_{CDp}(r_a, x)$ in 10^{19} cm^{-3} ↗	7.3269999, 2.8749111, 0.89246911	7.398868, 2.9031100, 0.90122304
$|RD|$ in 10^{-7}	2.71, 2.59, 2.77	2.72, 2.61, 2.70