EJTAS
ISSN 2786-7447
EUROPEAN JOURNAL OF THEORETICAL AND APPLIED SCIENCES
OPEN ACCESS
PEER REVIEWED

Critical Impurity Density in the Mott Metal-Insulator Transition, obtained in the n(p)-Type Degenerate $Si_{1-x}Ge_x$- Crystalline Alloy, and Its Applications

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Suggested Citation
Van Cong, H. (2024). Critical Impurity Density in the Mott Metal-Insulator Transition, obtained in the n(p)-Type Degenerate $Si_{1-x}Ge_x$- Crystalline Alloy, and Its Applications. *European Journal of Theoretical and Applied Sciences, 2*(2), 130-148. DOI: 10.59324/ejtas.2024.2(2).12

Abstract:

By basing on the same physical model and treatment method, as used in our recent works (Van Cong, 2024; 2023; 2023), we investigate the critical impurity density in the metal-insulator transition (MIT), obtained in the n(p)-type degenerate $Si_{1-x}Ge_x$- crystalline alloy, $0 \leq x \leq 1$, and also applied to determine the optical band gap, being due to the effects of the size of donor (acceptor) d(a)-radius, $r_{d(a)}$, the x-Ge concentration, the temperature T, and finally the high d(a)-density, N, assuming that all the impurities are ionized even at T=0 K. In such the n(p)-type degenerate $Si_{1-x}Ge_x$- crystalline alloy, we will determine:

(i)-the critical impurity density $N_{CDn(CDp)}(r_{d(a)}, x)$ in the MIT, as that given in Eq. (10), by using the generalized empirical Mott parameters $M_{n(p)}(x)$,

(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 parameters $\mathcal{H}_{n(p)}(x)$, as those 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 9.99×10^{-6} (1.49×10^{-5}), as seen in Tables 1n and 1p, respectively, and

(iii)-the OBG, $E_{gn1(gp1)}(N^*, r_{d(a)}, x, T)$, $N^* \equiv N - N_{CDn(NDp)}$, as that given in Eq. (28); its numerical results are reported in Tables 2, 3n and 3p, showing, in particular, in Table 2, in which $r_{d(a)} \equiv r_{P(B)}$, x=0 and T=20 K, the numerical results of $E_{gn1(gp1)}$ are found to be in good agreement with the data, obtained by Wagner & del Alamo (1988), with maximal relative deviations: 1.428 % (4.556 %), respectively.

Keywords: *$Si_{1-x}Ge_x$-crystalline alloy; critical impurity density in the MIT; optical band gap.*

Introduction

By basing on the same physical model and treatment method, as used in our recent works (Van Cong, 2024; 2023; 2023), and also other works (Kitel, 1976; Van Cong et al., 2014, Van Cong & Debiais, 1993; Van Cong et al., 1984; Wagner & del Alamo, 1988), we will investigate the critical impurity density in the metal-insulator transition (MIT), obtained in the n(p)-type degenerate $Si_{1-x}Ge_x$- crystalline alloy, $0 \leq$

$x \leq 1$, and also applied to determine the optical band gap (OBG), being due to the effects of the size of donor (acceptor) d(a)-radius, $r_{d(a)}$, the x-Ge concentration, the temperature T, and finally the high d(a)-density, N, assuming that all the impurities are ionized even at T=0 K.

In the n(p)-type degenerate $Si_{1-x}Ge_x$- crystalline alloy, we will determine:

(i)-the critical impurity density $N_{CDn(CDp)}(r_{d(a)}, x)$ in the MIT, as that given in Eq. (10), by using the generalized empirical Mott parameters $M_{n(p)}(x)$,

(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 parameters $\mathcal{H}_{n(p)}(x)$, as those 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 9.99×10^{-6} (1.49×10^{-5}), as seen in Tables 1n and 1p, respectively, and

(iii)-the OBG, $E_{gn1(gp1)}(N^*, r_{d(a)}, x, T)$, $N^* \equiv N - N_{CDn(NDp)}$, as that given in Eq. (28); its numerical results are reported in Tables 2, 3n and 3p, showing, in particular, in Table 2, in which $r_{d(a)} \equiv r_{P(B)}$, x=0 and T=20 K, the numerical results of $E_{gn1(gp1)}$ are found to be in good agreement with the data, obtained by Wagner & del Alamo (1988), with maximal relative deviations: 1.428 % (4.556 %), respectively.

In the following, we will determine those functions: $N_{CDn(CDp)}(r_{d(a)}, x)$, $N^{EBT}_{CDn(CDp)}(r_{d(a)}, x)$, and finally, $E_{gn1(gp1)}(N^*, r_{d(a)}, x, T)$.

Critical Density in the MIT, $N_{CDn(CDp)}(r_{d(a)}, x)$

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-Ge Concentration

Here, the values of the intrinsic energy-band-structure parameters, such as: 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 $m_r(x)/m_o$, 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 $r_{d(a)} = r_{do(ao)} \equiv r_{Si} = 0.117$ nm, are given respectively in the following (Van Cong, 2024; 2023; 2023).

$$g_c(x) = 3 \times x + 3 \times (1 - x) = 3, g_v(x) = 2 \times x + 2 \times (1 - x) = 2, \quad (1)$$

$$m_c(x)/m_o = 0.12 \times x + 0.3216 \times (1 - x), m_v(x)/m_o = 0.3 \times x + 0.3664 \times (1 - x),$$

$$m_r(x)/m_o = \frac{m_c(x) \times m_v(x)}{m_c(x) + m_v(x)}, \quad (2)$$

$$\varepsilon_o(x) = 15.8 \times x + 11.4 \times (1-x), \quad (3)$$

$$E_{go}(x) \text{ in eV} = 0.7412 \times x + 1.17 \times (1-x), \quad (4)$$

$$E_{do(ao)}(x) = \frac{13600 \times [m_{c(v)}(x)/m_o]}{[\varepsilon_o(x)]^2} \text{ meV, and} \quad (5)$$

$$B_{do(ao)}(x) \equiv \frac{E_{do(ao)}(x)}{(4\pi/3) \times (r_{do(ao)})^3}. \quad (6)$$

Effects of Impurity Size, with a Given x

Here, one shows that the effect of the size of donor (acceptor) d(a)-radius, $r_{d(a)}$, and x-Ge concentration strongly affects the changes in all the energy-band-structure parameters, which can be represented by the effective relative static dielectric constant $\varepsilon(r_{d(a)}, x)$, 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 (Van Cong, 2023, 2023; Van Cong et al., 1984), 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: $\frac{d}{dV}\left(\frac{d\sigma}{dV}\right) = \frac{B}{V}$. Then, by an integration, one gets:

$$[\Delta\sigma(r_{d(a)}, x)]_{n(p)} = B_{do(ao)}(x) \times (V - V_{do(ao)}) \times \ln\left(\frac{V}{V_{do(ao)}}\right) = E_{do(ao)}(x) \times \left[\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 - 1\right] \times \ln\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 \geq 0. \quad (7a)$$

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

$$E_{gno(gpo)}(r_{d(a)},x)-E_{go}(x)=E_{d(a)}(r_{d(a)},x)-E_{do(ao)}(x)=E_{do(ao)}(x)\times\left[\left(\frac{\varepsilon_o(x)}{\varepsilon(r_{d(a)})}\right)^2-1\right]=$$
$$-\left[\Delta\sigma(r_{d(a)},x)\right]_{n(p)}. \quad (7b)$$

Therefore, from above Equations (7a) and (7b), 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 $\varepsilon(r_{d(a)},x)=\frac{\varepsilon_o(x)}{\sqrt{1+\left[\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3-1\right]\times\ln\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3}}\leq\varepsilon_o(x)$,

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

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

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

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:

$$a_{Bn(Bp)}(r_{d(a)},x)\equiv\frac{\varepsilon(r_{d(a)},x)\times\hbar^2}{m_{c(v)}(x)\times q^2}=0.53\times10^{-8}\ \text{cm}\times\frac{\varepsilon(r_{d(a)},x)}{m_{c(v)}(x)/m_o}, \quad (9)$$

where $-q$ is the electron charge.

In the n(p)-type degenerate $Si_{1-x}Ge_x$- crystalline alloy, the critical donor (acceptor)-density in the MIT, $N_{CDn(NDp)}(r_{d(a)},x)$, is determined, using the generalized empirical Mott parameters $M_{n(p)}(x)$, as:

$N_{CDn}(r_d,x)^{1/3}\times a_{Bn}(r_d,x)=M_n(x)$, $M_n(x)=0.25\times x+0.290364495\times(1-x)$, and

$$N_{CDp}(r_a,x)^{1/3}\times a_{Bp}(r_a,x)=M_p(x),\ M_p(x)=0.25\times x+0.3687018\times(1-x). \quad (10)$$

It should be noted in Eq. (10) that, for the Mott criterion in the MIT, his empirical parameter is found to be equal to: M_{Mott}=0.25, while, from Eq. (10), $M_n(x=0)=0.290364495$ and $M_p(x=1)=0.25$ are chosen such that we can obtain the experimental values of critical densities of the Si-crystal, as (Van Cong, 2023; Van Cong et al., 2014): $N_{CDn}(r_d=r_P,x=0)=3.52\times10^{18}\ cm^{-3}$ and $N_{CDp}(r_a=r_B,x=0)=4.06\times10^{18}\ cm^{-3}$.

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

$N^{EBT}_{CDn(CDp)}(r_{d(a)},x)$- 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 the n(p)-type degenerate $Si_{1-x}Ge_x$- crystalline alloy, if denoting the Fermi wave number by: $k_{Fn(Fp)}(N,x)\equiv\left(3\pi^2N/g_{c(v)}(x)\right)^{1/3}$, the effective reduced Wigner-Seitz radius $r_{sn(sp)}$, characteristic of interactions, is defined by:

$$r_{sn(sp)}(N,r_{d(a)},x)\equiv\left(\frac{3g_{c(v)}(x)}{4\pi N}\right)^{1/3}\times\frac{1}{a_{Bn(Bp)}(r_{d(a)},x)}=1.1723\times10^8\times\left(\frac{g_{c(v)}(x)}{N}\right)^{1/3}\times\frac{m_{c(v)}(x)/m_o}{\varepsilon(r_{d(a)},x)}. \quad (11)$$

So, the ratio of the inverse effective screening length $k_{sn(sp)}$ to Fermi wave number $k_{Fn(kp)}$ at 0 K is defined by:

$$R_{sn(sp)}(N,r_{d(a)},x)\equiv\frac{k_{sn(sp)}}{k_{Fn(Fp)}}=\frac{k^{-1}_{Fn(Fp)}}{k^{-1}_{sn(sp)}}=R_{snWS(spWS)}+\left[R_{snTF(spTF)}-R_{snWS(spWS)}\right]e^{-r_{sn(sp)}}<1. \quad (12)$$

These ratios, $R_{snTF(spTF)}$ and $R_{snWS(spWS)}$, are determined in following Equations (13, 14).

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

$$R_{snTF}(N,r_{d(a)},x)\equiv\frac{k_{snTF(spTF)}}{k_{Fn(Fp)}}=\frac{k^{-1}_{Fn(Fp)}}{k^{-1}_{snTF(spTF)}}=\sqrt{\frac{4\gamma r_{sn(sp)}(N,r_{d(a)},x)}{\pi}}\ll1, \quad (13)$$

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 (Van Cong, 2023; 2023):

$$R_{snWS(spWS)}(N, r_{d(a)}, x) \equiv \frac{k_{snWS(spWS)}}{k_{Fn}(k_{Fp})} = \left(\frac{3}{2\pi} - \gamma \frac{d\left[r_{sn(sp)}^2 \times E_{CE}\right]}{dr_{sn(sp)}}\right) \times 1\ (0.389856828), \quad (14)$$

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

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

So, the n(p)-type degenerate $Si_{1-x}Ge_x$- crystalline alloy, the physical conditions are found to be given by :

$$\frac{k_{Fn(Fp)}^{-1}}{a_{Bn(Bp)}} < \frac{\eta_{n(p)}}{\mathbb{E}_{Fno(Fpo)}} \equiv \frac{1}{A_{n(p)}} < \frac{k_{Fn(Fp)}^{-1}}{k_{sn(sp)}^{-1}} \equiv R_{sn(sp)}(N, r_{d(a)}, x) < 1,\ A_{n(p)}(N, r_{d(a)}, x) \equiv \frac{\pm \mathbf{E_{Fno(Fpo)}}}{\eta_{n(p)}}. \quad (15)$$

Here, $\pm \mathbf{E_{Fno(Fpo)}}$ is the Fermi energy at 0 K, and $\eta_{n(p)}$ is defined in next Eq. (17), as:$\pm \mathbf{E_{Fno(Fpo)}}(N, x) = \frac{\hbar^2 \times k_{Fn(Fp)}(N,x)^2}{2 \times m_{c(v)}(x)}$, $\eta_{n(p)}(N, r_{d(a)}, x) = \frac{\sqrt{2\pi N}}{\varepsilon(r_{d(a)}, x)} \times q^2 k_{sn(sp)}^{-1/2}$.

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 the $Si_{1-x}Ge_x$- crystalline alloy, is defined by

$$V(r) \equiv \sum_{j=1}^{\mathbb{N}} v_j(r) + V_o, \quad (16)$$

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:

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

where $k_{sn(sp)}$ is the inverse screening length determined in Eq. (12).

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

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

where Ω is the total $Si_{1-x}Ge_x$- crystalline alloy volume.

Then, the effective auto-correlation function for potential fluctuations, $W_{n(p)}(\nu_{n(p)}, N, r_d) \equiv \langle V(r)V(r')\rangle$, was determined, (Van Cong, 2023 ; 2023) as :

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

$$\nu_{n(p)}(E, N, x) \equiv \frac{\mp E}{\pm E_{Fno(Fpo)}(N,x)}, \; \mathcal{H}_n(x) = 4.36698 \times x^{1.069} + 3.320313702 \times (1 - x^{1.069}), \text{ and}$$

$$\mathcal{H}_p(x) = 10.9385 \times x^{1.3053} + 3.320313702 \times (1 - x^{1.3053}). \quad (17)$$

Here, E is the total electron energy, $\varepsilon(r_{d(a)})$ is determined in Equations (8a, 8b), $R_{sn(sp)}(N, r_{d(a)}, x)$ in Eq. (12), and the empirical Heisenberg parameters $\mathcal{H}_{n(p)}(x)$ were 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:

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

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

$$\langle E_k^{a-\frac{1}{2}} \rangle_{KIM} = \frac{\exp(-y^2/4) \times W_{n(p)}^{\frac{2a-1}{4}}}{\sqrt{2\pi}} \times \Gamma(a + \tfrac{1}{2}) \times D_{-a-\frac{1}{2}}(y) = \frac{\exp(-y^2/4) \times \eta_{n(p)}^{a-\frac{1}{2}}}{\sqrt{2\pi}} \times \exp\left(-\frac{\mathcal{H}_{n(p)} \times R_{sn(sp)} \times (2a-1)}{8 \times \sqrt{|\nu_{n(p)}|}}\right) \times \Gamma(a + \tfrac{1}{2}) \times D_{-a-\frac{1}{2}}(y). \quad (18)$$

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. (18).

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. (18), one gets:

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

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

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

Therefore, as $E \to \pm 0$, from Eq. (18), one gets: $\langle E_k^{a-\frac{1}{2}} \rangle_{KIM} \to 0$.

Thus, in this case, one gets:

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

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:

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

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. (18), one gets:

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

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:

$$F_{n(p)}(\nu_{n(p)},N,r_{d(a)},x,a)=K_{n(p)}(\nu_{n(p)},N,r_{d(a)},x,a)+\left[H_{n(p)}(\nu_{n(p)},N,r_{d(a)},x,a)-K_{n(p)}(\nu_{n(p)},N,r_{d(a)},x,a)\right]\times\exp\left[-c_1\times\left(A_{n(p)}\nu_{n(p)}\right)^{c_2}\right], \quad (22)$$

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.

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

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

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

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

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

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

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

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

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

Where

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

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

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

Finally, Eq. (25) now yields:

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

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

In n(p)-type degenerate $Si_{1-x}Ge_x$- crystalline alloy, the numerical results of $N^{EBT}_{CDn(CDp)}[N = N_{CDn(NDp)}(r_{d(a)}, x), r_{d(a)}, x] \equiv N^{EBT}_{CDn(CDp)}(r_{d(a)}, x)$, for a simplicity of presentation, evaluated using Eq. (26), are given in following Tables 1n and 1p 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 (6), (8a), (8b), and (10), respectively, noting that the relative deviations in absolute values are defined by: $|RD| \equiv \left|1 - \frac{N^{EBT}_{CDn(CDp)}}{N_{CDn(CDp)}}\right|$.

Tables 1n and 1p in Appendix 1

Here, some concluding remarks are given and discussed in the following.

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

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

(3)-Here, one notes that the maximal value of $|RD|$ is found to be respectively given by: $9.99 \times 10^{-6}(1.49 \times 10^{-5})$, meaning that $N^{EBT}_{CDn} \cong N_{CDn}$. In other word, this critical d(a)-density $N_{CDn(NDp)}(r_{d(a))}, x)$, determined in Eq. (10) is just the density of electrons (holes) localized in the EBT, $N^{EBT}_{CDn(CDp)}(r_{d(a)}, x)$, respectively.

(4)-In particular, in the n(p)-type degenerate $Si_{1-x}Ge_x$- crystalline alloy, for x=1 and $r_{d(a)} = r_{P(B)}$, we get:

$\frac{r_{P(B)}}{r_{Si}} = \frac{11(8.8)}{11.7} = 0.940\ (0.75)$, while, in the n(p)-type degenerate Ge-crystal (Van Cong, 2023), $\frac{r_{P(B)}}{r_{Ge}} = \frac{11(8.8)}{12.2} = 0.902$ (0.721), meaning: $\frac{r_{P(B)}}{r_{Si}} > \frac{r_{P(B)}}{r_{Ge}}$, due to the atom size effect: $r_{Si} = 0.117\ nm < r_{Ge} = 0.122\ nm$. As a result, in those Tables 1n and 1p, we get: $\varepsilon(r_{P(B)}, x = 1) = 16.053\ (22.144)$, $E_{gno(gpo)}(r_{P(B)}, x = 1)$ =0.741 eV (0.733 eV), and $N_{CDn(CDp)}(r_{P(B)}, x = 1)$ in $10^{16}\ cm^{-3} = 4.384\ (26.95)$, while in the n(p)-type degenerate Ge-crystal (Van Cong, 2023) one has the corresponding results as: $\varepsilon(r_{P(B)}) = 16.499\ (25.373)$, $E_{gno(gpo)}(r_{P(B)})$ =0.64 eV (0.6305 eV), and $N_{CDn(CDp)}(r_{P(B)})$ in $10^{16}\ cm^{-3} = 4.038\ (17.347)$, meaning that, due to the atom size effect: $r_{Si} = 0.117\ nm < r_{Ge} = 0.122\ nm$, while $\varepsilon(r_{P(B)}, x = 1) < \varepsilon(r_{P(B)})$, therefore, $E_{gno(gpo)}(r_{P(B)}, x = 1) > E_{gno(gpo)}(r_{P(B)})$ and $N_{CDn(CDp)}(r_{P(B)}, x = 1) > N_{CDn(CDp)}(r_{P(B)})$. This remark is important.

Finally, the effective density of free electrons (holes), N^*, given in the parabolic conduction (valence) band of the n(p)-type degenerate $Si_{1-x}Ge_x$- crystalline alloy, can thus be expressed by:

$$N^* \equiv N - N_{CDn(NDp)} \cong N - N^{EBT}_{CDn(CDp)}. \quad (27)$$

Optical Band Gap

Here, the optical band gap, $E_{gn1(gp1)}(N^*, r_{d(a)}, x, T)$, is defined by (Van Cong, 2023; 2023):

$$E_{gn1(gp1)}(N^*, r_{d(a)}, x, T) \equiv E_{gn2(gp2)}(N^*, r_{d(a)}, x, T) \pm E_{Fn(Fp)}(N^*, x, T),$$
$$E_{gn2(gp2)}(N^*, r_{d(a)}, x, T) \equiv E_{gno(gpo)}(r_{d(a)}, x) - \Delta T(T) - \Delta E_{gn(gp)}(N^*, r_{d(a)}, x), \quad (28)$$

where $E_{gn2(gp2)}$ is the reduced band gap, meaning that the band gap $E_{gno(gpo)}$, given in Eq. (10), is reduced by the effect of temperature, $\Delta T(T)$, being given in next Eq. (30), and that of high doping, $\Delta E_{gn(gp)}(N^*, r_{d(a)}, x)$, being determined in next Equations (31n, 31p), and finally, $\pm E_{Fn(Fp)}(N^*, x, T)$ is the Fermi energy, being determined in next Eq. (32). Then, it should be noted that, in the calculation of $\Delta E_{gn(gp)}$ and $E_{Fn(Fp)}$, the effective mass $m_{c(v)}(x)$ is now replaced by the reduced mass $m_r(x)$, being determined in Eq. (2). Further, the effective reduced Wigner-Seitz radius $r_{sn(sp)}$, characteristic of interactions, determined in Eq. (11), is now replaced by:

$$r_{sn(sp)}(N^*, r_{d(a)}, x) \equiv 1.1723 \times 10^8 \times \left(\frac{g_{c(v)}(x)}{N^*}\right)^{1/3} \times \frac{m_r(x)/m_o}{\varepsilon(r_{d(a)},x)}, \quad (29)$$

replacing $m_{c(v)}(x)$ by $m_r(x)$.

Now, the expressions of ΔT, $\Delta E_{gn(gp)}$ and $\pm E_{Fn(Fp)}$ are determined as follows.

$\Delta T(T)$-Determination

Here, we have (Van Cong, 2024):

$$\Delta T(T) = 10^{-4} \times T^2 \times \left[\frac{3.525 \times x}{T+94\ K} + \frac{2.54 \times (1-x)}{T+204\ K}\right]. \quad (30)$$

$\Delta E_{gn(gp)}(N^*, r_{d(a)}, x)$ −Determination

Then, the band gap narrowing $\Delta E_{gn}(N^*, x, T)$ is found to be given by (Van Cong, 2023; 2023):

$$\Delta E_{gn}(N^*, r_d, x) \simeq a_1 \times \frac{\varepsilon_o(x)}{\varepsilon(r_d,x)} \times N_r^{1/3} + a_2 \times \frac{\varepsilon_o(x)}{\varepsilon(r_d,x)} \times N_r^{\frac{1}{3}} \times (2.503 \times [-E_{cn}(r_{sn}) \times r_{sn}]) + a_3 \times \left[\frac{\varepsilon_o(x)}{\varepsilon(r_d,x)}\right]^{5/4} \times \sqrt{\frac{m_v}{m_r}} \times N_r^{1/4} + a_4 \times \sqrt{\frac{\varepsilon_o(x)}{\varepsilon(r_d,x)}} \times N_r^{1/2} \times 2 + a_5 \times \left[\frac{\varepsilon_o(x)}{\varepsilon(r_d,x)}\right]^{\frac{3}{2}} \times N_r^{\frac{1}{6}}, \quad N_r \equiv \left(\frac{N^*}{9.999 \times 10^{17}\ cm^{-3}}\right), \quad (31n)$$

where $a_1 = 6.506 \times 10^{-3}(eV)$, $a_2 = 1.113 \times 10^{-3}(eV)$, $a_3 = 4.794 \times 10^{-3}(eV)$, $a_4 = 9.582 \times 10^{-3}(eV)$ and $a_5 = 1.387 \times 10^{-3}(eV)$, and

$$\Delta E_{gp}(N^*, r_a, x) \simeq a_1 \times \frac{\varepsilon_o(x)}{\varepsilon(r_a,x)} \times N_r^{1/3} + a_2 \times \frac{\varepsilon_o(x)}{\varepsilon(r_a,x)} \times N_r^{\frac{1}{3}} \times \left(2.503 \times [-E_{cp}(r_{sp}) \times r_{sp}]\right) + a_3 \times \left[\frac{\varepsilon_o(x)}{\varepsilon(r_a,x)}\right]^{5/4} \times \sqrt{\frac{m_c}{m_r}} \times N_r^{1/4} + 2a_4 \times \sqrt{\frac{\varepsilon_o(x)}{\varepsilon(r_a,x)}} \times N_r^{1/2} + a_5 \times \left[\frac{\varepsilon_o(x)}{\varepsilon(r_a,x)}\right]^{\frac{3}{2}} \times N_r^{\frac{1}{6}}, \quad N_r \equiv \left(\frac{N^*}{9.999 \times 10^{17}\ cm^{-3}}\right), \quad (31p)$$

where $a_1 = 1.113 \times 10^{-2}(eV)$, $a_2 = 1.904 \times 10^{-3}(eV)$, $a_3 = 8.526 \times 10^{-3}(eV)$, $a_4 = 1.640 \times 10^{-2}(eV)$ and $a_5 = 2.373 \times 10^{-3}(eV)$.

Further, the correlation energy of an effective electron gas, $E_{cn(cp)}(N^*, r_{d(a)}, x)$, is given as (Van Cong, 2023; 2023):

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

and $r_{sn(rp)}$ is determined in Eq. (29).

It should be noted in Equations (31n) and (31p) that, for given $r_{d(a)}\ and\ x$, the values of $\Delta E_{gn(gp)}$ increase with increasing N.

$\pm\ \mathbf{E_{Fn(Fp)}(N^*, x, T)}$ −Determination

Here, as given in our previous works (Van Cong, 2023; Van Cong & Debiais, 1993), for the n(p)-type, the Fermi energy $\pm\ \mathrm{E_{Fn(Fp)}}$ was investigated, with a precision of the order of 2.11×10^{-4}, as:

$$\frac{E_{Fn}(u)}{k_BT}\left(\frac{-E_{Fp}(u)}{k_BT}\right) = \frac{G(u)+Au^BF(u)}{1+Au^B},\ A = 0.0005372 \text{ and } B = 4.82842262, \quad (32)$$

where u is the reduced electron density, $u(N^*,T,x) \equiv \frac{N^*}{N_{c(v)}(T,x)}$, $N_{c(v)}(T,x) = 2 \times g_{c(v)}(x) \times \left(\frac{m_r(x)\times k_BT}{2\pi\hbar^2}\right)^{\frac{3}{2}}\ (cm^{-3})$, $F(u) = au^{\frac{2}{3}}\left(1 + bu^{-\frac{4}{3}} + cu^{-\frac{8}{3}}\right)^{-\frac{2}{3}}$, $a = \left[(3\sqrt{\pi}/4) \times u\right]^{2/3}$, $b = \frac{1}{8}\left(\frac{\pi}{a}\right)^2$, $c = \frac{62.3739855}{1920}\left(\frac{\pi}{a}\right)^4$, and $G(u) \simeq Ln(u) + 2^{-\frac{3}{2}} \times u \times e^{-du}$; $d = 2^{3/2}\left[\frac{1}{\sqrt{27}} - \frac{3}{16}\right] > 0$.

Here, one notes that:

(i) as $u \gg 1$, according to the degenerate case, Eq. (32) is reduced to the function F(u),

(ii) $\frac{E_{Fn}(u\ll1)}{k_BT}\left(\frac{-E_{Fp}(u\ll1)}{k_BT}\right) \ll -1$, to the non-degenerate case, Eq. (32) is reduced to the function G(u), and

(ii) for given $r_{d(a)}\ and\ x$, the values of $\pm\ E_{Fn(Fp)}$ increase with increasing N.

Now, going back to Eq. (28),

(1)-the numerical results of $\mathrm{E_{gn1(gp1)}(N^*, r_{d(a)}, x = 0, T = 20\ K)}$ are calculated, being in good agreement with experimental ones obtained by Wagner and del Alamo (1988), with a precision of the order of 1.428 % (4.556 %), respectively, as observed in the following Table 2 in Appendix 1.

Table 2 in Appendix 1

(2)-for $\mathbf{N > N_{CDn(CDp)}(r_{d(a)}, x)}$, the numerical results of the optical band gap, given in the n(p)-type, $\mathrm{E_{gn1}(N^*, r_{d(a)}, x, T = 20\ K)}$, are obtained, as functions of N and $\mathrm{r_{d(a)}}$, for x=0, 0.5, 1, respectively, being reported in following Tables 3n and 3p in Appendix 1.

Tables 3n and 3p in Appendix 1

Finally, as noted in Equations (31n), (31p) and (32), because both two functions: $\mathrm{\Delta E_{gn(gp)}}$ and $\mathrm{\pm\ E_{Fn(Fp)}}$, for given $\mathrm{r_{d(a)}\ and\ x}$, increase with increasing N, the optical band gap, $\mathrm{E_{gn1}(N^*, r_{d(a)}, x, T = 20\ K)}$, determined in Eq. (28), and expressed as functions of N, thus randomly varies.

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Appendix

Table 1n. The numerical results of B_{do}, ε, E_{gno}, N_{CDn}, and N_{CDn}^{EBT} are computed, using Equations (6), (8a), (8b), (10), and (26), respectively, noting that the relative deviations in absolute values are defined by: $|RD| \equiv \left|1 - \frac{N_{CDn}^{EBT}}{N_{CDn}}\right|$

Donor		P	**Si**	Te
r_d (nm)	↗	0.110	**r_{do}=0.117**	0.132
x	↗	0, 0.5, 1	0, 0.5, 1	0, 0.5, 1
$B_{do}(x)$ in 10^8 (N/m^2)	↘		8.036400, 3.876827, 1.5610697	
$\varepsilon(r_d, x)$	↘	11.58254, 13.81777, 16.052996	11.4, 13.6, 15.8	10.59472, 12.63931, 14.683906
$E_{gno}(r_d, x)$ eV	↗	1.168948, 0.955092, 0.7409956	1.17, 0.9556, 0.7412	1.175310, 0.958162, 0.7422316
$N_{CDn}(r_d, x)$ in 10^{18} cm^{-3}	↗	3.519998, 0.5405417, 0.0438400	3.6918109, 0.566926, 0.0459799	4.599238, 0.706273, 0.0572815
$N_{CDn}^{EBT}(r_d, x)$ in 10^{18} cm^{-3}	↗	3.519975, 0.5405384, 0.0438396	3.6917862, 0.566922, 0.0459794	4.599222, 0.706269, 0.0572809
$\|RD\|$ in 10^{-6}		7.10, 6.04, 9.29	6.71, 6.03, 9.30	3.47, 6.04, 9.30
Donor		Sb	Sn	
r_d (nm)	↗	0.136	0.140	
x	↗	0, 0.5, 1	0, 0.5, 1	
$\varepsilon(r_d, x)$	↘	10.165683, 12.12748, 14.089280	9.6901858, 11.65602, 13.430257	
$E_{gno}(r_d, x)$ eV	↗	1.1786689, 0.959782, 0.7428839	1.1829244, 0.961835, 0.7437106	
$N_{CDn}(r_d, x)$ in 10^{18} cm^{-3}	↗	5.2064812, 0.799523, 0.0648444	1.1829244, 0.961835, 0.7437106	
$N_{CDn}^{EBT}(r_d, x)$ in 10^{18} cm^{-3}	↗	5.2064292, 0.799518, 0.0648438	6.0111115, 0.923085, 0.0748655	
$\|RD\|$ in 10^{-6}		9.99, 6.03, 9.30	6.7, 6.03, 9.30	

Table 1p. The numerical results of B_{ao}, ε, E_{gpo}, N_{CDp}, and N_{CDp}^{EBT} are computed, using Equations (6), (8a), (8b), (10), and (26), respectively, noting that the relative deviations in absolute values are defined by: $|RD| \equiv \left|1 - \frac{N_{CDp}^{EBT}}{N_{CDp}}\right|$

Acceptor		B	**Si**	Mg
r_a (nm)	↗	0.088	**r_{ao}=0.117**	0.140
x	↗	0, 0.5, 1	0, 0.5, 1	0, 0.5, 1
$B_{ao}(x)$ in 10^8 (N/m^2)	↘		9.155899, 5.850357, 3.902674	

$\varepsilon(r_a, x)$	↘	15.9777, 19.0611, 22.1445	11.4, 13.6, 15.8	9.690186, 11.5602, 13.4302
$E_{gpo}(r_a, x)$ eV	↗	1.15118, 0.94357, 0.73318	1.17, 0.9556, 0.7412	1.184725, 0.96501, 0.74748
$N_{CDp}(r_a, x)$ in 10^{18} cm^{-3}	↗	4.060003, 1.062187, 0.260952	11.17771, 2.924339, 0.718436	18.19999, 4.761524, 1.169785
$N_{CDp}^{EBT}(r_a, \mathbf{x})$ in 10^{18} cm^{-3}	↗	4.060012, 1.062182, 0.260956	11.17774, 2.924324, 0.718446	18.20003, 4.761500, 1.169803
$\|RD\|$ in 10^{-6}		2.28, 5.03, 14.9	2.30, 5.01, 14.9	2.30, 5.02, 14.9
Acceptor		In	Cd	
r_a (nm)	↗	0.144	0.148	
x	↗	0, 0.5, 1	0, 0.5, 1	
$\varepsilon(r_a, x)$	↘	9.191081, 10.9648, 12.73851	8.687132, 10.36360, 12.0401	
$E_{gpo}(r_a, x)$ eV	↗	1.190645, 0.96879, 0.749999	1.197687, 0.973291, 0.75300	
$N_{CDp}(r_a, x)$ in 10^{18} cm^{-3}	↗	21.328877, 5.580108, 1.3708900	25.260281, 6.608653, 1.623578	
$N_{CDp}^{EBT}(r_a, \mathbf{x})$ in 10^{18} cm^{-3}	↗	21.328916, 5.580080, 1.370910	25.260339, 6.608620, 1.623602	
$\|RD\|$ in 10^{-6}		2.30, 5.02, 14.9	2.30, 5.02, 14.9	

Table 2. Here, the numerical results of the optical band gap, given in the n(p)-type, $E_{gn1(gp1)}(N^*, r_{d(a)} = r_{P(B)}, x = 0, T = 20\ K)$, are obtained by using Eq. (28), respectively, noting that the maximal values of $\left|RD = 1 - \frac{E_{gn1(gp1)}}{E_{gn1(gp1)}^{Exp.}}\right|$, $E_{gn1(gp1)}^{Exp.}$ being the experimental values given by Wagner and del Alamo (1988), are found to be given respectively by: 1.428 % (4.556 %)

N in 10^{18} cm^{-3}	4	8.5	15	50	80	150	
$E_{gn1}^{Exp.}(N^*, r_P, T)$ in eV	1.138	1.138	1.129	1.131	1.132	1.133	
$E_{gn1}(N^*, r_P; x = 0, T)$ in eV	1.1375	1.120	1.114	1.115	1.123	1.149	
$\|RD\|$ in %	0.041	1.105	1.291	**1.428**	0.755	1.415	
N in 10^{18} cm^{-3}	6.5	11	15	26	60	170	400
$E_{gp1}^{Exp.}(N^*, r_B, T)$ in eV	1.142	1.140	1.139	1.142	1.142	1.162	1.178
$E_{gp1}(N^*, r_B, x = 0, T)$ in eV	1.115	1.102	1.097	1.090	1.090	1.129	1.231
$\|RD\|$ in %	2.341	3.312	3.714	**4.556**	4.505	2.825	4.492

Table 3n. Here, for $N > N_{CDn}(r_d, x)$, the numerical results of the optical band gap, $E_{gn1}(N^*, r_d, x, T = 20\ K)$, are obtained by using Eq. (28), as functions of N and r_d , for x=0, 0.5, 1, respectively

N in 10^{18} cm^{-3}	4	8.5	15	50	80	150
x=0						
$E_{gn1}(N^*, r_P, T)$ in eV	1.1375	1.120	1.114	1.115	1.123	1.149
$E_{gn1}(N^*, r_{Si}, T)$ in eV	1.139	1.120	1.113	1.113	1.121	1.146
$E_{gn1}(N^*, r_{Te}, T)$ in eV		1.118	1.109	1.104	1.110	1.131
$E_{gn1}(N^*, r_{Sb}, T)$ in eV		1.118	1.107	1.099	1.104	1.123
$E_{gn1}(N^*, r_{Sn}, T)$ in eV		1.119	1.104	1.092	1.096	1.113
x=0.5						
$E_{gn1}(N^*, r_P, T)$ in eV	0.921	0.920	0.922	0.946	0.970	1.024
$E_{gn1}(N^*, r_{Si}, T)$ in eV	0.921	0.919	0.920	0.944	0.967	1.021
$E_{gn1}(N^*, r_{Te}, T)$ in eV	0.918	0.914	0.915	0.935	0.956	1.006
$E_{gn1}(N^*, r_{Sb}, T)$ in eV	0.916	0.912	0.911	0.929	0.949	0.998
$E_{gn1}(N^*, r_{Sn}, T)$ in eV	0.914	0.908	0.907	0.923	0.941	0.987
x=1						
$E_{gn1}(N^*, r_P, T)$ in eV	0.726	0.737	0.752	0.830	0.890	1.013
$E_{gn1}(N^*, r_{Si}, T)$ in eV	0.725	0.736	0.751	0.828	0.887	1.010
$E_{gn1}(N^*, r_{Te}, T)$ in eV	0.722	0.731	0.745	0.819	0.876	0.995
$E_{gn1}(N^*, r_{Sb}, T)$ in eV	0.720	0.728	0.742	0.813	0.869	0.987
$E_{gn1}(N^*, r_{Sn}, T)$ in eV	0.717	0.724	0.737	0.806	0.806	0.976

Table 3p. Here, for $N > N_{CDp}(r_a, x)$, the numerical results of $E_{gp1}(N^*, r_a, x, T = 20\ K)$, are obtained by using Eq. (28), as functions of N and r_a , for x=0, 0.5, 1, respectively

N in 10^{18} cm^{-3}	6.5	11	15	26	60	170	400
x=0							
$E_{gp1}(N^*, r_B, T)$ in eV	1.115	1.102	1.097	1.090	1.090	1.129	1.231
$E_{gp1}(N^*, r_{Si}, T)$ in eV	1.094	1.073	1.063	1.046	1.027	1.129	1.085
$E_{gp1}(N^*, r_{Mg}, T)$ in eV				1.054	0.999	0.970	0.998

$E_{gp1}(N^*, r_{In}, T)$ in eV				1.064	0.990	0.951	0.969
$E_{gp1}(N^*, r_{Cd}, T)$ in eV				1.102	0.982	0.930	0.936
x=0.5							
$E_{gp1}(N^*, r_{B}, T)$ in eV	0.910	0.909	0.909	0.915	0.943	1.043	1.237
$E_{gp1}(N^*, r_{Si}, T)$ in eV	0.884	0.877	0.873	0.870	0.879	0.943	1.092
$E_{gp1}(N^*, r_{Mg}, T)$ in eV	0.891	0.868	0.858	0.846	0.841	0.883	1.006
$E_{gp1}(N^*, r_{In}, T)$ in eV	0.898	0.865	0.853	0.837	0.828	0.862	0.977
$E_{gp1}(N^*, r_{Cd}, T)$ in eV		0.864	0.849	0.829	0.814	0.840	0.944
x=1							
$E_{gp1}(N^*, r_{B}, T)$ in eV	0.732	0.745	0.757	0.789	0.880	1.126	1.545
$E_{gp1}(N^*, r_{Si}, T)$ in eV	0.706	0.714	0.722	0.745	0.817	1.027	1.401
$E_{gp1}(N^*, r_{Mg}, T)$ in eV	0.691	0.694	0.699	0.716	0.778	0.968	1.318
$E_{gp1}(N^*, r_{In}, T)$ in eV	0.686	0.687	0.691	0.707	0.764	0.948	1.288
$E_{gp1}(N^*, r_{Cd}, T)$ in eV	0.680	0.680	0.683	0.696	0.749	0.925	1.256