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Accurate expressions for optical coefficients, due to the impurity-size effect, and obtained in n(p)-type degenerate Si crystals, taking into account their correct asymptotic behavior, as the photon energy E (→ ∞)

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Abstract

In our three previous papers [1, 2, 3], referred to as I, II and III. In I and II, our new expression for the static dielectric constant, $\varepsilon(r_{d(a)})$, $r_{d(a)}$ being the donor (acceptor) d(a)-radius, was determined by using an effective Bohr model, suggesting that, for an increasing $r_{d(a)}$, $\varepsilon(r_{d(a)})$, due to such the impurity size effect, decreases, and affecting strongly the critical d(a)-density in the metal-insulator transition (MIT), $N_{CDn(CDp)}(r_{d(a)})$, determined by Eq. (3), and also the optical coefficients, given in the n(p)-type degenerate Si crystal, at low temperature T and high d(a)-density N, according to the reduced Fermi energy $\xi_{n(p)}(\geqq 1)$, since those coefficients are expressed in terms of $(E^* \equiv E - \mathbb{E}_{gn(gp)})^2$. Here, E^* is the effective photon energy, E is the photon energy and $\mathbb{E}_{gn(gp)}$ is the band gap, which can be equal to the intrinsic band gap $\mathbb{E}_{gni(gpi)}(r_{d(a)})$, and optical band gap $\mathbb{E}_{gn1(gp1)}(N^*, r_{d(a)}, T)$, as those defined in Eq. (5), noting that N^* is the effective d(a)-density, defined by: $N^* \equiv N - N_{CDn(CDp)}(r_{d(a)})$, being the effective density of free electrons (holes), given in the parabolic conduction (valence) bands of the n(p)-type degenerate d(a)-Si crystals.

Then, using the same physical model and same mathematical methods and taking into account the corrected values of energy-band-structure parameters, all the numerical results of the optical coefficients, obtained in III, are now revised and performed, giving rise to some important concluding remarks, as follows.

(i) The physical MIT-condition for N, is found to be given by: $N^* \equiv N - N_{CDn(CDp)}(r_{d(a)})=0$ or $N = N_{CDn(CDp)}(r_{d(a)})$, which can be explained by the density of electrons (holes) localized in the exponential conduction(valence)-band tails, $N^{EBT}_{CDn(CDp)}(r_{d(a)})$, determined in Eq. (21), with a precision of the order of 10^{-5}, as given in Table 1.

(ii) By basing on correct asymptotic behaviors of the refraction index n and extinction coefficient κ, as those proposed in Equations (28, 29), we have investigated all the optical coefficients, being determined in Equations (24, 25, 28, 29),

and then their numerical results given in different physical conditions have been tabulated and discussed in Tables 2a(b, c), 3a(b, c), 4n(p), 5n(p), and 6n(p), in which $\mathbb{E}_{gni(gpi)}$ and $\mathbb{E}_{gn1(gp1)}$, defined in Eq. (5), play a very important role.

(iii) As given in Eq. (30), at T=0K, the physical MIT-condition for E, is that $\kappa(E^* = 0, r_{d(a)}) = 0$, at $E^* \equiv E - \mathbb{E}_{gni(gpi)} = 0$, according to the critical photon energy $E = E_{CPE} = \mathbb{E}_{gni(gpi)}$, being similar to the physical MIT-condition for N, as that given in (i).

(iv) As showed in Tables 3a, 3b and 3c, our expressions for optical coefficients are found to be more accurate than the corresponding ones, being obtained from the physical model proposed by Forouhi and Bloomer [11].

(v) Finally, as showed in Tables 4n and 4p, the extrema values of real (imaginary) parts of the complex dielectric functions, $\varepsilon_{1(2)}(E, r_{d(a)})$, given in any d(a)-Si systems, occur at the same photon energy E.

Keywords: Effects of the impurity-size and heavy doping; effective autocorrelation function for potential fluctuations; optical coefficients; critical photon energy

1. Introduction

In our two previous papers [1, 2, 3], referred here to as I, II and III.

In I and II, our new expression for the extrinsic static dielectric constant, $\varepsilon(r_{d(a)})$, $r_{d(a)}$ being the donor (acceptor) d(a)-radius, was determined by using an effective Bohr model, suggesting that, with an increasing $r_{d(a)}$, $\varepsilon(r_{d(a)})$, due to such the impurity size effect, decreases, affecting strongly the critical impurity density in the metal-insulator transition, and also the optical coefficients, given in n(p)-type degenerate Si crystal, for the reduced Fermi energy [4], $\boldsymbol{\xi}_{\mathbf{n(p)}}(\geqq \mathbf{1})$. Therefore, all the numerical results of those obtained and given in III are now revised and performed, in comparison with those obtained in [5-12], as given in the following Sections 1-5.

2. Energy-band-structure parameters

First of all, we present in the following Table 1 the values of the energy-band-structure parameters, given in the n(p)-type Si-crystal, such as: (i) if denoting the free electron mass by m_o, the relative effective electron (hole) mass, $m^*_{n(p)}/m_o$, which is equal to the relative effective mass, $m_{n(p)}/m_o$ [5], as used in this Sections 2 and 4 to determine the critical impurity density in the MIT, and (ii) to the reduced effective mas, $m_r = \frac{m_n \times m_p}{m_n + m_p} \times m_o$, as used in Sections 3 and 5 to determine the optical band gap and the optical coefficients in the n(p)-type degenerate Si. Further, $\mathbb{E}_{go}(r_{d(a)} = r_{Si}) = 1.17 eV$ [4] is the unperturbed intrinsic band gap, as used in Section 3 to determine the optical band gap, $\varepsilon_o = 11.4$ [6] is the relative intrinsic dielectric constant, the critical impurity density in the MIT, $N_{CDn(CDp)}(r_{P(B)}) = 3.52(4.06 \times 10^{18} cm^{-3}$ [3, 7], and finally, the effective averaged numbers of equivalent conduction (valence)-band edge, $g_{c(v)} = 3(2)$ [4, 7], used here.

Table 1. For increasing $r_{d(a)}$, while $\varepsilon(r_d)$ decreases, the functions: $\mathbb{E}_{gni(gpi)}(r_{d(a)})$, $N_{CDn(NDp)}(r_{d(a)})$ and $N^{EBT}_{CDn(CDp)}(r_{d(a)})$ increase. The relative deviations between the numerical results of $N_{CDn}(r_d)$ and $N^{EBT}_{CDn}(r_d)$, calculated using Equations (3, 21), are verry small, of the order of 9.8×10^{-6}, suggesting that $N_{CDn(NDp)}(r_{d(a)})$ can be well explained by $N^{EBT}_{CDn}(r_d)$, being localized in the EBT.

Donor		P	Si	As	Te	Sb	Sn
r_d (nm) [4]	↗	0.110	0.117	0.118	0.132	0.136	0.140
$\varepsilon(r_d)$	↘	11.58	11.4	11.396	10.59	10.16	9.69
$\mathbb{E}_{gni}(r_d)$ in meV	↗	1168.9	1170	1170.02	1175.04	1178.67	1182.9
$N_{CDn}(r_d)$ in 10^{18} cm^{-3}	↗	3.52 [7]	3.69181	3.69547	4.59924	5.20648	6.011
$N^{EBT}_{CDn}(r_d)$ in 10^{18} cm^{-3}	↗	3.52 [7]	3.69179	3.695468	4.599223	5.20643	6.01109
$\lvert RD\rvert$ in 10^{-6}		0	6.5	0.4	3.7	**9.8**	9.4

Acceptor		**B**	**Si**	**Ga(Al)**	**Mg**	**In**
r_a (nm) [4]	↗	0.088	0.117	0.126	0.140	0.14
$\varepsilon(r_a)$	↘	15.98	11.4	11.1	9.69	9.19
$\mathbb{E}_{gpi}(r_a)$ in meV	↗	1151.2	1170	1172.1	1184.7	1190.6
$N_{CDp}(r_a)$ in 10^{18} cm^{-3}	↗	4.06 [7]	11.177705	12.118516	18.199979	21.328851
$N^{EBT}_{CDp}(r_a)$ in 10^{18} cm^{-3}	↗	4.06 [7]	11.177737	12.118572	18.199970	21.32881
$\lvert RD\rvert$ in 10^{-6}		0	2.8	**4.58**	0.49	1.9

We now determine our expression for extrinsic static dielectric constant, $\varepsilon(r_{d(a)})$, due to the impurity size effect, and the expression for critical density, $N_{CDn(CDp)}(r_{d(a)})$, characteristic of the MIT, as follows.

2.1. Expression for $\varepsilon(r_{d(a)})$

In the [d(a)-semiconductors]-systems, since $r_{d(a)}$, given in tetrahedral covalent bonds, is usually either larger or smaller than $r_{do(ao)} \equiv r_{Si}$, a local mechanical strain (or deformation potential energy) is induced, according to a compression (dilation) for: $r_{d(a)} > r_{do(ao)}$ ($r_{d(a)} < r_{do(ao)}$), due to the d(a)-size effect, respectively [1]. Then, we have shown that this $r_{d(a)}$-effect affects the changes in all the energy-band-structure parameters, expressed in terms of the static dielectric constant, $\varepsilon(r_{d(a)})$, determined as follows.

At T=0K, we shown [1, 2] that, as $r_{d(a)} > r_{do(ao)}$($r_{d(a)} < r_{do(ao)}$), such the compression (dilatation) corresponding the repulsive (attractive) force increases (decreases) the intrinsic energy gap $\mathbb{E}_{gni(gpi)}(r_{d(a)})$ and the effective donor(acceptor)-ionization energy $\mathbb{E}_{d(a)}(r_{d(a)})$ in absolute values, obtained in an effective Bohr model, as [1]:

$$\mathbb{E}_{gni(gpi)}(r_{d(a)}) - \mathbb{E}_{go}(r_{Si}) = \mathbb{E}_{d(a)}(r_{d(a)}) - \mathbb{E}_{do(ao)}(r_{Si}) = \mathbb{E}_{do(ao)}(r_{Si}) \times \left[\left(\frac{\varepsilon_o}{\varepsilon(r_{d(a)})}\right)^2 - 1\right], \quad (1)$$

where $\mathbb{E}_{do(ao)}(r_{Si}) \equiv \frac{13600\, meV \times (m_{n(p)}/m_o)}{\varepsilon_o^2}$ and

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

$$\varepsilon(r_{d(a)}) = \frac{\varepsilon_o}{\sqrt{1-\left[\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3-1\right]\times\ln\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3}} \geq \varepsilon_o,\ \left[\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3-1\right]\times\ln\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 < 1, \text{ for } r_{d(a)} \leq r_{do(ao)}. \quad (2)$$

One notes that $\varepsilon(r_{d(a)})$ decreases with an increasing $r_{d(a)}$.

2.2. Our expressions for the critical density in the MIT

In the n(p)-type degenerate Si-crystals, the critical donor(acceptor)-density, $N_{CDn(NDp)}(r_{d(a)})$, is determined from the generalized effective Mott criterion in the MIT, as:

$$N_{CDn(NDp)}(r_{d(a)})^{1/3} \times a_{Bn(Bp)}(r_{d(a)}) = z,\ z{=}0.290364495(0.3687017088), \quad (3)$$

and the effective Bohr radius $a_{Bn(Bp)}(r_{d(a)})$ is given by:

$$a_{Bn(Bp)}(r_{d(a)}) \equiv \frac{\varepsilon(r_{d(a)})\times\hbar^2}{(m^*_{n(p)}/m_o)\times q^2} = 0.53\times10^{-8}\ \text{cm}\times\frac{\varepsilon(r_{d(a)})}{(m^*_{n(p)}/m_o)}, \quad (4)$$

where $-q$ is the electron charge, $\varepsilon(r_{d(a)})$ is determined in Eq. (2), and $m^*_{n(p)}/m_o = m_{n(p)}/m_o = 0.3216(0.3664)$. It should be noted in Eq. (3) that, for the Mott criterion in the MIT, z_{Mott}=0.25, while in the present work, z= 0.290364495(0.3687017088), is chosen so that we can obtain the exact values of $N_{CDn(CDp)}(r_{P(B)}) = 3.52\ (4.06)\times10^{18}\ \text{cm}^{-3}$ [3, 7], as those given in Table 1. Further, these obtained results can also be justified by those of the densities of electrons (holes) localized in exponential conduction (valance)-band (EBT) tails, $N^{EBT}_{CDn(CDp)}(r_{P(B)}) \equiv N_{CDn(CDp)}(r_{P(B)}) = 3.52\ (4.06)\times10^{18}\ \text{cm}^{-3}$, obtained using Eq. (21), as investigated in Section 4, and reported also in Table 1. In this Table, we also present various values of $\varepsilon(r_{d(a)})$, $\mathbb{E}_{gni(gpi)}(r_{d(a)})$, $N_{CDn(NDp)}(r_{d(a)})$, and $N^{EBT}_{CDn(CDp)}(r_{d(a)})$, noting that the maximal relative deviations, in absolute values, $|RD|$, between $N_{CDn(NDp)}(r_{d(a)})$ and $N^{EBT}_{CDn(CDp)}(r_{d(Ba)})$ are found to be equal to: $9.8(0.49)\times10^{-6}$, respectively. In other word, $N_{CDn(NDp)}(r_{d(a)})$, determined in Eq. (3), can be explained by the densities of electrons (holes) localized in exponential conduction (valance)-band (EBT) tails, $N^{EBT}_{CDn(CDp)}(r_{d(a)})$, determined in Eq. (21). Furthermore, in our recent work [7], we showed that, in the n(p)-type degenerate Si, the critical densities of electrons (holes) can also be determined from the spin-susceptibility singularities (SSS), obtained at $N = N^{SSS}_{CDn(CDp)}(r_{d(a)})$, at which the MITs occur.

Table 1 also indicates that, for increasing $r_{d(a)}$, $\varepsilon(r_{d(a)})$ decreases, while $\mathbb{E}_{gni(gpi)}(r_{d(a)})$, $N_{CDn(NDp)}(r_{d(a)})$ and $N^{EBT}_{CDn(CDp)}(r_{d(a)})$ increase, affecting strongly all the physical properties, as those given in following Sections 3-5 .

3. Optical band gap

Here, $m^*_{n(p)}/m_o$ is chosen as: $m^*_{n(p)}/m_o = m_r/m_o = 0.1713$, and then, if denoting $N^* \equiv N - N_{CDn(NDp)}(r_{d(a)})$, the optical band gap (**OBG**) is found to be given by:

$$\mathbb{E}_{gn1(gp1)}(N^*, r_{d(a)}, T) \equiv \mathbb{E}_{gn2(gp2)}(N^*, r_{d(a)}, T) + \mathbb{E}_{Fn(Fp)}(N^*, T), \quad (5)$$

where the Fermi energy $\mathbb{E}_{Fn(Fp)}(N^*,T)$ is determined in Eq. (A3) of the Appendix A and the reduced band gap is defined by:

$\mathbb{E}_{gn2(gp2)}(N^*, r_{d(a)}, T) \equiv \mathbb{E}_{gnei(gpei)}(r_{d(a)}, T) - \Delta\mathbb{E}_{gn(gp)}(N^*, r_{d(a)})$.

Here, the effective intrinsic band gap $\mathbb{E}_{gnei(gpei)}$ is determined by:

$$\mathbb{E}_{gnei(gpei)}(r_{d(a)}, T) \equiv \mathbb{E}_{gni(gpi)}(r_{d(a)}) - 0.071\text{eV} \times \left\{\left(1 + \left[\frac{2T}{440.6913}\right]^{2.201}\right)^{\frac{1}{2.201}} - 1\right\},$$

and the band gap narrowing, $\Delta\mathbb{E}_{gn(gp)}(N^*, r_{d(a)})$, are determined in Equations (B3, B4) of the Appendix B and the intrinsic energy gap $\mathbb{E}_{gni(gpi)}(r_{d(a)})$ is defined in in Eq. (1).

Then, as noted in the Appendix A and B, at T=0K, as $N^* = 0$, one has: $\mathbb{E}_{Fn(Fp)}(N^*,T) = \mathbb{E}_{Fno(Fpo)}(N^*) = 0$, as given in Eq. (A4), and $\Delta\mathbb{E}^*_{gni(gpi)}(N^*, r_{d(a)}, T) = 0$, or $\Delta\mathbb{E}_{gn(gp)}(N^*, r_{d(a)}) = 0$, according to the MIT, as noted in Appendix A and B. Therefore, $\mathbb{E}_{gn1(gp1)} = \mathbb{E}_{gn2(gp2)} = \mathbb{E}_{gnei(gpei)}(r_{d(a)}) = \mathbb{E}_{gni(gpi)}(r_{d(a)})$ at T=0K and $N^* = 0$, according also to the MIT.

Finally, the numerical results of $\mathbb{E}_{gn1(gp1)}(N^* > 0, r_{d(a)}, T)$ at T=20K, calculated using Eq. (5), expressed as functions of N and $r_{d(a)}$, and reported in Table 3 of I, being also compared with the corresponding data [8], obtained in the P(B)-type degenerate Si, giving rise to the accuracies of the order of 1.16% (2.68%), respectively. Here, we also showed that, in the n(p)-type degenerate Si and for a given photon energy $E \equiv \hbar\omega$, since the extinction coefficient, $\kappa_{n(p)}$, and other optical coefficients, as discussed in III, are expressed in terms of the function $(E - \mathbb{E}_{gn1(gp1)})^2$. Therefore, if the values of $\mathbb{E}_{gn1(gp1)}$ obtained in Table 3 of III, increase (decrease), $(E - \mathbb{E}_{gn})^2$ and other optical coefficients then decrease (increase), respectively, as showed in Figures 3a, 3b and 3c of our previous paper II.

4. Physical model and mathematical methods

4.1. Physical model

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

$$\gamma \times r_{sn(sp)}(N^*, r_{d(a)}, m^*_{n(p)}) \equiv \frac{k^{-1}_{Fn(Fp)}}{a_{Bn(Bp)}} < 1, \tag{6}$$

being proportional to $N^{*-1/3}$. Here, $\gamma = (4/9\pi)^{1/3}$, $k^{-1}_{Fn(Fp)}$ means the averaged distance between ionized donors (acceptors), and $a_{Bn(Bp)}(r_{d(a)})$ is determined in Eq. (4).

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

$$R_{sn(sp)}(N^*, r_{d(a)}) \equiv \frac{k_{sn(sp)}}{k_{Fn(Fp)}} = \frac{k^{-1}_{Fn(Fp)}}{k^{-1}_{sn(sp)}} = R_{snWS(spWS)} + [R_{snTF(spTF)} - R_{snWS(spWS)}]e^{-r_{sn(sp)}} < 1. \tag{7}$$

These ratios, $R_{snTF(spTF)}$ *and* $R_{snWS(spWS)}$, can be determined as follows.

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

$$R_{snTF}(N^*, r_{d(a)}) \equiv \frac{k_{snTF(spTF)}}{k_{Fn(Fp)}} = \frac{k_{Fn(Fp)}^{-1}}{k_{snTF(spTF)}^{-1}} = \sqrt{\frac{4\gamma r_{sn(sp)}}{\pi}} \ll 1, \quad (8)$$

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

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

$$R_{sn(sp)WS}(N^*, r_{d(a)}) \equiv \frac{k_{sn(sp)WS}}{k_{Fn}} = \left(\frac{3}{2\pi} - \gamma \frac{d\left[r_{sn(sp)}^2 \times \mathbb{E}_{CE}(N^*, r_{d(a)})\right]}{dr_{sn(sp)}}\right), \quad (9)$$

where $\mathbb{E}_{CE}(N^*, r_{d(a)})$ is the majority-carrier correlation energy (CE), being determined in Eq. (B2) of the Appendix B.

Furthermore, as given in II, in the highly degenerate case, the physical conditions are found to be given by :

$$\frac{k_{Fn(Fp)}^{-1}}{a_{Bn(Bp)}} < \frac{\eta_{n(p)}}{\mathbb{E}_{Fno(Fpo)}} \equiv \frac{1}{A_{n(p)}} < \frac{k_{Fn(Fp)}^{-1}}{k_{sn(sp)}^{-1}} \equiv R_{sn(sp)} < 1, \; A_{n(p)} \equiv \frac{\mathbb{E}_{Fno(Fpo)}}{\eta_{n(p)}}, \quad (10)$$

being needed to determine the expression for electrical conductivity, as investigated in Section 5. Here, $R_{sn(sp)}$ is determined in Eq. (7).

Then, in degenerate d(a)-Si systems, 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 crystal, is defined by

$$V(r) \equiv \sum_{j=1}^{\mathbb{N}} v_j(r) + V_o, \quad (11)$$

where $\mathbb{N}$ is the total number of ionized donors(acceptors), V_o is a constant potential energy, and $v_j(r)$ is a screened Coulomb potential energy for each d(a)-Si system, 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. (7).

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-crystal 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 in II, as :

$$W_{n(p)}(\nu_{n(p)}, N^*, r_{d(a)}) \equiv \eta_{n(p)}^2 \times \exp\left(\frac{-\mathcal{H} \times R_{sn(sp)}(N^*, r_{d(a)})}{2\sqrt{|\nu_{n(p)}|}}\right), \eta_{n(p)}(N^*, r_{d(a)}) \equiv \frac{\sqrt{2\pi N^*}}{\varepsilon(r_{d(a)})} \times q^2 k_{sn(sp)}^{-1/2}, \nu_{n(p)} \equiv \frac{-\mathbb{E}}{\mathbb{E}_{Fno(Fpo)}}. \quad (12)$$

Here, $\varepsilon(r_{d(a)})$ is determined in Eq. (2), $R_{sn(sp)}(N^*, r_{d(a)})$in Eq. (7), the empirical Heisenberg parameter $\mathcal{H} = 3.320313702$ will be chosen such that the determination of the density of electrons localized in the conduction(valence)-band tails, determined in Section 5 would be accurate, and finally $\nu_{n(p)} \equiv \frac{-\mathbb{E}}{\mathbb{E}_{Fno(Fpo)}}$, where $\mathbb{E}$ is the total electron energy and $\mathbb{E}_{Fno(Fpo)}$ is the Fermi energy at 0 K, determined in Eq. (A4) of the Appendix A.

In the following, we will calculate the ensemble average of the function: $(\mathbb{E}-V)^{a-\frac{1}{2}} \equiv \mathbb{E}_k^{a-\frac{1}{2}}$, for $a \geq 1$, $\mathbb{E}_k \equiv \frac{\hbar^2 \times k^2}{2 \times m_{n(p)}^*}$ being the kinetic energy of the electron (hole), and $V(r)$ determined in Eq. (11), by using the two following integration methods, as developed in II, which strongly depend on $W_{n(p)}(\nu_{n(p)}, N^*, r_{d(a)})$.

4.2. Mathematical methods and their application (Critical impurity density)

A. Kane integration method (KIM)

In heavily doped d(a)-Si systems, 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 $(\mathbb{E}-V)^{a-\frac{1}{2}} \equiv \mathbb{E}_k^{a-\frac{1}{2}}$ is defined by

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

Then, by variable changes: $s = (\mathbb{E}-V)/\sqrt{W_{n(p)}}$ and $x = -\mathbb{E}/\sqrt{W_{n(p)}} \equiv A_{n(p)} \times \nu_{n(p)} \times \exp\left(\frac{\mathcal{H} \times R_{sn(sp)}}{4 \times \sqrt{|\nu_{n(p)}|}}\right)$,

and using an identity:

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

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

$$\langle\mathbb{E}_k^{a-\frac{1}{2}}\rangle_{KIM} = \frac{\exp(-x^2/4) \times W_{n(p)}^{\frac{2a-1}{4}}}{\sqrt{2\pi}} \times \Gamma\left(a+\frac{1}{2}\right) \times D_{-a-\frac{1}{2}}(x) = \frac{\exp(-x^2/4) \times \eta_{n(p)}^{a-\frac{1}{2}}}{\sqrt{2\pi}} \times \exp\left(-\frac{\mathcal{H} \times R_{sn(sp)} \times (2a-1)}{8 \times \sqrt{|\nu_{n(p)}|}}\right) \times \Gamma\left(a+\frac{1}{2}\right) \times D_{-a-\frac{1}{2}}(x). \quad (13)$$

B. Feynman path-integral method (FPIM)

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

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

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 $x = -\mathbb{E}/\sqrt{W_{n(p)}}$, and then using an identity:

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

one finally obtains: $\langle\mathbb{E}_k^{a-\frac{1}{2}}\rangle_{FPIM} \equiv \langle\mathbb{E}_k^{a-\frac{1}{2}}\rangle_{KIM}$, $\langle\mathbb{E}_k^{a-\frac{1}{2}}\rangle_{KIM}$ being determined in Eq. (13).

In the following, with use of asymptotic forms for $D_{-a-\frac{1}{2}}(x)$, those given for $\langle(\mathbb{E}-V)^{a-\frac{1}{2}}\rangle_{KIM}$ will be obtained in the two cases: $\mathbb{E}\geq 0$ and $\mathbb{E}\leq 0$.

(i) $\mathbb{E}\geq 0$-case

As $\mathbb{E}\to+\infty$, one has: $\nu_n\to-\infty$ and $x\to-\infty$. In this case, one gets:

$$D_{-a-\frac{1}{2}}(x\to-\infty)\approx\frac{\sqrt{2\pi}}{\Gamma(a+\frac{1}{2})}\times e^{\frac{x^2}{4}}\times(-x)^{a-\frac{1}{2}}.$$

Therefore, Eq. (13) becomes: $\langle\mathbb{E}_k^{a-\frac{1}{2}}\rangle_{KIM}\approx\mathbb{E}^{a-\frac{1}{2}}$. Further, as $\mathbb{E}\to+0$, one has: $\nu_{n(p)}\to-0$ and $x\to-\infty$. So, one gets :

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

Thus, as $\mathbb{E}\to+0$, from Eq. (13), one gets: $\langle\mathbb{E}_k^{a-\frac{1}{2}}\rangle_{KIM}\to 0$.

In summary, for $\mathbb{E}\geq 0$, the expression of $\langle\mathbb{E}_k^{a-\frac{1}{2}}\rangle_{KIM}$ can be approximated by:

$$\langle\mathbb{E}_k^{a-\frac{1}{2}}\rangle_{KIM}\cong\mathbb{E}^{a-\frac{1}{2}},\quad \mathbb{E}_k\equiv\frac{\hbar^2\times k^2}{2\times m^*}. \tag{14}$$

(ii) $\mathbb{E}\leq 0$ – case.

As $\mathbb{E}\to-0$, from Eq. (13), one has: $\nu_{n(p)}\to+0$ and $x\to+\infty$. Thus, one first obtains, for any $a\geq 1$,

$D_{-a-\frac{1}{2}}(x\to\infty)\simeq\beta(a)\times\exp\left[-(\sqrt{a}+\frac{1}{16a^{\frac{3}{2}}})\,x-\frac{x^2}{16a}-\frac{x^3}{24\sqrt{a}}\right]\to 0,\ \beta(a)=\frac{\sqrt{\pi}}{2^{\frac{2a+1}{4}}\Gamma(\frac{a}{2}+\frac{3}{4})]}$, noting that $\beta(1)=\frac{\sqrt{\pi}}{2^{\frac{3}{4}}\times\Gamma(5/4)}$ and $\beta(5/2)=\frac{\sqrt{\pi}}{2^{3/2}}$.

Then, 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. (13) yields

$$H_{n(p)}(\nu_{n(p)}\to+0\,,r_{d(a)},a)=\frac{\langle\mathbb{E}_k^{a-\frac{1}{2}}\rangle_{KIM}}{f(a)}=\exp\left[-\frac{\mathcal{H}\times R_{sn(sp)}\times(2a-1)}{8\times\sqrt{|\nu_{n(p)}|}}-\left(\sqrt{a}+\frac{1}{16a^{\frac{3}{2}}}\right)x-\left(\frac{1}{4}+\frac{1}{16a}\right)x^2-\frac{x^3}{24\sqrt{a}}\right]\to 0. \tag{15}$$

Further, as $\mathbb{E}\to-\infty$, one has: $\nu_{n(p)}\to+\infty$ and $x\to\infty$. Thus, one gets:

$D_{-a-\frac{1}{2}}(x\to\infty)\approx x^{-a-\frac{1}{2}}\times e^{-\frac{x^2}{4}}\to 0$. Therefore, Eq. (13) yields

$$K_{n(p)}(\nu_{n(p)}\to+\infty\,,r_{d(a)},a)\equiv\frac{\langle\mathbb{E}_k^{a-\frac{1}{2}}\rangle_{KIM}}{f(a)}\simeq\frac{1}{\beta(a)}\times\exp\left(-\frac{(A_{n(p)}\times\nu_{n(p)})^2}{2}\right)\times(A_{n(p)}\times\nu_{n(p)})^{-a-\frac{1}{2}}\to 0. \tag{16}$$

It should be noted that, as $\mathbb{E}\leq 0$, the ratios (15) and (16) can be taken in an approximate form as:

$$F_{n(p)}(\nu_{n(p)},r_{d(a)},a)=K_{n(p)}(\nu_{n(p)},r_{d(a)},a)+\left[H_{n(p)}(\nu_{n(p)},r_{d(a)},a)-K_{n(p)}(\nu_{n(p)},r_{d(a)},a)\right]\times\exp\left[-c_1\times\left(A_{n(p)}\nu_{n(p)}\right)^{c_2}\right], \tag{17}$$

such that: $F_{n(p)}(\nu_{n(p)},r_{d(a)},a)\to H_{n(p)}(\nu_{n(p)},r_{d(a)},a)$ for $0\leq\nu_n\leq 16$, and $F_{n(p)}(\nu_{n(p)},r_{d(a)},a)\to K_{n(p)}(\nu_{n(p)},r_{d(a)},a)$ for $\nu_{n(p)}\geq 16$. 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), $N^{EBT}_{CDn(CDp)}(N, r_{d(a)})$, in the following.

C. Critical impurity density in the MIT

In degenerate d(a)-Si systems at T=0 K, in which $m^*_{n(p)}/m_o = m_{n(p)}/m_o = 0.3216(0.3664)$, as given in Table 1, using Eq. (13), for a=1, the density of states $\mathcal{D}(\mathbb{E})$ is defined by:

$$\langle \mathcal{D}(\mathbb{E}_k)\rangle_{KIM} \equiv \frac{g_{c(v)}}{2\pi^2}\left(\frac{2m_{n(p)}}{\hbar^2}\right)^{\frac{3}{2}} \times \langle \mathbb{E}_k^{\frac{1}{2}}\rangle_{KIM} = \frac{g_{c(v)}}{2\pi^2}\left(\frac{2m_{n(p)}}{\hbar^2}\right)^{\frac{3}{2}} \times \frac{\exp\left(-\frac{x^2}{4}\right)\times W_n^{\frac{1}{4}}}{\sqrt{2\pi}} \times \Gamma\left(\tfrac{3}{2}\right) \times D_{-\frac{3}{2}}(x) = \mathcal{D}(\mathbb{E}), \quad (18)$$

where x is defined in Eq. (13), as: $x = -\mathbb{E}/\sqrt{W_{n(p)}} \equiv A_{n(p)} \times \nu_{n(p)} \times \exp\left(\frac{\mathcal{H}\times R_{sn(sp)}}{4\times\sqrt{|\nu_{n(p)}|}}\right)$.

Here, $\mathbb{E}_{Fno}$ is determined in Eq. (A4) of the Appendix A, with $m^*_{n(p)}/m_o = m_{n(p)}/m_o$ and $\mathcal{H} = 3.320313702$, being chosen such that the following determination of $N^{EBT}_{CDn(CDp)}(N, r_{d(a)})$ would be accurate. Going back to the functions: H_n, K_n and F_n, given respectively in Equations (15-17), in which the factor $\frac{\langle \mathbb{E}_k^{\frac{1}{2}}\rangle_{KIM}}{f(a=1)}$ is now replaced by:

$$\frac{\langle \mathbb{E}_k^{\frac{1}{2}}\rangle_{KIM}}{f(a=1)} = \frac{\mathcal{D}(\mathbb{E}\le 0)}{\mathcal{D}_o} = F_{n(p)}\left(\nu_{n(p)}, r_{d(a)}, a=1\right),\ \mathcal{D}_o = \frac{g_{c(v)}\times\left(m_{n(p)}\times m_o\right)^{3/2}\times\sqrt{\eta_{n(p)}}}{2\pi^2\hbar^3} \times \beta(a=1),\ \beta(a=1) = \frac{\sqrt{\pi}}{2^{\frac{3}{4}}\times\Gamma(5/4)}. \quad (19)$$

Therefore, $N^{EBT}_{CDn(CDp)}(N, r_{d(a)})$ can be defined by

$N^{EBT}_{CDn(CDp)}(N, r_{d(a)}) = \int_{-\infty}^{0} \mathcal{D}(\mathbb{E}\le 0)\, d\mathbb{E}$,

where $\mathcal{D}(\mathbb{E}\le 0)$ is determined in Eq. (19). Then, by a variable change: $\nu_{n(p)} \equiv \frac{-\mathbb{E}}{\mathbb{E}_{Fno(Fpo)}}$, one obtains:

$$N^{EBT}_{CDn(CDp)}(N, r_{d(a)}) = \frac{g_{c(v)}\times\left(m_{n(p)}\right)^{3/2}\sqrt{\eta_{n(p)}}\times\mathbb{E}_{Fno(Fpo)}}{2\pi^2\hbar^3} \times \left\{\int_0^{16} \beta(a=1) \times F_{n(p)}\left(\nu_{n(p)}, r_{d(a)}, a=1\right) d\nu_{n(p)} + I_{n(p)}\right\}, \quad (20)$$

where

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

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

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

$$I_{n(p)} = \frac{1}{2^{5/4}A_{n(p)}} \times \int_{y_{n(p)}}^{\infty} t^{b-1}\, e^{-t} dt \equiv \frac{\Gamma(b, y_{n(p)})}{2^{5/4}\times A_{n(p)}},$$

where $b = -1/4$, $y_{n(p)} = \left[16A_{n(p)}/\sqrt{2}\right]^2$, and $\Gamma(b, y_{n(p)})$ is the incomplete Gamma function, defined by:

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

Finally, Eq. (20) now yields:

$$N^{EBT}_{CDn(CDp)}[N = N_{CDn(NDp)}(r_{d(a)}), r_{d(a)}] = \frac{g_{c(v)} \times (m_{n(p)})^{3/2} \sqrt{\eta_{n(p)}} \times \mathbb{E}_{Fno(Fpo)}}{2\pi^2 \hbar^3} \times \left\{ \int_0^{16} \beta(a = 1) \times F_{n(p)}(\nu_{n(p)}, r_{d(a)}, a = 1)\, d\nu_{n(p)} + \frac{\Gamma(b,\ y_{n(p)})}{2^{5/4} \times A_{n(p)}} \right\}, \quad (21)$$

being the density of electrons(holes) localized in the exponential conduction(valence)-band tails (EBT), respectively.

The numerical results of $N^{EBT}_{CDn(CDp)}[N = N_{CDn(NDp)}(r_{d(a)}), r_{d(a)}] \equiv N^{EBT}_{CDn(CDp)}(r_{d(a)})$, for a simplicity of presentation, evaluated using Eq. (21), are given in Table 2 of III, confirming thus those of $N_{CDn(NDp)}(r_{d(a)})$, calculated using Eq. (3), with a precision of the order of $9.8(4.91) \times 10^{-6}$, respectively. In other word, this critical d(a)-density $N_{CDn(NDp)}(r_{d(a)})$ can thus be explained by the density of electrons(holes) localized in the EBT, $N^{EBT}_{CDn(CDp)}(r_{d(a)})$, respectively.

So, the effective density of free electrons (holes), N^*, given in the parabolic conduction (valence) band of the degenerate d(a)-Si systems, can thus be expressed by:

$$N^* \equiv N - N_{CDn(NDp)} \cong N - N^{EBT}_{CDn(CDp)}. \quad (22)$$

Then, if $N^* = N_{CDn(NDp)}$, according to the Fermi energy, $\mathbb{E}_{Fno(Fpo)}(N^* = N_{CDn(NDp)}) \equiv \frac{\hbar^2 \times k^2_{Fn(Fp)}(N^*)}{2 \times m^*_{n(p)}}$, then the value of the density of electrons(holes), $N^{EBT}_{CDn(CDp)}$, localized in the EBT for $\mathbb{E} \leq 0$, is almost equal to $N_{CDn(NDp)}$, given in this parabolic conduction (valence) band, for $\mathbb{E} \geq 0$. This can be expressed as:

$$N^{EBT}_{CDn(CDp)} \cong N_{CDn(NDp)}, \text{ as } N^* \equiv N_{CDn(NDp)}. \quad (23)$$

5. Optical coefficients

Optical properties of any medium can be described by the complex refraction index $\mathbb{N}$ and the complex dielectric function ε, $\mathbb{N} \equiv n - i\kappa$ and $\varepsilon \equiv \varepsilon_1 - i\varepsilon_2$, where $i^2 = -1$ and $\varepsilon \equiv \mathbb{N}^2$. Therefore, the real and imaginary parts of ε denoted by ε_1 and ε_2 can thus be expressed in terms of the refraction index n and the extinction coefficient κ as: $\varepsilon_1 \equiv n^2 - \kappa^2$ and $\varepsilon_2 \equiv 2n\kappa$. One notes that the optical absorption coefficient α is related to ε_2, n, κ, and the optical conductivity σ_O by [3]

$$\alpha(E) \equiv \frac{\hbar q^2 \times |v(E)|^2}{n(E) \times \varepsilon_{free\ space} \times cE} \times J(E^*) = \frac{E \times \varepsilon_2(E)}{\hbar c n(E)} \equiv \frac{2E \times \kappa(E)}{\hbar c} \equiv \frac{4\pi\sigma_O(E)}{cn(E) \times \varepsilon_{free\ space}}, \ \varepsilon_1 \equiv n^2 - \kappa^2 \text{ and } \varepsilon_2 \equiv 2n\kappa, \quad (24)$$

where the effective photon energy: $E^* = E - \mathbb{E}_{gn(gp)} = \mathbb{E}$ is the reduced photon energy, the band gap $\mathbb{E}_{gn(gp)}$ can be equal to the optical band gap $\mathbb{E}_{gn1(gp1)}$ and intrinsic band gap $\mathbb{E}_{gni(gpi)}$, determined in Eq. (5). Here, $E \equiv \hbar\omega$, -q, $\hbar$, $|v(E)|$, ω, $\varepsilon_{free\ space}$, c and $J(E^*)$ respectively represent: the photon energy, electron charge, Dirac's constant, matrix elements of the velocity operator between valence (conduction)-and-conduction (valence) bands in n(p)-type semiconductors, photon frequency, permittivity of free space, velocity of light, and joint density of states. It should be noted that, if the three functions such as: $|v(E)|^2$, $J(E^*)$ and $n(E)$ are known, then the other optical dispersion functions given in Eq. (24) can thus be determined. Moreover, the normal-incidence reflectance, R(E), can be expressed in terms of κ(E) and n(E) as:

$$R(E) = \frac{[n(E)-1]^2+\kappa(E)^2}{[n(E)+1]^2+\kappa(E)^2}. \quad (25)$$

From Equations (24, 25), if the two optical functions, ε_1 and ε_2, (or n and κ), are both known, the other ones defined above can thus be determined.

Then, using a transformation for the joint density of states, given in allowed indirect Si-transitions, for a=5/2, as discussed in II, one has:

$$J_{n(p)}\left(E \geq \mathbb{E}_{gn(gp)}\right) = \frac{1}{2\pi^2} \times \left(\frac{2m_r}{\hbar^2}\right)^{3/2} \times \frac{(E-\mathbb{E}_{gn(gp)})^{a-(1/2)}}{E_{gni(gpi)}^{a-1}} = \frac{1}{2\pi^2} \times \left(\frac{2m_r}{\hbar^2}\right)^{3/2} \times \frac{(E-\mathbb{E}_{gn(gp)})^2}{E_{gni(gpi)}^{3/2}}, \text{ for a=5/2.} \quad (26)$$

Therefore, from Equations (24, 26), for $E \geq \mathbb{E}_{gn(gp)}$, or for $E^* = E - \mathbb{E}_{gn(gp)} = \mathbb{E} \geq 0$, the extinction coefficient κ can be determined by:

$$\kappa\left(E \geq \mathbb{E}_{gn(gp)}\right) = f(E) \times (E^* = E - \mathbb{E}_{gn(gp)})^2, \ f(E)= \frac{q^2 \times m_r^{3/2} \times |v(E)|^2}{\sqrt{2}\times\pi^2\times\varepsilon_o\times\hbar\times n(E)\times E^2\times E_{gni(gpi)}^{3/2}}, \quad (27)$$

noting that the optical function such as: n(E) and $\kappa\left(E \geq \mathbb{E}_{gn(gp)}\right)$, were parameterized by various authors [10-12]. First of all, one notes that, as $E \to \infty$, Forouhi and Bloomer (FB) [11] claimed model that $\kappa(E \to \infty) \to$ a constant, while Jellison and Modine [12] and Van Cong [3] showed that their proposed expressions quickly go to 0 as E^{-3}, and consequently, the optical functions such as: $\sigma_0(E)$ and α(E), given in Eq. (24), both go 0 as E^{-2}.

In the following, we will propose: $\kappa(E \to \infty) \to 0$ as E^{-1} so that $\sigma_0(E \to \infty)$ and $\alpha(E \to \infty)$ both go to their appropriate limiting constants.

Then, if defining the band gap $\mathbb{E}_{gn(gp)}$, equal to the optical band gap $\mathbb{E}_{gn1(gp1)}$ or to the intrinsic band gap $\mathbb{E}_{gni(gpi)}$, and taking into account the above remarks, we now propose:

$$\kappa(E^* \geq 0) = f(E) \times \left(E^* \equiv E - \mathbb{E}_{gn(gp)}\right)^2, \ f(E)=\sum_{i=1}^{4} \frac{A_i}{E^2\times(1+10^{-4}\times\frac{E}{6})-B_i E+C_i}, \quad (28)$$

being equal to 0 for $E^* = 0$ (or for $E = \mathbb{E}_{gn(gp)}$) and also going to 0 as E^{-1} as $E \to \infty$, and then,

$$n(E) = n_\infty(r_{d(a)}) + \sum_{i=1}^{4} \frac{B_{oi}E+C_{oi}}{E^2-B_i E+C_i}, \quad (29)$$

going to a constant as $E \to \infty$, since $n(E \to \infty, r_{d(a)}) = n_\infty(r_{d(a)}) = \sqrt{\varepsilon(r_{d(a)})} \times \frac{\omega_T}{\omega_L}$, $\omega_T = 9.9 \times 10^{13}\ s^{-1}$ [5] and $\omega_L = 16.8464 \times 10^{13}\ s^{-1}$, according to $n_\infty(r_P) = 2$, being obtained from the Lyddane-Sachs-Teller relation [5], from which T(L) represents the transverse (longitudinal) optical phonon mode.

Here, other parameters are determined by: $B_{oi} = \frac{A_i}{Q_i} \times \left[-\frac{B_i^2}{2} + E_{gnei(gpei)}B_i - E_{gnei(gpei)}^2 + C_i\right]$, $C_{oi} = \frac{A_i}{Q_i} \times \left[\frac{B_i\times(E_{gnei(gpei)}^2+C_i)}{2} - 2\mathbb{E}_{gnei(gpei)}C_i\right]$, $Q_i = \frac{\sqrt{4C_i-B_i^2}}{2}$, where, for i=(1, 2, 3, and 4), $A_i = 0.004374,\ 0.0154, 0.0738\ and\ 0.1889$, $B_i = 6.885, 7.401, 8.634$ and 10.652, and $C_i =$ 11.864, 13.754, 18.812, and 29.841.

The important numerical results of the above optical functions, at T=0K, $N = N_{CDn(CDp)}$, and for $E = \mathbb{E}_{gni(gi)}$, are reported in following Tables 2a, 2b and 2c, and Tables 3a, 3b and 3c, in which they are also discussed, and compared with the corresponding ones, calculated and obtained from FB-model [11], and also with the corresponding data given by Aspnes and Studna [9].

Table 2a. At the MIT, T=0K, $N=N_{CDn(p)}(r_{d(a)})$, and the critical photon energy $E_{CPE} = E = \mathbb{E}_{gni(gpi)}(r_{d(a)})$, $\kappa_{MIT}(\mathbb{E}_{gni(gpi)}, r_{d(a)}) = 0$, $\varepsilon_{2(MIT)}(\mathbb{E}_{gni(gpi)}, r_{d(a)}) = 0$, $\sigma_{O(MIT)}(\mathbb{E}_{gni(gpi)}, r_{d(a)}) = 0$ and $\propto_{MIT}(\mathbb{E}_{gni(gpi)}, r_{d(a)}) = 0$, and the other functions such as : $n_{MIT}(\mathbb{E}_{gni(gpi)}, r_{d(a)})$, $\varepsilon_{1(MIT)}(\mathbb{E}_{gni(gpi)}, r_{d(a)})$, and $R_{MIT}(\mathbb{E}_{gni(gpi)}, r_{d(a)})$ decrease with increasing $r_{d(a)}$ and $\mathbb{E}_{gni}(r_{d(a)})$.

Donor	P	Si	As	Te	Sb	Sn
At the MIT, T=0K, $N=N_{CDn}(r_d)$, and the critical photon energy $E_{CPE} = E = \mathbb{E}_{gni}(r_a)$, on has :						
$\mathbb{E}_{gni}(r_d)$ in meV ↗	1168.9	1170	1170.02	1175.04	1178.67	1182.9
$n_{MIT}(\mathbb{E}_{gni}, r_d)$ ↘	3.4463	3.43	3.4279	3.3565	3.3158	3.2696
$\kappa_{MIT}(\mathbb{E}_{gni}, r_d)$	0	0	0	0	0	0
$\varepsilon_{1(MIT)}(\mathbb{E}_{gni}, r_d)$ ↘	11.8768	11.7649	11.7626	11.2658	10.9943	10.6902
$\varepsilon_{2(MIT)}(\mathbb{E}_{gni}, r_d)$	0	0	0	0	0	0
$\sigma_{O(MIT)}(\mathbb{E}_{gni}, r_d)$	0	0	0	0	0	0
$\propto_{MIT}(\mathbb{E}_{gni}, r_d)$	0	0	0	0	0	0
$R_{MIT}(\mathbb{E}_{gni}, r_d)$ ↘	0.3027	0.3009	0.3009	0.2926	0.2879	0.2826

Acceptor	**B**	**Si**	**Ga(Al)**	**Mg**	**In**
At the MIT, T=0K, $N=N_{CDp}(r_a)$, and the critical photon energy $E_{CPE} = E = \mathbb{E}_{gpi}(r_a)$, on has :					
$\mathbb{E}_{gpi}(r_a)$ in meV ↗	1151.2	1170	1172.1	1184.7	1190.6
$n_{MIT}(\mathbb{E}_{gpi}, r_a)$ ↘	3.8030	3.43	3.4026	3.2688	3.2185
$\kappa_{MIT}(\mathbb{E}_{gpi}, r_a)$	0	0	0	0	0
$\varepsilon_{1(MIT)}(\mathbb{E}_{gpi}, r_a)$ ↘	14.4626	11.7649	11.5774	10.6851	10.3589
$\varepsilon_{2(MIT)}(\mathbb{E}_{gpi}, r_a)$	0	0	0	0	0
$\sigma_{O(MIT)}(\mathbb{E}_{gpi}, r_a)$	0	0	0	0	
$\propto_{MIT}(\mathbb{E}_{gpi}, r_a)$	0	0	0	0	0
$R_{MIT}(\mathbb{E}_{gpi}, r_a)$ ↘	0.3406	0.3009	0.2978	0.2825	0.2766

Table 2b. In d(a)-Si systems, the values of the following optical coefficients at $\mathbb{E} \leq 0$, expressed as functions of $r_{d(a)}$, and calculated using Equations (31-36, 24), for $E^* = \mathbb{E}_{gni(gpi)}(r_{d(a)})$, present the exponential tail-states for κ^{EEC-T} , ε_2^{EImD-T}, σ_O^{EOC-T} , σ_O^{EOC-T} , $\propto^{EOAC-T}$ and R^{NIR-T}, and their variations with increasing $r_{d(a)}$ are represented by the arrows: ↗ and ↘, suggesting that the obtained results of n^{ERI-T}, ε_1^{EReD-T}, and R^{NIR-T} are almost equal to the corresponding ones given in the above Table 2a.

d-Si systems	P-Si	As-Si	Te-Si	Sb-Si	Sn-Si
$n^{ERI-T}(r_d)$ ↘	3.4463	3.4297	3.3565	3.3158	3.2696
$\kappa^{EEC-T}(r_d)$ ↗	0.0282	0.0282	0.0286	0.0288	0.0291

$\varepsilon_1^{EReD-T}(r_d)$ ↘	11.8761	11.7618	11.2650	10.9935	10.6893
$\varepsilon_2^{EImD-T}(r_d)$ ↘	0.1941	0.1936	0.1917	0.1909	0.1901
$\sigma_O^{EOC-T}(r_d)$ in $\Omega^{-1}cm^{-1}$ ↘	2.4286	2.4251	2.4108	2.4086	2.4067
$\propto^{EOAC-T}(r_d)$ in $10^3\ cm^{-1}$ ↗	3.3361	3.3473	3.4002	3.4389	3.4847
$R^{NIR-T}(r_d)$ ↘	0.3027	0.3009	0.2926	0.2880	0.2826

a-Si systems	B-Si	Ga-Si	Mg-Si	In-Si
$n^{ERI-T}(r_a)$ ↘	3.803	3.4026	3.2688	3.2185
$\kappa^{EEC-T}(r_a)$ ↗	0.027	0.0284	0.0292	0.0296
$\varepsilon_1^{EReD-T}(r_a)$ ↘	14.4619	11.5766	10.6843	10.3580
$\varepsilon_2^{EImD-T}(r_a)$ ↘	0.2057	0.193	0.1908	0.1904
$\sigma_O^{EOC-T}(r_a)$ in $\Omega^{-1}cm^{-1}$ ↘	2.5343	2.4216	2.4194	2.4261
$\propto^{EOAC-T}(r_a)$ in $10^3\ cm^{-1}$ ↗	3.1548	3.3692	3.5039	3.5684
$R^{NIR-T}(r_a)$ ↘	0.3406	0.2978	0.2825	0.2766

Table 2c. Here, the choice of the real refraction index: $n(E \to \infty, r_{d(a)}) = n_\infty(r_{d(a)}) = \sqrt{\varepsilon(r_{d(a)})} \times \frac{\omega_T}{\omega_L}$, $\omega_T = 9.9 \times 10^{13}\ s^{-1}$ [5] and $\omega_L = 16.8464 \times 10^{13}\ s^{-1}$, obtained from the Lyddane-Sachs-Teller relation [5], from which T(L) represents the transverse (longitudinal) optical phonon mode, giving rise to $n_\infty(r_P) = 2$, and further, that of the asymptotic behavior, given for the extinction coefficient: $\kappa_\infty(E \to \infty, r_{d(a)}) \to 0$, as E^{-1}, so that $\sigma_0(E \to \infty, r_{d(a)})$ and $\alpha(E \to \infty, r_{d(a)})$ both go to their appropriate limiting constants, are found to be very important, affecting strongly the numerical results of the other optical coefficients.

Donor	P	Si	As	Te	Sb	Sn
$\varepsilon(r_d)$ ↘	11.58	11.4	11.396	10.59	10.16	9.69
$n_\infty(r_d)$ ↘	2	1.9842	1.9838	1.9128	1.8737	1.8293
$\kappa_\infty(r_d)$	0	0	0	0	0	0
$\varepsilon_{1,\infty}(r_d)$ ↘	4	3.9370	3.9356	3.6589	3.5107	3.3465
$\varepsilon_{2,\infty}(r_d)$	0	0	0	0	0	0
$\sigma_{O,\infty}(r_d)$ in $\frac{10^5}{\Omega \times cm}$ ↘	7.2548	7.1974	7.1963	6.9385	6.7966	6.6357
$\propto_\infty(r_d)$ in $(10^9 \times cm^{-1})$	1.7172	1.7172	1.7172	1.7172	1.7172	1.7172
$R_\infty(r_d)$ ↘	0.1111	0.1088	0.1087	0.0982	0.0924	0.0859

Acceptor	B	Si	Ga(Al)	Mg	In
$\varepsilon(r_a)$ ↘	15.98	11.4	11.1	9.69	9.19
$n_\infty(r_a)$ ↘	2.349	1.9842	1.9576	1.8293	1.7816
$\kappa_\infty(r_a)$	0	0	0	0	0
$\varepsilon_{1,\infty}(r_a)$ ↘	5.5179	3.9370	3.8323	3.3465	3.1741
$\varepsilon_{2,\infty}(r_a)$	0	0	0	0	0
$\sigma_{O,\infty}(r_a)$ in $\frac{10^5}{\Omega \times cm}$ ↘	8.5208	7.1974	7.1011	6.6357	6.4626
$\propto_\infty(r_a)$ in $(10^9 \times cm^{-1})$	1.7172	1.7172	1.7172	1.7172	1.7172
$R_\infty(r_a)$ ↘	0.1623	0.1088	0.1048	0.0859	0.0790

Table 3a. In the P-Si system, at T=0K, our numerical results of the following optical coefficients, expressed as functions of E, and calculated using Equations (24, 25, 28, 29), for $\mathbb{E}_{gn}(r_P) = \mathbb{E}_{gni}(r_P)[= 1.1689 \text{ eV}]$, and the corresponding ones, obtained from the FB-model [11], are reported in the following Table 2a, in which the relative deviations (RDs) of those are also given and calculated, for $1.5 \leq E(eV) \leq 6$, using the Aspnes-and-Studna (AS)-data [9]. Here, as noted in above Table 2c, one obtains: $\kappa_\infty(E \to \infty, \mathrm{r_P}) \to 0$ and $\varepsilon_{2,\infty}(E \to \infty, \mathrm{r_P}) \to 0$, while, in the FB-model, $\kappa_{\infty(FB)}(E \to \infty, \mathrm{r_P}) = 0.2615$ and $\varepsilon_{2,\infty(FB)}(E \to \infty, \mathrm{r_P}) = 1.0196$.

E in eV	n (RD%)	κ (RD%)	ε_1 (RD%)	ε_2 (RD%)	n_{FB} (RD%)	κ_{FB} (RD%)	$\varepsilon_{1(FB)}$ (RD%)	$\varepsilon_{2(FB)}$ (RD%)
1.5	3.605 (1.8)	**0.003 (45)**	12.999 (3.6)	**0.020 (47.8)**	3.535 (3.7)	0.004 (10)	12.497 (7.3)	0.032 (16.2)
1.6	3.661 (1.4)	0.005 (37.8)	13.401 (2.8)	0.036 (36.1)	3.590 (3.3)	0.007 (9.6)	12.887 (6.6)	0.052 (8.9)
1.7	3.720 (0.8)	0.008 (19.2)	13.839 (1.7)	0.060 (22.9)	3.648 (2.8)	0.011 (8.6)	13.312 (5.4)	0.079 (1.6)
1.8	3.784 (0.3)	0.012 (5.9)	14.319 (0.6)	0.093 (6.5)	3.712 (2.2)	0.016 (19.8)	13.777 (4.4)	0.116 (16.8)
1.9	3.853 (0.2)	0.018 (10.4)	14.847 (0.3)	0.136 (8.0)	3.780 (1.7)	0.022 (34.9)	14.288 (3.4)	0.163 (29.5)
2	3.98 (0.6)	0.025 (12.0)	15.429 (1.1)	0.194 (12.5)	3.854 (1.3)	0.029 (32.7)	14.854 (2.6)	0.225 (30.8)
2.1	4.010 (1.0)	0.033 (11.7)	16.076 (2.0)	0.269 (13.9)	3.935 (0.9)	0.039 (29.1)	15.482 (1.7)	0.305 (29.1)
2.2	4.099 (1.4)	0.045 (39.9)	16.798 (2.8)	0.367 (41.1)	4.023 (0.5)	**0.051 (58.3)**	16.183 (0.9)	**0.408 (56.8)**
2.3	4.197 (1.8)	0.059 (22.8)	17.611 (3.6)	0.495 (24.9)	4.120 (0.1)	0.066 (36.7)	16.973 (0.1)	0.541 (36.5)
2.4	4.305 (2.1)	0.077 (28.2)	18.532 (4.3)	0.662 (30.4)	4.228 (0.3)	0.084 (40.6)	17.868 (0.6)	0.508 (40.4)
2.5	4.427 (2.5)	0.100 (36.6)	19.585 (4.9)	0.883 (40.1)	4.348 (0.6)	0.108 (48.1)	18.893 (1.2)	0.940 (49.2)
2.6	4.863 (2.7)	0.129 (43.3)	20.804 (5.5)	1.177 (46.6)	4.483 (0.9)	0.138 (53.7)	20.080 (1.8)	1.240 (54.5)
2.7	4.718 (2.9)	0.167 (28.5)	22.232 (5.9)	1.576 (32.1)	4.637 (1.2)	0.177 (36.5)	21.472 (2.3)	1.646 (38.0)
2.8	4.897 (3.0)	0.217 (33.4)	23.933 (6.1)	2.130 (37.6)	4.815 (1.3)	0.229 (40.6)	23.130 (2.5)	2.208 (42.6)
2.9	5.107 (2.9)	0.286 (41.1)	25.999 (5.8)	2.926 (45.1)	5.024 (1.2)	0.300 (47.7)	25.147 (2.3)	3.013 (49.4)
3	5.359 (2.6)	0.385 (43.2)	28.572 (5.1)	4.128 (47.1)	5.275 (1.0)	0.401 (48.9)	27.663 (1.7)	4.226 (50.5)
3.1	5.671 (1.8)	0.536 (38.6)	31.873 (3.2)	6.084 (40.8)	5.586 (0.3)	0.555 (43.4)	30.891 (0.06)	6.200 (43.5)
3.2	6.068 (0.1)	0.797 (26.4)	36.188 (0.4)	9.668 (26.6)	5.982 (1.3)	0.821 (30.4)	35.109 (3.4)	9.825 (28.7)
3.3	6.549 (2.4)	1.329 (0.7)	41.127 (4.9)	17.412 (1.7)	6.461 (3.7)	1.372 (3.9)	39.869 (7.8)	17.725 (0.04)
3.4	6.650 (1.9)	2.440 (9.8)	38.265 (8.6)	32.454 (8.0)	6.550 (0.4)	2.550 (5.7)	36.400 (3.3)	33.404 (5.3)
3.5	5.662 (0.9)	2.896 (3.9)	23.666 (5.7)	32.798 (3.0)	5.535 (1.3)	3.006 (0.3)	21.599 (3.5)	33.270 (1.6)
3.6	5.532 (4.5)	2.828 (5.3)	22.608 (18.2)	31.295 (1.1)	5.396 (1.9)	2.888 (3.3)	20.777 (8.6)	31.163 (1.5)
3.7	5.399 (4.7)	3.105 (1.5)	19.501 (13.2)	33.531 (6.4)	5.254 (1.9)	3.156 (3.2)	17.643 (2.4)	33.165 (5.2)
3.8	5.155 (1.8)	3.208 (0.8)	16.282 (4.8)	33.075 (2.6)	5.003 (1.2)	3.245 (2.0)	14.502 (6.6)	32.470 (0.7)
3.9	5.149 (2.7)	3.255 (2.7)	15.921 (14.0)	33.519 (0.1)	4.992 (0.5)	3.275 (2.1)	14.197 (1.7)	32.704 (2.5)
4	5.273 (5.2)	3.527 (1.6)	15.363 (25.5)	37.201 (3.5)	5.112 (2.0)	3.537 (1.4)	13.620 (11.3)	36.159 (0.6)
4.1	5.276 (5.1)	4.060 (2.0)	11.354 (21.2)	42.842 (7.2)	5.110 (1.8)	4.062 (2.1)	9.613 (2.7)	41.515 (3.9)
4.2	4.963 (1.5)	4.715 (1.6)	2.403 (1.3)	46.796 (3.2)	4.795 (1.9)	4.710 (1.5)	**0.803 (66.1)**	45.166 (0.4)
4.3	4.280 (4.7)	5.231 (3.0)	**−9.048 (27.1)**	44.773 (1.5)	4.114 (0.7)	5.218 (3.3)	−10.309 (17.0)	42.937 (2.6)
4.4	3.409 (9.2)	5.375 (0.6)	−17.275 (8.2)	36.644 (9.9)	3.250 (4.2)	5.352 (0.1)	−18.079 (3.9)	34.792 (4.3)
4.5	2.646 (7.9)	5.146 (1.2)	−19.475 (1.7)	27.232 (9.3)	2.498 (1.9)	5.110 (0.6)	−19.878 (0.3)	25.527 (2.4)
4.6	2.151 (8.2)	4.732 (1.1)	−17.764 (0.9)	20.359 (9.4)	2.011 (1.1)	4.687 (0.2)	−17.919 (0.1)	18.852 (1.3)
4.7	1.901 (7.8)	4.315 (0.9)	−15.004 (1.2)	16.407 (8.7)	1.767 (0.2)	4.262 (0.4)	−15.042 (1.0)	15.067 (0.2)
4.8	1.805 (8.9)	3.980 (0.01)	−12.577 (3.9)	14.370 (8.9)	1.676 (1.1)	3.921 (1.4)	−12.568 (4.0)	13.145 (0.4)
4.9	1.784 (11.7)	3.742 (0.2)	−10.820 (6.0)	13.347 (11.5)	1.657 (3.8)	3.679 (1.9)	−10.792 (6.2)	12.194 (1.8)
5	**1.783 (13.6)**	3.587 (0.6)	−9.690 (5.4)	12.793 (14.3)	1.659 (5.7)	3.521 (1.2)	−9.645 (5.8)	11.684 (4.4)
5.1	1.775 (13.0)	3.494 (1.9)	−9.056 (2.5)	12.403 (15.0)	1.653 (5.2)	3.424 (0.1)	−8.987 (3.4)	11.322 (5.1)
5.2	1.745 (9.8)	3.439 (2.5)	−8.778 (0.6)	12.004 (12.7)	1.627 (2.4)	3.365 (0.3)	−8.675 (0.6)	10.947 (2.7)
5.3	1.690 (7.0)	3.403 (1.5)	−8.724 (0.3)	11.501 (8.6)	1.575 (0.3)	3.325 (0.8)	−8.577 (2.0)	10.473 (1.1)
5.4	1.610 (9.5)	3.371 (0.2)	−8.773 (4.3)	10.859 (9.6)	1.500 (1.9)	3.290 (2.2)	−8.578 (6.4)	9.868 (0.4)
5.5	1.513 (12.9)	3.334 (0.9)	−8.824 (3.1)	10.086 (14.0)	1.407 (5.0)	3.250 (1.6)	−8.582 (5.8)	9.142 (3.3)
5.6	1.404 (12.6)	3.283 (2.4)	−8.806 (0.9)	9.219 (15.2)	1.303 (5.0)	3.197 (0.3)	−8.521 (2.3)	8.331 (4.1)
5.7	1.292 (8.9)	3.217 (3.1)	−8.678 (4.2)	8.310 (12.3)	1.196 (4.1)	3.129 (2.4)	−8.359 (4.2)	7.484 (6.4)
5.8	1.182 (4.4)	3.135 (3.0)	−8.430 (5.5)	7.414 (7.5)	1.092 (3.6)	3.046 (0.004)	−8.087 (1.3)	6.654 (3.5)
5.9	1.081 (0.2)	3.040 (1.9)	−8.074 (4.6)	6.574 (1.8)	0.996 (8.0)	2.951 (1.0)	−7.717 (0.05)	5.880 (9.0)

6	0.991 (1.8)	2.935 (0.9)	−7.633 (2.6)	5.819 (0.9)	**0.911 (9.8)**	2.847 (2.1)	−7.273 (2.3)	5.189 (11.7)
…								
10^{21}	2	0	4	0	1.95	0.2615	3.7341	1.0198
…								
10^{22}	2	0	4	0	1.95	0.2615	3.7341	1.0198
E in eV	n (RD%)	κ (RD%)	ε_1 (RD%)	ε_2 (RD%)	n_{FB} (RD%)	κ_{FB} (RD%)	$\varepsilon_{1(FB)}$ (RD%)	$\varepsilon_{2(FB)}$ (RD%)

Table 3b. In the P-Si system, at T=0K, our numerical results of the following optical coefficients, expressed as functions of E, and calculated using Equations (24, 25, 28, 29), for $\mathbb{E}_{gn}(r_P) = \mathbb{E}_{gni}(r_P)[=1.1689$ eV], and the corresponding ones, obtained from the FB-model [11], are reported in the following Table 2a, in which the relative deviations (RDs) of those are also given and calculated, for $1.5 \leq E(eV) \leq 6$, using the Aspnes-and-Studna (AS)-data [9]. Here, as noted in above Table 2c, one obtains: $\propto_{\infty}(E \to \infty, \mathrm{r_P}) = 1.7122 \times 10^9\ cm^{-1}$ and $\sigma_{0,\infty}(E \to \infty, \mathrm{r_P}) = 7.2548 \times 10^5 \left(\frac{1}{\Omega \times cm}\right)$, while, in the FB-model, $\propto_{FB} \to \infty$, and $\sigma_{O(FB)} \to \infty$, which should be not correct.

E in eV	$\propto (10^3 \times cm^{-1})$; RD%	R; RD%	$\sigma_O \left(\frac{1}{\Omega \times cm}\right)$	$\sigma_{O(FB)} \left(\frac{1}{\Omega \times cm}\right)$	$\propto_{FB}(10^3 \times cm^{-1})$; RD%	R_{FB}; RD%
1.5	**0.418; 46.4%**	0.3200; 2.1%	0.3186	0.5110	0.684; 12.3%	**0.3125; 4.4%**
1.6	0.807; 35.4%	0.3259; 1.5%	0.6241	0.8893	1.173; 6.2%	0.3184; 3.8%
1.7	1.392; 22.7%	0.3321; 0.9%	1.0937	1.4525	1.872; 4.0 %	0.3246; 3.1%
1.8	2.231; 6.2%	0.3387; 0.4%	1.7837	2.2277	2.841; 19.4 %	0.3321; 2.6%
1.9	3.401; 7.9 %	0.3456; 0.2%	2.7680	3.3197	4.157; 32.0 %	0.3383; 1.9%
2	4.994; 11.7 %	0.3530; 0.6%	4.1440	4.8168	5.916; 32.4 %	0.3457; 1.5%
2.1	7.134; 12.9 %	0.3609; 1.1%	6.0425	6.8509	8.242; 30.4 %	0.3537; 0.9%
2.2	9.979; 39.2 %	0.3694; 1.5%	8.6404	9.6004	**11.297; 57.5 %**	0.3623; 0.5%
2.3	13.741; 22.8 %	0.3785; 1.7%	12.182	13.311	15.293; 36.7 %	0.3715; 0.1%
2.4	18.705; 27.7 %	0.3883; 2.2%	17.012	18.328	20.522; 40.1 %	0.3814; 0.4%
2.5	25.265; 36.7 %	0.3989; 2.3%	23.625	25.150	27.383; 48.2 %	0.3922; 0.5%
2.6	33.986; 42.7 %	0.4105; 2.6%	32.758	34.517	36.447; 53.1 %	0.4039; 1.0%
2.7	45.703; 28.3 %	0.4233; 2.7%	45.549	47.570	48.564; 36.3 %	0.4169; 1.2%
2.8	61.719; 33.5 %	0.4375; 2.7%	63.843	66.165	65.054; 40.7 %	0.4313; 1.2%
2.9	84.199; 40.9 %	0.4535; 2.6%	90.832	93.513	88.121; 47.5 %	0.4476; 1.3%
3	117.09; 43.3 %	0.4718; 2.3%	132.55	135.69	121.78; 49.0%	0.4663; 1.1%
3.1	168.51; 38.6 %	0.4935; 1.5%	201.87	205.72	174.36; 43.4%	0.4885; 0.5%
3.2	258.32; 26.5 %	0.5202; 0.4%	331.13	336.52	266.32; 30.4%	0.5158; 0.4%
3.3	444.54; 0.6 %	0.5542; 1.2%	615.00	626.05	458.68; 3.8%	0.5509; 1.8%
3.4	840.79; 9.8 %	0.5874; 0.8%	1181.0	1215.6	878.58; 5.7%	0.5874; 0.8%
3.5	1027.3; 3.9 %	0.5708; 0.7%	1228.7	1246.3	1066.0; 0.3%	0.5721; 0.5%
3.6	1031.8; 5.3 %	0.5633; 0.1%	1205.9	1200.7	1053.5; 3.3%	0.5617; 0.4%
3.7	1164.4; 1.5 %	0.5731; 1.8%	1327.9	1313.4	1183.4; 3.2%	0.5717; 1.5%
3.8	1235.4; 0.8 %	0.5720; 0.7%	1345.2	1320.7	1249.6; 2.0%	0.5702; 0.4%
3.9	1286.3; 2.7 %	0.5745; 0.4%	1399.2	1365.2	1294.5; 2.1%	0.5718; 0.9%
4	1429.8; 1.7 %	0.5928; 0.3%	1592.7	1548.1	1433.7; 1.4%	0.5899; 0.2%
4.1	1686.9; 2.0 %	0.6223; 1.3%	1880.1	1821.8	1687.7; 2.1%	0.6203; 1.0%
4.2	2006.6; 1.6 %	0.6564; 0.7%	2103.6	2030.4	2004.7; 1.5%	0.6561; 0.6%
4.3	2279.4; 3.1 %	0.6901; 1.8%	2060.6	1976.1	2274.0; 3.3%	0.6918; 1.6%
4.4	2396.8; 0.6 %	0.7179; 1.1%	1725.7	1638.5	2386.4; 0.1%	0.7217; 0.6%
4.5	2346.5; 1.2 %	0.7339; 0.8%	1311.6	1229.5	2330.4; 0.5%	0.7395; 0.07%
4.6	2205.9; 1.1 %	0.7338; 1.1%	1002.4	928.16	2184.7; 0.2%	0.7408; 0.2%
4.7	2055.2; 0.8 %	0.7187; 1.3%	825.37	757.95	2030.0; 0.4%	0.7262; 0.2%
4.8	1935.8; 0.1 %	0.6954; 2.1%	738.28	675.34	1907.5; 1.5%	0.7025; 1.0%
4.9	1858.0; 0.2 %	0.6720; 3.0%	700.02	639.53	1827.0; 1.9%	0.6782; 2.1%

5	1817.7; 0.6 %	**0.6540; 3.1%**	684.66	627.27	1784.1; 1.2%	0.6591; 2.3%
5.1	1805.7; 1.9 %	0.6433; 2.2%	677.05	618.03	1769.4; 0.2%	0.6475; 1.6%
5.2	1812.1; 2.5 %	0.6394; 1.0%	668.08	609.28	1773.1; 0.3 %	0.6429; 0.5%
5.3	1827.7; 1.5 %	0.6407; 0.9%	652.43	594.12	1786.0; 0.8 %	0.6439; 0.5%
5.4	1845.0; 0.1 %	0.6457; 2.6%	627.65	570.38	1800.6; 2.3 %	0.6487; 2.2%
5.5	1858.0; 0.9 %	0.6528; 3.0%	693.75	538.17	1811.3; 1.6 %	0.6559; 2.5%
5.6	1863.0; 2.4 %	0.6608; 2.1%	552.55	499.32	1814.1; 0.3%	0.6642; 1.6%
5.7	1858.0; 3.1 %	0.6688; 0.6%	506.98	456.62	1807.3; 0.3%	0.6726; 0.06%
5.8	1842.7; 2.9 %	0.6759; 0.6%	460.23	413.08	1790.5; 003%	0.6801; 1.2%
5.9	1817.7; 1.9 %	0.6814; 1.2%	415.13	371.32	1764.5; 1.1%	0.6861; 1.9%
6	1784.8; 0.9 %	0.6848; 1.2%	373.72	333.21	1730.9; 2.2%	0.6899; 1.9%
…						
10^{21}	1.7122×10^6	0.1111	7.2548×10^5	$\mathbf{1.0916 \times 10^{22}}$	$\mathbf{2.65 \times 10^{22}}$	0.1107
…						
10^{22}	1.7122×10^6	0.1111	7.2548×10^5	$\mathbf{1.0916 \times 10^{23}}$	$\mathbf{2.65 \times 10^{23}}$	0.1107
E in eV	$\propto (10^3 \times cm^{-1})$; RD%	R; RD%	$\sigma_O \left(\frac{1}{\Omega \times cm}\right)$	$\sigma_{O(FB)} \left(\frac{1}{\Omega \times cm}\right)$	$\propto_{FB}(10^3 \times cm^{-1})$; RD%	R_{FB}; RD%

Table 3c. Here, our maximal relative deviation (MRD)-values and those of $(\mathrm{MRD})_{\mathrm{FB}}$ are reported, suggesting that our obtained numerical results of these optical coefficients are found be more accurate than the corresponding ones, obtained from the FB-model.

MRD	n	κ	ε_1	ε_2	$\propto$	R
E (eV)						
1.5		45%		**47.8%**	46.4%	
4.3			27.1%			
5	13.6%					3.1%

$(MRD)_{FB}$	n_{FB}	κ_{FB}	$\varepsilon_{1(FB)}$	$\varepsilon_{2(FB)}$	$\propto_{FB}$	R_{FB}
E (eV)						
1.5						4.4%
2.2		58.3%		56.8%	57.5%	
4.2			**66.1%**			
6	9.8%					

Some important cases, given in various physical conditions, are considered as follows.

5.1. Metal-insulator transition (MIT)-case

As discussed in Equations (21-23) and Eq. (A4) of the Appendix A, the physical conditions used for the MIT are: T=0K, $N^* = 0$ or $N = N_{CDn(CDp)} \cong N^{EBT}_{CDn(CDp)}$, vanishing the Fermi energy: $\mathbb{E}_{Fno(Fpo)}(N^*) \equiv \frac{\hbar^2 \times k^2_{Fn(Fp)}(N^*)}{2\times m^*_{n(p)}}$=0. Further, from the discussions given Eq. (5) for the optical band gap:

$\mathbb{E}_{gn1(gp1)}(N^* = 0, r_{d(a)}, T = 0) = \mathbb{E}_{gnei(gpei)}(r_{d(a)}) = \mathbb{E}_{gni(gpi)}(r_{d(a)})$, according also to the MIT.

Then, in this MIT-case, replacing both $\mathbb{E}_{gnei(gpei)}$ and $\mathbb{E}_{gn1(gp1)}$, by $\mathbb{E}_{gni(gpi)}$, given in Equations (28, 29), and consequently from Eq. (24), one gets, for the effective photon energy $E^* \equiv E - \mathbb{E}_{gni(gpi)} = 0$:

$\kappa(E^*, r_{d(a)}) = 0$, $\varepsilon_2(E^*, r_{d(a)}) = 0$, $\sigma_O(E^*, r_{d(a)}) = 0$ and $\alpha(E^*, r_{d(a)}) = 0$, corresponding also to the MIT. Thus, in this case, the photon energy E becomes the critical photon energy, defined by:

$E_{CPE}(r_{d(a)}) \equiv \mathbb{E}_{gni(gpi)}(r_{d(a)})$. Therefore, Equations (28, 29), obtained in the MIT-case, become:

$$\kappa(E^* = 0) = f(E_{gni(gpi)}) \times (E^* \equiv E_{CPE} - \mathbb{E}_{gni(gpi)} = 0)^2 = 0, \quad (30)$$

$$n(E = \mathbb{E}_{gni(gpi)}) = n_\infty + \sum_{i=1}^{4} \frac{B_{oi}E + C_{oi}}{E^2 - B_i E + C_i}, \text{ in which } \mathbb{E}_{gnei(gpei)} = \mathbb{E}_{gni(gpi)}. \quad (31)$$

Then, going back to the remark given in Eq. (23), we can determine the values of some optical coefficients for $\mathbb{E} \leq 0$, representing the exponential tail-states, which can be deduced from Eq. (30), by putting: $E^* = \mathbb{E}_{gni(gpi)}(r_{d(a)})$, as:

$$\kappa^{EEC-T}(\mathbb{E}_{gni(gpi)}) = f(\mathbb{E}_{gni(gpi)}) \times \mathbb{E}^2_{gni(gpi)}. \quad (32)$$

Now, replacing Equations (31, 32) into Equations (24, 25), one obtains for $\mathbb{E} \leq 0$ the expressions, obtained for the following exponential tail-states of ε_2, $\sigma_O(E)$, α, and R as:

$$\varepsilon_2^{EImDC-T}(\mathbb{E}_{gni(gpi)}) = 2 \times \kappa^{EEC-T}(\mathbb{E}_{gni(gpi)}) \times n(E = \mathbb{E}_{gni(gpi)}), \quad (33)$$

$$\sigma_O^{EOC-T}(\mathbb{E}_{gni(gpi)}) = \frac{\varepsilon_{free\ space} \times \mathbb{E}_{gni(gpi)} \times \varepsilon_2^{EImD-T}(\mathbb{E}_{gni(gpi)})}{4\pi\hbar}, \quad (34)$$

$$\alpha^{EOAC-T}(\mathbb{E}_{gni(gpi)}) = \frac{2\times \mathbb{E}_{gni(gpi)} \times \kappa^{EEC-T}(\mathbb{E}_{gni(gpi)})}{\hbar \times c}, \text{ and} \quad (35)$$

$$R^{NIR-T}(\mathbb{E}_{gni(gpi)}) = \frac{[n(\mathbb{E}_{gni(gpi)}) - 1]^2 + \kappa^{EEC-T}(\mathbb{E}_{gni(gpi)})^2}{[n(\mathbb{E}_{gni(gpi)}) + 1]^2 + \kappa^{EEC-T}(\mathbb{E}_{gni(gpi)})^2}. \quad (36)$$

The numerical results of those optical functions, determined by Equations (31-36, 24), were discussed and reported in the above Table 2b.

5.2. Extrema values of $\varepsilon_{1(2)}$ as functions of photon energy E

From Equations (24, 28, 29), we can determine the extrema values of typical optical functions $\varepsilon_{1(2)}(E, r_{d(a)})$ in following physical conditions by: T=0K and $N = N_{CDn(NDp)}$, and by: T=20K and $N = 1.5(1.7) \times 10^{20} cm^{-3}$, respectively, as given in following Tables 4n and 4p, in which the arrows (↑↓) indicates the maximum, and (↓↑) the minimum and the extrema-values of those occur at the same corresponding photon energy E.

Table 4n. In d-Si systems, and for two types of physical conditions such as: (T=0K and $N = N_{CDn}(r_d)$) and (T=20K, $N = 1.5 \times 10^{20}\ cm^{-3}$), the extrema values of $\varepsilon_1(E)$ and $\varepsilon_2(E)$, calculated using Equations (24, 28, 29), vary with increasing E, represented by the arrows: ↑ or ↓ , suggesting that their extrema occur at the same E.

E in eV	3	**3.34**	**3.44**	**3.56**	**3.712**	**3.87**	**4.215**	**4.5**	10	100	10^{21}
In the P-Si system, at T=0K and N = $N_{CDn}(r_P) = 3.52 \times 10^{18}$ cm^{-3}, $\mathbb{E}_{gn}(r_P) \equiv \mathbb{E}_{gni}(r_P)$[= 1.1689 eV]											
$\varepsilon_1(E)$	28.57	↑ 42.11	↓ 31.22	22.72	18.98	15.88	0.72	↓ −19.47	↑ 0.73	3.71	4
$\varepsilon_2(E)$	4.13	22.81	↑ 35.58	↓ 30.81	↑ 33.60	↓ 33.06	↑ 46.95	↓ 27.23	2.03	1.19	0
In the As-Si system, at T=0K and N = $N_{CDn}(r_{As}) = 3.6955 \times 10^{18}$ cm^{-3}, $\mathbb{E}_{gn}(r_{As}) \equiv \mathbb{E}_{gni}(r_{As})$[= 1.1170 eV]											
$\varepsilon_1(E)$	28.37	↑ 41.85	↓ 31.00	22.53	18.81	15.71	0.58	↓ −19.52	↑ 0.69	3.65	3.9356
$\varepsilon_2(E)$	4.11	22.72	↑ 35.44	↓ 30.68	↑ 33.46	↓ 32.92	↑ 46.75	↓ 27.05	2.01	1.18	0
In the Te-Si system, at T=0K and N = $N_{CDn}(r_{Te}) = 4.59924 \times 10^{18}$ cm^{-3}, $\mathbb{E}_{gn}(r_{Te}) \equiv \mathbb{E}_{gni}(r_{Te})$[= 1.1750 eV]											
$\varepsilon_1(E)$	27.51	↑ 40.74	↓ 30.03	21.72	18.05	15.01	0.005	↓ −19.72	↑ 0.54	3.38	3.6589
$\varepsilon_2(E)$	4.02	22.32	↑ 34.81	↓ 30.11	↑ 32.84	↓ 2.30	↑ 45.87	↓ 26.27	1.89	1.13	0
In the Sb-Si system, at T=0K and N = $N_{CDn}(r_{Sb}) = 5.20648 \times 10^{18}$ cm^{-3}, $\mathbb{E}_{gn}(r_{Sb}) \equiv \mathbb{E}_{gni}(r_{Sb})$[= 1.1787 eV]											
$\varepsilon_1(E)$	27.02	↑ 40.09	↓ 29.50	21.28	17.64	14.62	−0.29	↓ −19.80	↑ 0.45	3.23	3.5107
$\varepsilon_2(E)$	3.97	22.08	↑ 34.43	↓ 29.77	↑ 32.47	↓ 31.94	↑ 45.35	↓ 25.83	1.83	1.11	0
In the Sn-Si system, at T=0K and N = $N_{CDn}(r_{Sn}) = 6.01115 \times 10^{18}$ cm^{-3}, $\mathbb{E}_{gn}(r_{Sn}) \equiv \mathbb{E}_{gni}(r_{Sn})$[= 1.1829 eV]											
$\varepsilon_1(E)$	26.47	↑ 39.37	↓ 28.89	20.78	17.17	14.20	−0.62	↓ −19.87	↑ 0.37	3.07	3.3465
$\varepsilon_2(E)$	3.91	21.80	↑ 33.99	↓ 29.38	↑ 32.05	↓ 31.52	↑ 44.77	↓ 25.33	1.75	1.08	0

E in eV	3	**3.34**	**3.44**	**3.56**	**3.712**	**3.87**	**4.215**	**4.5**	10	100	10^{21}
In the P-Si system, at T=20K and N = 1.5×10^{20} cm^{-3}, $\mathbb{E}_{gn}(r_P) \equiv \mathbb{E}_{gn1}(r_P)$[= 1.1467 eV]											
$\varepsilon_1(E)$	28.57	↑ 41.99	↓ 30.91	22.43	18.64	15.53	0.04	↓ −20.19	↑ 0.72	3.71	4
$\varepsilon_2(E)$	4.23	23.28	↑ 36.28	↓ 31.39	↑ 34.20	↓ 33.61	↑ 47.64	↓ 27.59	2.04	1.19	0
In the As-Si system, at T=20K and N = 1.5×10^{20} cm^{-3}, $\mathbb{E}_{gn}(r_{As}) \equiv \mathbb{E}_{gn1}(r_{As})$[= 1.144eV]											
$\varepsilon_1(E)$	28.37	↑ 41.72	↓ 30.64	22.20	18.41	15.32	−0.196	↓ −20.34	↑ 0.68	3.65	3.9356
$\varepsilon_2(E)$	4.22	23.26	↑ 36.24	↓ 31.34	↑ 34.14	↓ 33.55	↑ 47.54	↓ 27.47	2.02	1.18	0
In the Te-Si system, at T=20K and N = 1.5×10^{20} cm^{-3}, $\mathbb{E}_{gn}(r_{Te}) \equiv \mathbb{E}_{gn1}(r_{Te})$[= 1.1346 eV]											
$\varepsilon_1(E)$	27.50	↑ 40.52	↓ 29.45	21.19	17.42	14.37	−1.24	↓ −21.02	↑ 0.52	3.38	3.6589
$\varepsilon_2(E)$	4.20	23.17	↑ 36.07	↓ 31.14	↑ 33.90	↓ 33.28	↑ 47.10	↓ 26.91	1.91	1.14	0
In the Sb-Si system, at T=20K and N = 1.5×10^{20} cm^{-3}, $\mathbb{E}_{gn}(r_{Sb}) \equiv \mathbb{E}_{gn1}(r_{Sb})$[= 1.129 eV]											
$\varepsilon_1(E)$	27.01	↑ 39.84	↓ 28.79	20.63	16.87	13.85	−1.81	↓ −21.387	↑ 0.44	3.23	3.5107
$\varepsilon_2(E)$	4.19	23.10	↑ 35.95	↓ 31.01	↑ 33.75	↓ 33.12	↑ 46.84	↓ 26.60	1.85	1.11	0
In the Sn-Si system, at T=20K and N = 1.5×10^{20} cm^{-3}, $\mathbb{E}_{gn}(r_{Sn}) \equiv \mathbb{E}_{gn1}(r_{Sn})$[= 1.123 eV]											
$\varepsilon_1(E)$	26.46	↑ 39.05	↓ 28.02	19.99	16.23	13.26	−2.47	↓ −21.81	↑ 0.35	3.07	3.3465
$\varepsilon_2(E)$	4.18	23.03	↑ 35.82	↓ 30.88	↑ 33.59	↓ 32.94	↑ 46.56	↓ 26.25	1.78	1.08	0
E in eV	3	**3.34**	**3.44**	**3.56**	**3.712**	**3.87**	**4.215**	**4.5**	10	100	10^{21}

Table 4p. In a-Si systems, and for two types of physical conditions such as: (T=0K and $\mathrm{N} = \mathrm{N_{CDp}(r_a)}$) and (T=20K, $\mathrm{N} = 1.5\,\mathrm{x}10^{20}\ \mathrm{cm}^{-3}$), the extrema values of $\varepsilon_1(E)$ and $\varepsilon_2(E)$, calculated using Equations (24, 28, 29), vary with increasing E, represented by the arrows: ↑ or ↓ , suggesting that their extrema occur at the same E.

E in eV	3	**3.34**	**3.44**	**3.56**	**3.712**	**3.87**	**4.215**	**4.5**	10	100	10^{21}
In the B-Si system, at T=0K and $\mathrm{N} = \mathrm{N_{CDp}(r_B)} = 4.06\,\mathrm{x}10^{18}\ \mathrm{cm}^{-3}$, $\mathbb{E}_{gp}(\mathrm{r_B}) \equiv \mathbb{E}_{gpi}(\mathrm{r_B})[= 1.1512\ \mathrm{eV}]$											
$\varepsilon_1(E)$	32.85	↑ 47.57	↓ 36.05	26.82	22.88	19.54	3.88 ↓	−18.13 ↑	1.65	5.19	5.5179
$\varepsilon_2(E)$	4.51	24.57	↑ 38.40	↓ 33.42	↑ 36.46	↓ 35.92	↑ 51.05	↓ 31.06	2.62	1.40	0
In the Ga-Si system, at T=0K and $\mathrm{N} = \mathrm{N_{CDp}(r_{Ga})} = 1.2119\,\mathrm{x}10^{19}\ \mathrm{cm}^{-3}$, $\mathbb{E}_{gp}(\mathrm{r_{Ga}}) \equiv \mathbb{E}_{gpi}(\mathrm{r_{Ga}})[= 1.1721\ \mathrm{eV}]$											
$\varepsilon_1(E)$	28.05	↑ 41.43	↓ 30.64	22.23	18.53	15.45	0.37 ↓	−19.59 ↑	0.63	3.55	3.8323
$\varepsilon_2(E)$	4.08	22.57	↑ 35.20	↓ 30.46	↑ 33.23	↓ 32.68	↑ 46.42	↓ 26.76	1.96	1.16	0
In the Mg-Si system, at T=0K and $N = \mathrm{N_{CDp}(r_{Mg})} = 1.82\,\mathrm{x}10^{19}\ \mathrm{cm}^{-3}$, $\mathbb{E}_{gp}(\mathrm{r_{Mg}}) \equiv \mathbb{E}_{gpi}(\mathrm{r_{Mg}})[= 1.1847eV]$											
$\varepsilon_1(E)$	26.44	↑ 39.32	↓ 28.86	20.77	17.17	14.20	−0.58 ↓	−19.81 ↑	0.37	3.07	3.3465
$\varepsilon_2(E)$	3.90	21.75	↑ 33.91	↓ 29.31	↑ 31.99	↓ 31.46	↑ 44.70	↓ 25.31	1.75	1.08	0
In-Si system, at T=0K and $\mathrm{N} = \mathrm{N_{CDp}(r_{In})} = 2.133\,\mathrm{x}10^{19}\ \mathrm{cm}^{-3}$, $\mathbb{E}_{gp}(\mathrm{r_{In}}) \equiv \mathbb{E}_{gpi}(\mathrm{r_{In}})[= 1.1906\ \mathrm{eV}]$											
$\varepsilon_1(E)$	25.82	↑ 38.50	↓ 28.19	20.23	16.68	13.75	−0.90 ↓	−19.85 ↑	0.28	2.91	3.1741
$\varepsilon_2(E)$	3.83	21.41	↑ 33.39	↓ 28.85	↑ 31.49	↓ 30.98	↑ 44.02	↓ 24.76	1.68	1.05	0
E in eV	3	**3.34**	**3.44**	**3.56**	**3.712**	**3.87**	**4.215**	**4.5**	10	100	10^{21}
In the B-Si system, at T=20K and $\mathrm{N} = 1.7\,\mathrm{x}10^{20}\ \mathrm{cm}^{-3}$, $\mathbb{E}_{gp}(\mathrm{r_B}) \equiv \mathbb{E}_{gp1}(\mathrm{r_B})[= 1.193\ \mathrm{eV}]$											
$\varepsilon_1(E)$	32.87	↑ 47.80	↓ 36.65	27.37	23.53	20.19	5.15 ↓	−16.80 ↑	1.67	5.19	5.5179
$\varepsilon_2(E)$	4.31	23.64	↑ 37.01	↓ 32.27	↑ 35.28	↓ 34.82	↑ 49.67	↓ 30.29	2.60	1.40	0
In the Ga-Si system, at T=20K and $\mathrm{N} = 1.7\,\mathrm{x}10^{20}\ \mathrm{cm}^{-3}$, $\mathbb{E}_{gp}(\mathrm{r_{Ga}}) \equiv \mathbb{E}_{gp1}(\mathrm{r_{As}})[= 1.119\mathrm{eV}]$											
$\varepsilon_1(E)$	28.04	↑ 41.14	↓ 29.86	21.52	17.68	14.61	−1.28 ↓	−21.32 ↑	0.62	3.55	3.8323
$\varepsilon_2(E)$	4.32	23.69	↑ 36.88	↓ 31.84	↑ 34.64	↓ 33.99	↑ 48.06	↓ 27.63	2.00	1.16	0
In the Mg-Si system, at T=20K and $\mathrm{N} = 1.7\,\mathrm{x}10^{20}\ \mathrm{cm}^{-3}$, $\mathbb{E}_{gp}(\mathrm{r_{Mg}}) \equiv \mathbb{E}_{gp1}(\mathrm{r_{Mg}})[= 1.089\mathrm{eV}]$											
$\varepsilon_1(E)$	26.41	↑ 38.79	↓ 27.45	19.48	15.65	12.68	−3.57 ↓	−22.94 ↑	0.34	3.07	3.3465
$\varepsilon_2(E)$	4.32	23.72	↑ 36.85	↓ 31.72	↑ 34.45	↓ 33.74	↑ 47.56	↓ 26.79	1.79	1.09	0
In the In-Si system, at T=20K and $\mathrm{N} = 1.7\,\mathrm{x}10^{20}\ \mathrm{cm}^{-3}$, $\mathbb{E}_{gp}(\mathrm{r_{In}}) \equiv \mathbb{E}_{gp1}(\mathrm{r_{In}})[= 1.078\mathrm{eV}]$											
$\varepsilon_1(E)$	25.79	↑ 37.88	↓ 26.52	18.70	14.87	11.95	−4.44 ↓	−23.55 ↑	0.24	2.91	3.1741
$\varepsilon_2(E)$	4.32	23.72	↑ 36.82	↓ 31.66	↑ 34.37	↓ 33.64	↑ 47.36	↓ 26.48	1.72	1.06	0
E in eV	3	**3.34**	**3.44**	**3.56**	**3.712**	**3.87**	**4.215**	**4.5**	10	100	10^{21}

5.3. Variations of various optical coefficients as functions of N, typically for some d(a)-Si systems

Also, from Equations (24, 28, 29), we can determine the variations of various optical coefficients at 20K, as functions of N, typically for E=3.34 eV and for some (P, Te, Sn)-Si systems and (B, Ga, In)-Si ones, being indicated by the arrows: ↗ and ↘ , as tabulated in following Tables 5n and 5p, in which the physical condition $\mathrm{N} > \mathrm{N_{CDn(NDp)}}$ (or $\mathrm{N}^* > 0$) must be respected, and their variations thus depend on the ones of the optical band gap, $\mathbb{E}_{gn1(gp1)}(\mathrm{N}^*, \mathrm{r_{d(a)}})$.

Table 5n. In (P, Te, Sn)-Si systems, our numerical results of the following optical coefficients, expressed as functions of N, and calculated using Equations (31-36, 24), for E=3.34 eV and T=20K, present the variations by arrows, (↘ and ↗), since those of the optical gap $\mathbb{E}_{gn1}(N^*, r_d)$, are presented by (↗ and ↘) or by (↘ and ↗).

$N\ (10^{18}\ cm^{-3})$	4		8.5		15		50		80		150
$\mathbb{E}_{gn1}(N^*, r_P, 20K)$ in eV	1.1489	↘	1.1294	↘	1.1219	↘	1.1184	↗	1.1248	↗	1.1467
$n(r_P)$=6.7086											
$\kappa(N, r_P)$	1.732	↗	1.763	↗	1.774	↗	1.780	↘	1.770	↘	1.735
$\varepsilon_1(N, r_P)$	42.007	↘	41.898	↘	41.856	↘	41.836	↗	41.873	↗	41.995
$\varepsilon_2(N, r_P)$	23.233	↗	23.649	↗	23.809	↗	23.885	↘	23.746	↘	23.279
$\sigma_O(N, r_P)$ in $10^2\ \Omega^{-1}cm^{-1}$	8.306	↗	8.454	↗	8.511	↗	8.539	↘	8.489	↘	8.322
$\propto (N, r_P)$ in $10^5\ cm^{-1}$	5.861	↗	5.966	↗	6.006	↗	6.025	↘	5.990	↘	5.873
$R(N, r_P)$	0.570	↗	0.571	↗	0.5711	↗	0.5713	↘	0.571	↘	0.5702
$\mathbb{E}_{gn1}(N^*, r_{Te}, 20K)$ in eV			1.1334	↘	1.1225	↘	1.1132	↗	1.117	↗	1.135
$n(r_{Te})$=6.6031											
$\kappa(N, r_{Te})$			1.756	↗	1.773	↗	1.788	↘	1.782	↘	1.754
$\varepsilon_1(N, r_{Te})$			40.517	↘	40.456	↘	40.402	↗	40.424	↗	40.524
$\varepsilon_2(N, r_{Te})$			23.192	↗	23.421	↗	23.619	↘	23.538	↘	23.168
$\sigma_O(N, r_{Te})$ in $10^2\ \Omega^{-1}cm^{-1}$			8.291	↗	8.373	↗	8.443	↘	8.415	↘	8.282
$\propto (N, r_{Te})$ in $10^5\ cm^{-1}$			5.944	↗	6.003	↗	6.053	↘	6.033	↘	5.938
$R(N, r_{Te})$			0.566	↗	0.5667	↗	0.5671	↘	0.5669	↘	0.5662
$\mathbb{E}_{gn1}(N^*, r_{Sn}, 20K)$ in eV			1.1421	↘	1.1256	↘	1.1092	↗	1.1101	↗	1.123
$n(r_{Sn})$=6.4960											
$\kappa(N, r_{Sn})$			1.742	↗	1.769	↗	1.7949	↘	1.7935	↘	1.773
$\varepsilon_1(N, r_{Sn})$			39.163	↘	39.071	↘	38.977	↗	38.982	↗	39.056
$\varepsilon_2(N, r_{Sn})$			22.637	↗	22.978	↗	23.319	↘	23.301	↘	23.032
$\sigma_O(N, r_{Sn})$ in $10^2\ \Omega^{-1}cm^{-1}$			8.092	↗	8.214	↗	8.336	↘	8.330	↘	8.234
$\propto (N, r_{Sn})$ in $10^5\ cm^{-1}$			5.897	↗	5.986	↗	6.075	↘	6.070	↘	6.000
$R(N, r_{Sn})$			0.5613	↗	0.562	↗	0.5626	↘	0.5625	↘	0.5621
$N\ (10^{18}\ cm^{-3})$	4		8.5		15		50		80		150

Table 5p. In (B, Ga, In)-Si systems, the numerical results of the following optical coefficients, expressed as functions of N, and calculated using Equations (31-36, 24), for E=3.34eV and T=20K, present the variations by arrows, (↘ and ↗), since those of the optical gap $\mathbb{E}_{gp1}(N^*, r_a)$, are presented by (↗ and ↘) or by (↘ and ↗).

$N\ (10^{18}\ cm^{-3})$	6.5		11		15		26		60		170
$\mathbb{E}_{gp1}(N^*, r_B, 20K)$ in eV	1.120	↘	1.113	↘	1.111	↘	1.112	↗	1.127	↗	1.193
$n(r_B)$=7.1111											
$\kappa(N, r_B)$	1.777	↗	1.789	↗	1.7917	↘	1.7907	↘	1.766	↘	1.662

$\varepsilon_1(N, r_B)$	47.408	↘	47.368	↘	47.357	↗	47.361	↗	47.448	↗	47.804
$\varepsilon_2(N, r_B)$	25.279	↗	25.439	↗	25.482	↘	25.467	↘	25.121	↘	23.642
$\sigma_O(N, r_B)$ in $10^2\ \Omega^{-1}cm^{-1}$	9.037	↗	9.094	↗	9.109	↘	9.104	↘	8.981	↘	8.452
$\propto (N, r_B)$ in $10^5\ cm^{-1}$	6.016	↗	6.054	↗	6.0644	↘	6.061	↘	5.979	↘	5.627
$R(N, r_B)$	0.5875	↗	0.5877	↗	0.5878	↘	0.5877	↘	0.5872	↘	0.5851
$\mathbb{E}_{gp1}(N^*, r_{Ga}, 20K)$ in **eV**					1.121	↘	1.098	↘	1.088	↗	1.119
$n(r_{Ga})=6.6568$											
$\kappa(N, r_{Ga})$					1.7756	↗	1.8128	↗	1.8283	↘	1.780
$\varepsilon_1(N, r_{Ga})$					41.1598	↘	41.0261	↘	40.9697	↗	41.145
$\varepsilon_2(N, r_{Ga})$					23.639	↗	24.135	↗	24.3416	↘	23.694
$\sigma_O(N, r_{Ga})$ in $10^2\ \Omega^{-1}cm^{-1}$					8.451	↗	8.628	↗	8.702	↘	8.470
$\propto (N, r_{Ga})$ in $10^5\ cm^{-1}$					6.0098	↗	6.136	↗	6.188	↘	6.024
$R(N, r_{Ga})$					0.5690	↗	0.5699	↗	0.5703	↘	0.569
$\mathbb{E}_{gp1}(N^*, r_{In}, 20K)$ in eV							1.118	↘	1.074	↗	1.078
$n(r_{In})=6.4254$											
$\kappa(N, r_{In})$							1.7806	↗	1.8511	↘	1.846
$\varepsilon_1(N, r_{In})$							38.115	↘	37.859	↗	37.879
$\varepsilon_2(N, r_{In})$							22.882	↗	23.788	↘	23.7185
$\sigma_O(N, r_{In})$ in $10^2\ \Omega^{-1}cm^{-1}$							8.181	↗	8.504	↘	8.479
$\propto (N, r_{In})$ in $10^5\ cm^{-1}$							6.027	↗	6.265	↘	6.247
$R(N, r_{In})$							0.5592	↗	0.5611	↘	0.5610
$N\ (10^{18}\ cm^{-3})$	6.5		11		15		26		60		170

5.4. Variations of various optical coefficients as functions of T, typically for some d(a)-Si systems

Here, from Equations (24, 28, 29), we can determine the variations of various optical coefficients at $N = 1.5(3) \times 10^{19} cm^{-3}$, respectively, as functions of T, typically for E=3.34 eV and for some (P, Te, Sn)-Si systems and (B, Ga, In)-Si ones, being indicated by the arrows: ↗ and ↘ , as given in following Tables 6n and 6p, in which their variations thus depend on the ones of the reduced Fermi energy, $\xi_{n(p)}(r_{d(a)}, T)$.

Table 6n. In (P, Te, Sn)-Si systems, our numerical results of the following optical coefficients, expressed as functions of T, and calculated using Equations (31-36, 24), for E=3.34eV and $N = 1.5 \times 10^{19}\ cm^{-3}$, increase with increasing T, since the optical band gap $\mathbb{E}_{gn1}(T, r_d)$ decreases with increasing T.

T in K	20	30	50	100	200	300
$\mathbb{E}_{gn} \equiv \mathbb{E}_{gn1}(T, r_P)$ in eV ↘	1.1219	1.1218	1.1212	1.1185	1.1091	1.1024
$n(r_P, T)$ ↗	6.7086	6.7093	6.7118	6.724	6.774	6.8457
$\kappa(r_P, T)$ ↗	1.774	1.7747	1.7756	1.780	1.795	1.8059
$\varepsilon_1(r_P, T)$ ↗	41.856	41.865	41.895	42.049	42.668	43.603
$\varepsilon_2(r_P, T)$ ↗	23.809	23.814	23.835	23.939	24.320	24.725

$\sigma_O(r_P, T)$ in $10^2\ \Omega^{-1}cm^{-1}$ ↗	8.511	8.513	8.521	8.558	8.694	8.8389
$\propto (r_P, T)$ in $10^5\ cm^{-1}$ ↗	6.006	6.007	6.0098	6.0248	6.0757	6.1124
$R(r_P, T)$ ↗	0.5711	0.5712	0.5713	0.5719	0.5744	0.5775
$\mathbb{E}_{gn} \equiv \mathbb{E}_{gn1}(T, r_{Te})$ in eV ↘	1.1225	1.1224	1.1219	1.1192	1.1106	1.1063
$n(r_{Te}, T)$ ↗	6.6031	6.6038	6.606	6.6189	6.6686	6.740
$\kappa(r_{Te}, T)$ ↗	1.773	1.7737	1.774	1.7787	1.7926	1.7996
$\varepsilon_1(r_{Te}, T)$ ↗	40.456	40.464	40.494	40.6458	41.2569	42.189
$\varepsilon_2(r_{Te}, T)$ ↗	23.421	23.426	23.4458	23.5467	23.9077	24.258
$\sigma_O(r_{Te}, T)$ in $10^2\ \Omega^{-1}cm^{-1}$ ↗	8.373	8.3746	8.3816	8.4177	8.5467	8.6721
$\propto (r_{Te}, T)$ in $10^5\ cm^{-1}$ ↗	6.0027	6.0034	6.0062	6.0206	6.0673	6.0911
$R(r_{Te}, T)$ ↗	0.5667	0.5667	0.5668	0.5675	0.5699	0.5731
$\mathbb{E}_{gn} \equiv \mathbb{E}_{gn1}(T, r_{Sn})$ in eV ↘	1.1256	1.1255	1.1250	1.1225	1.1153	1.1152
$n(r_{Sn}, T)$ ↗	6.496	6.4967	6.4992	6.5118	6.5613	6.6326
$\kappa(r_{Sn}, T)$ ↗	1.7686	1.7688	1.7696	1.7735	1.7851	1.7853
$\varepsilon_1(r_{Sn}, T)$ ↗	39.0706	39.0790	39.1082	39.2579	39.8646	40.8037
$\varepsilon_2(r_{Sn}, T)$ ↗	22.9776	22.9828	23.0014	23.0970	23.4256	23.6817
$\sigma_O(r_{Sn}, T)$ in $10^2\ \Omega^{-1}cm^{-1}$ ↗	8.2142	8.2161	8.2227	8.2569	8.3744	8.4659
$\propto (r_{Sn}, T)$ in $10^5\ cm^{-1}$ ↗	5.9862	5.9869	5.9895	6.0027	6.0421	6.0426
$R(r_{Sn}, T)$ ↗	0.5620	0.5620	0.5621	0.5628	0.5652	0.5682
T in K	20	30	50	100	200	300

Table 6p. In (B, Ga, In)-Si systems, our numerical results of the following optical coefficients, expressed as functions of T, and calculated using Equations (31-36, 24), for E=3.34eV and $N = 3 \times 10^{19}\ cm^{-3}$, increase with increasing T, since the optical band gap $\mathbb{E}_{gp1}(T, r_a)$ decreases with increasing T.

T in K	20	30	50	100	**200**	300
$\mathbb{E}_{gp} \equiv \mathbb{E}_{gp1}(T, r_B)$ in eV ↘	1.1130	1.1128	1.1121	1.1085	1.0945	1.0755
$n(r_B, T)$ ↗	7.1111	7.1118	7.1143	7.127	7.177	7.249
$\kappa(r_B, T)$ ↗	1.7888	1.7891	1.7902	1.796	1.8186	1.849
$\varepsilon_1(r_B, T)$ ↗	47.368	47.3769	47.4082	47.568	48.203	49.128
$\varepsilon_2(r_B, T)$ ↗	25.440	25.448	25.472	25.600	26.105	26.813
$\sigma_O(r_B, T)$ in $10^2\ \Omega^{-1}cm^{-1}$ ↗	9.095	9.097	9.106	9.152	9.332	9.585
$\propto (r_B, T)$ in $10^5\ cm^{-1}$ ↗	6.0546	6.0556	6.0594	6.079	6.156	6.260
$R(r_B, T)$ ↗	0.5877	0.5877	0.5879	0.5885	0.5909	0.5943
$\mathbb{E}_{gp} \equiv \mathbb{E}_{gp1}(T, r_{Ga})$ in eV ↘	1.0948	1.0946	1.0939	1.0905	1.0773	1.0603
$n(r_{Ga}, T)$ ↗	6.6568	6.6575	6.6599	6.673	6.722	6.794
$\kappa(r_{Ga}, T)$ ↗	1.8182	1.8185	1.8195	1.825	1.846	1.874
$\varepsilon_1(r_{Ga}, T)$ ↗	41.007	41.015	41.044	41.192	41.780	42.642
$\varepsilon_2(r_{Ga}, T)$ ↗	24.206	24.213	24.236	24.356	24.826	25.470
$\sigma_O(r_{Ga}, T)$ in $10^2\ \Omega^{-1}cm^{-1}$ ↗	8.653	8.656	8.664	8.707	8.875	9.105

$\propto(r_{Ga},T)$ in $10^5\ cm^{-1}$	↗	6.154	6.155	6.1586	6.1774	6.250	6.345
$R(r_{Ga},T)$	↗	0.5701	0.5701	0.5702	0.5709	0.5735	0.5771
$\mathbb{E}_{gp} \equiv \mathbb{E}_{gp1}(T, r_{In})$ in eV	↘	1.1050	1.1049	1.1043	1.0912	1.0773	1.0820
$n(r_{In},T)$	↗	6.4254	6.4261	6.4285	6.441	6.490	6.562
$\kappa(r_{In},T)$	↗	1.8016	1.8019	1.8028	1.8074	1.824	1.839
$\varepsilon_1(r_{In},T)$	↗	38.040	38.048	38.076	38.220	38.800	39.672
$\varepsilon_2(r_{In},T)$	↗	23.152	23.158	23.178	23.283	23.676	24.132
$\sigma_O(r_{In},T)$ in $10^2\ \Omega^{-1}cm^{-1}$	↗	8.276	8.279	8.286	8.323	8.464	8.627
$\propto(r_{In},T)$ in $10^5\ cm^{-1}$	↗	6.098	6.0988	6.102	6.118	6.173	6.224
$R(r_{In},T)$	↗	0.5598	0.5598	0.5599	0.5606	0.5632	0.5666
T in K		20	30	50	100	200	300

6. Concluding remarks

In the n(p)-type degenerate Si-crystal, by using the same physical model, as that given in Eq. (7), and same mathematical methods, as those proposed in I, II and III, and further, by taking into account the corrected values of energy-band-structure parameters, and mainly the correct asymptotic behaviors of the refraction index n and extinction coefficient κ, as the photon energy $E(\to\infty)$, all the numerical results, obtained in III, are now revised and performed.

So, by basing on our following basic expressions, as:

(i)the effective static dielectric constant, $\varepsilon(r_{d(a)})$, due to the impurity size effect, determined by an effective Bohr model [1], and given in Eq. (2),

(ii) the critical donor(acceptor)-density, $N_{CDn(NDp)}(r_{d(a)})$, determined from the generalized effective Mott criterion in the MIT, and as given in Eq. (3), being used to determine the effective d(a)-density: $N^* \equiv N - N_{CDn(CDp)}(r_{d(a)})$, which gives a physical condition, needed to define the metal-insulator transition (**MIT**) at T=0K, as: $N^* \equiv N - N_{CDn(CDp)} = 0$ or $N = N_{CDn(CDp)}$, noting that $N_{CDn(CDp)}$ can also be explained as the density of electrons(holes) localized in the exponential conduction(valence)-band tails (EBT), $N^{EBT}_{CDn(CDp)}$, as that determined in Eq. (21), with a precision of the order of 10^{-5}, being observed in Table 1,

(iii) the Fermi energy, $\mathbb{E}_{Fn(Fp)}(N^*, T)$, determined in Eq. (A3) of the Appendix A, with a precision of the order of 2.11×10^{-4} [3], and finally,

(iv) the refraction index n and the extinction coefficient κ, determined in Equations (28, 29), verifying their correct asymptotic behaviors,

we have investigated the optical coefficients, determined from Equations (24, 25, 28, 29), and their numerical results, given in different physical conditions, have been obtained and discussed in above Tables 2a, 2b, 2c, 3a, 3b, 3c, 4n(4p), 5n(5p), and finally 6n(6p). In particular, in Tables 3a, 3b and 3c, our numerical results for those optical coefficients are found to be more accurate than the corresponding ones, calculated from the physical model, proposed by Forouhi and Bloomer (FB) [11].

Finally, one notes that the MIT occurs in the degenerate case, in which:

(a) $\mathbb{E}_{Fno(Fpo)}(N^* = 0, T = 0) = 0$, determined by Eq. (A4) of the Appendix A, since it is proportional to $(N^*)^{2/3}$,

(b) as discussed in Eq. (5), in the MIT, in which $\mathbb{E}_{gn1(gp1)}(N^* = 0, r_{d(a)}, T = 0) = \mathbb{E}_{gni(gpi)}(r_{d(a)})$, where $\mathbb{E}_{gn1(gp1)}$ and $\mathbb{E}_{gni(Fgpi)}$ are the optical band gap and intrinsic band gap, respectively, and

c) as discussed in Section 5.1, as $E = E_{CPE}(r_{d(a)}) \equiv \mathbb{E}_{gni(gpi)}(r_{d(a)})$ or the effective photon energy $E^* \equiv E - \mathbb{E}_{gni(gpi)}(r_{d(a)}) = 0$, one has: $\kappa(E^* = 0, r_{d(a)}) = 0$, $\varepsilon_2(E^* = 0, r_{d(a)}) = 0$, $\sigma_O(E^* = 0, r_{d(a)}) = 0$ and $\alpha(E^* = 0, r_{d(a)}) = 0$, since those optical coefficients expressed in terms of $(E^* \equiv E - \mathbb{E}_{gni(gpi)} = 0)^2$, according also to the MIT-case, being new results.

In summary, all the numerical results, given in III [3], are now revised and performed in the present work.

Appendix

Appendix A. Fermi Energy and generalized Einstein relation

A1. In the n(p)-type Si-crystals, the Fermi energy $\mathbb{E}_{Fn(Fp)} \equiv [\mathbb{E}_{fn} - \mathbb{E}_c](\mathbb{E}_{Fp} \equiv [\mathbb{E}_v - \mathbb{E}_{fp}])$, $\mathbb{E}_{c(v)}$ being the conduction (valence) band edges, obtained for any T and donor (acceptor) density N, being investigated in our previous paper, with a precision of the order of 2.11×10^{-4} [3], is now summarized in the following. In this work, N is replaced by the effective density N^*, $N^* \equiv N - N_{CDn(CDp)}(r_{d(a)})$, $N_{CDn(CDp)}(r_{d(a)})$ being the critical density, characteristic of the insulator-metal transition phenomenon. It means that $N^* = 0$ at this transition.

First of all, we define the reduced electron density by:

$$u(N^*, r_{d(a)}, T) \equiv u(N^*, T) \equiv \frac{N^*}{N_{c(v)}},\ N_{c(v)}(T) = 2 \times g_{c(v)} \times \left(\frac{m^*_{n(p)} \times k_B T}{2\pi\hbar^2}\right)^{\frac{3}{2}}\ (cm^{-3}), \quad (A1)$$

where $N_{c(v)}(T)$ is the conduction (valence)-band density of states, and the values of $g_{c(v)}$ and $m^*_{n(p)}$ are defined and given in Table 1. Then, the reduced Fermi energy in the n(p)-type Si is determined by :

$$\frac{\mathbb{E}_{Fn}(u)}{k_B T}\left(\frac{\mathbb{E}_{Fp}(u)}{k_B T}\right) = \frac{G(u) + Au^B F(u)}{1 + Au^B} = \theta_n(u) \equiv \frac{V(u)}{W(u)},\ A = 0.0005372 \text{ and } B = 4.82842262, \quad (A2)$$

where $F(N^*, r_{d(a)}, T) = au^{\frac{2}{3}}\left(1 + bu^{-\frac{4}{3}} + cu^{-\frac{8}{3}}\right)^{-\frac{2}{3}}$, obtained for $u \gg 1$, according to the degenerate cas, $a = [(3\sqrt{\pi}/4)]^{2/3}$, $b = \frac{1}{8}\left(\frac{\pi}{a}\right)^2$, $c = \frac{62.3739855}{1920}\left(\frac{\pi}{a}\right)^4$, and then $G(u) \simeq Ln(u) + 2^{-\frac{3}{2}} \times u \times e^{-du}$ for $u \ll 1$, according to the non − degenerate case, with: $d = 2^{3/2}\left[\frac{1}{\sqrt{27}} - \frac{3}{16}\right] > 0$.

So, in the present degenerate case ($u \gg 1$), one has:

$$\mathbb{E}_{Fn(Fp)}(N^*, r_{d(a)}, T) \equiv \mathbb{E}_{Fn(Fp)}(N^*, T) = \mathbb{E}_{Fno(Fpo)}(u) \times \left(1 + bu^{-\frac{4}{3}} + cu^{-\frac{8}{3}}\right)^{-\frac{2}{3}}. \quad (A3)$$

Then, at T=0K, since $u^{-1} = 0$, Eq. (A.3) is reduced to:

$$\mathbb{E}_{Fno(Fpo)}(N^*) \equiv \frac{\hbar^2 \times k^2_{Fn(Fp)}(N^*)}{2 \times m^*_{n(p)}}, \quad (A4)$$

being proportional to $(N^*)^{2/3}$, and equal to 0, $\mathbb{E}_{Fno(Fpo)}(N^* = 0) = 0$, according to the MIT, as discussed in Section 2 and 3.

Appendix B. Approximate forms for band gap narrowing (BGN)

First of all, in the n(p)-type Si-crystals, we define the effective reduced Wigner-Seitz radius $r_{sn(sp)}$, characteristic of the interactions, by:

$$r_{sn(sp)}(N^*, r_{d(a)}) \equiv \left(\frac{3g_{c(v)}}{4\pi N^*}\right)^{1/3} \times \frac{1}{a_{Bn(Bp)}(r_{d(a)})} = 1.1723 \times 10^8 \times \left(\frac{g_{c(v)}}{N^*}\right)^{1/3} \times \frac{m^*_{n(p)}/m_o}{\varepsilon(r_{d(a)})}. \quad (B1)$$

Here, the values of $g_{c(v)} = 3(2)$ and $(m^*_{n(p)}/m_o)$ are defined and given in Table 1.

In particular, in the following, $m^*_{n(p)}/m_o = m_r/m_o = 0.1713$, is taken for evaluating the band gap narrowing (BGN), as used in Section 3. Therefore, the correlation energy of an effective electron gas, $\mathbb{E}_{CE}(r_{sn(sp)})$, is found to be given by [1]:

$$\mathbb{E}_{CE}(r_{sn(sp)}) \equiv \mathbb{E}_{CE}(N^*, r_{d(a)}) = \frac{-0.87553}{0.0908 + r_{sn(sp)}} + \frac{\frac{0.87553}{0.0908 + r_{sn(sp)}} + \left(\frac{2[1 - \ln(2)]}{\pi^2}\right) \times \ln(r_{sn(sp)}) - 0.093288}{1 + 0.03847728 \times r_{sn(sp)}^{1.67378876}}. \quad (B2)$$

Then, the band gap narrowing (BGN) can be determined by [1]:

$$\Delta\mathbb{E}_{gn}(N^*, r_d) \simeq a_1 \times \frac{\varepsilon_o}{\varepsilon(r_d)} \times N_r^{1/3} + a_2 \times \frac{\varepsilon_o}{\varepsilon(r_d)} \times N_r^{\frac{1}{3}} \times (2.503 \times [-\mathbb{E}_{CE}(r_{sn}) \times r_{sn}]) + a_3 \times \left[\frac{\varepsilon_o}{\varepsilon(r_d)}\right]^{5/4} \times \sqrt{\frac{m_v}{m_r}} \times N_r^{1/4} + a_4 \times \sqrt{\frac{\varepsilon_o}{\varepsilon(r_d)}} \times N_r^{1/2} \times 2 + a_5 \times \left[\frac{\varepsilon_o}{\varepsilon(r_d)}\right]^{\frac{3}{2}} \times N_r^{\frac{1}{6}},\ N_r \equiv \frac{N^* = N - N_{CDn}(r_d)}{9.999 \times 10^{17} cm^{-3}}, \quad (B3)$$

where $a_1 = 6.829 \times 10^{-3}$(eV), $a_2 = 1.168 \times 10^{-3}$(eV), $a_3 = 5.032 \times 10^{-3}$(eV), $a_4 = 10.058 \times 10^{-3}$(eV) and $a_5 = 1.455 \times 10^{-3}$(eV), and

$$\Delta\mathbb{E}_{gp}(N^*, r_a) \simeq a_1 \times \frac{\varepsilon_o}{\varepsilon(r_a)} \times N_r^{1/3} + a_2 \times \frac{\varepsilon_o}{\varepsilon(r_a)} \times N_r^{\frac{1}{3}} \times (2.503 \times [-\mathbb{E}_{CE}(r_{sp}) \times r_{sp}]) + a_3 \times \left[\frac{\varepsilon_o}{\varepsilon(r_a)}\right]^{5/4} \times \sqrt{\frac{m_c}{m_r}} \times N_r^{1/4} + 2a_4 \times \sqrt{\frac{\varepsilon_o}{\varepsilon(r_a)}} \times N_r^{1/2} + a_5 \times \left[\frac{\varepsilon_o}{\varepsilon(r_a)}\right]^{\frac{3}{2}} \times N_r^{\frac{1}{6}},\ N_r \equiv \left(\frac{N^* = N - N_{CDp}(r_a)}{9.999 \times 10^{17}\ cm^{-3}}\right), \quad (B4)$$

where $a_1 = 9.329 \times 10^{-3}$(eV), $a_2 = 1.596 \times 10^{-3}$(eV), $a_3 = 7.144 \times 10^{-3}$(eV), $a_4 = 13.741 \times 10^{-3}$(eV) and $a_5 = 1.988 \times 10^{-3}$(eV).

Therefore, in Equations (B3, B4), as T=0 and $N^* = 0$, and for any $r_{d(a)}$, $\Delta\mathbb{E}_{gn(gp)}(N^* = 0, r_{d(a)}) = 0$, according to the MIT.

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