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Accurate expressions of the optical coefficients, given in n(p)-type degenerate GaAs-crystals, due to the impurity-size effect, and obtained by an improved Forouhi-Bloomer parameterization model (FB-PM)

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Abstract

In the n(p)-type degenerate GaAs-crystals, at low temperature T and high d(a)-density N, our expression for the static dielectric constant, $\varepsilon(r_{d(a)})$, expressed as a function of the donor (acceptor) radius, $r_{d(a)}$, and determined by using an effective Bohr model, as that investigated in [1,2], suggests that, for an increasing $r_{d(a)}$, due to such the impurity size effect, $\varepsilon(r_{d(a)})$ decreases, affecting strongly the critical d(a)-density in the metal-insulator transition (MIT), $N_{CDn(CDp)}(r_{d(a)})$, determined by Eq. (3), and its values are reported in Table 1, and also our accurate expressions for optical coefficients, obtained in Equations (24, 25, 28, 29), and their numerical results are given in Tables 2-6. Furthermore, one notes that, as observed in Table 3c, our obtained results of those optical coefficients are found to be more accurate than the corresponding ones, obtained from the FB-PM [11], suggesting thus that the present model, used here to study the optical properties of the n(p)-type degenerate GaAs-crystals, is a good improved FB-PM.

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

1. Introduction

In our three 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

$r_{d(a)}$, due thus to such the impurity size effect, $\varepsilon(r_{d(a)})$ 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], $\boldsymbol{\xi_{n(p)}}(\geqq \mathbf{1})$. 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 2-5.

2. Energy-band-structure parameters

First of all, in the following Table 1, we present the values of the energy-band-structure parameters, given in the n(p)-type GaAs -crystal, such as: (i) if denoting the free electron mass by m_o, the effective electron (hole) mass, $m^*_{n(p)}/m_o$, which is respectively equal to the relative effective mass, $m_{n(p)}/m_o = 0.066\ (0.291)$ [2], as used in this Sections 2 and 4 to determine the critical impurity density in the metal-insulator transition (**MIT**), and (ii) to the reduced effective mas, $m_r/m_o = \frac{m_n \times m_p}{m_n + m_p} = 0.0538$, as used in Sections 3 and 5 to determine the optical band gap and the optical coefficients given in the n(p)-type degenerate GaAs. Further, $\mathbb{E}_{go} = \mathbb{E}_{goAs(goGa)} = 1.52$ eV [2] is the unperturbed intrinsic band gap, $\varepsilon_o = \varepsilon_{As(Ga)} = 13.13$ is the relative static intrinsic dielectric constant of the GaAs-crystal, and finally, the effective averaged numbers of equivalent conduction (valence)-band edge, $g_{c(v)} = 1(1)$.

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 2.35×10^{-3}, 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	As	Te	Sb	Sn
r_d (nm) [4]	↗	0.110	0.118	0.132	0.136	0.140
$\varepsilon(r_d)$	↘	13.40	13.13	12.33	11.86	11.33
$\mathbb{E}_{gni}(r_d)$ in meV	↗	1519.8	1520	1520.7	1521.2	1521.8
$N_{CDn}(r_d)$ in 10^{16} cm^{-3}	↗	1.2538	1.3330	1.6107	1.8099	2.0762
$N^{EBT}_{CDn}(r_d)$ in 10^{16} cm^{-3}	↗	1.2516	1.3305	1.6070	1.8058	2.0713
$\lvert RD \rvert$ in 10^{-3}		1.79	1.90	2.278	2.28	**2.35**

Acceptor		B	Ga(Al)	Mg	In
r_a (nm) [4]	↗	0.088	0.126	0.140	0.144
$\varepsilon(r_a)$	↘	24.3813	13.13	12.4205	11.9991
$\mathbb{E}_{gpi}(r_a)$ in meV	↗	1503.7	1520	1522.7	1524.5
$N_{CDp}(r_a)$ in 10^{17} cm^{-3}	↗	1.7845	11.426	13.497	14.970
$N^{EBT}_{CDp}(r_a)$ in 10^{17} cm^{-3}	↗	1.7850542	11.429526	13.50187	14.975094
$\lvert RD \rvert$ in 10^{-4}		3.1	3.08	**3.61**	3.40

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 $r_{do(ao)} \equiv r_{As(Ga)}$, 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, 2]. 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 have showed [1, 2] that such the compression (dilatation) corresponds to 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:

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

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 $r_{d(a)}$, as observed in the above Table 1.

2.2. Our expressions for the critical density in the MIT

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

$$N_{CDn(NDp)}(r_{d(a)})^{1/3} \times a_{Bn(Bp)}(r_{d(a)}) = z, \quad z=0.25, \quad (3)$$

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

$$a_{Bn(Bp)}(r_{d(a)}) \equiv \frac{\varepsilon(r_{d(a)}) \times \hbar^2}{m^*_{n(p)} \times q^2} = 0.53 \times 10^{-8}\ \text{cm} \times \frac{\varepsilon(r_{d(a)})}{(m^*_{n(p)}/m_o)}, \quad (4)$$

where $-q$ is the electron charge, $\varepsilon(r_{d(a)})$ is determined in Eq. (2), and $m^*_{n(p)}/m_o = m_{n(p)}/m_o = 0.066(0.291)$. From Eq. (3), the numerical results of $N_{CDn(NDp)}(r_{d(a)})$ are obtained and given in the above Table 1, in which we also report those of the densities of electrons (holes) localized in exponential conduction (valance)-band (EBT) tails, $N^{EBT}_{CDn(CDp)}(r_{d(a)})$, obtained using Eq. (21), as investigated in Section 4, noting that the maximal relative deviations (RD), in absolute values, between $N_{CDn(NDp)}(r_{d(a)})$ and $N^{EBT}_{CDn(CDp)}(r_{d(Ba)})$ are found to be equal to: $2.35(0.361) \times 10^{-3}$, respectively. Thus, $N_{CDn(NDp)}(r_{d(a)})$

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 also showed that, in the n(p)-type degenerate semiconductors, 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 MIT occur.

In summary, Table 1 also indicates that, for an 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 observed in following Sections 3-5 .

3. Optical band gap

Here, $m^*_{n(p)}/m_o$ is chosen as: $m^*_{n(p)}/m_o = m_r/m_o = 0.0538$, and then, if denoting $N^* \equiv N - N_{CDn(NDp)}(r_{d(a)})$, the optical band gap (**OBG**) is found to be given by:

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

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:

$$\mathbb{E}_{gnei(gpei)}(r_{d(a)}, T) \equiv \mathbb{E}_{gni(gpi)}(r_{d(a)}) - \frac{4.9\times10^{-4}\times T^2}{T+327\ K},$$

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 values of $\mathbb{E}_{gni(gpi)}(r_{d(a)})$ are given in Table 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 $\Delta\mathbb{E}_{gn(gp)}(N^*, r_{d(a)}) = 0$, 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.

4. Physical model and mathematical methods

4.1. Physical model

In the n(p)-type degenerate GaAs, 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

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

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

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

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

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

$$R_{sn(sp)WS}\big(N^{*}, r_{d(a)}\big) \equiv \frac{k_{sn(sp)WS}}{k_{Fn}} = 0.5\ (1) \times \left(\frac{3}{2\pi} - \gamma \frac{d\big[r_{sn(sp)}^{2} \times \mathbb{E}_{CE}\big(N^{*}, r_{d(a)}\big)\big]}{dr_{sn(sp)}}\right), \quad (9)$$

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

Furthermore, as given in I, 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)-GaAs 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)-GaAs system, defined as

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

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 GaAs -crystal volume.

Then, the effective auto-correlation function for potential fluctuations, $W_{n(p)}\big(\nu_{n(p)}, N^{*}, r_d\big) \equiv \langle V(r)V(r')\rangle$, was determined in II, as :

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

Here, $\varepsilon(\mathrm{r_{d(a)}})$ is determined in Eq. (2), $\mathrm{R_{sn(sp)}}\big(\mathrm{N^*}, \mathrm{r_{d(a)}}\big)$in Eq. (7), the empirical Heisenberg parameter $\mathcal{H} = 0.48302632\ (1.58)$, respectively, 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 $\nu_{\mathrm{n(p)}} \equiv \frac{-\mathbb{E}}{\mathbb{E}_{\mathrm{Fno(Fpo)}}}$, where $\mathbb{E}$ is the total electron energy and $\mathbb{E}_{\mathrm{Fno(Fpo)}}$ 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: $(\mathbb{E} - \mathrm{V})^{\mathrm{a}-\frac{1}{2}} \equiv \mathbb{E}_{\mathrm{k}}^{\mathrm{a}-\frac{1}{2}}$, for $\mathrm{a} \geq 1$, $\mathbb{E}_{\mathrm{k}} \equiv \frac{\hbar^2 \times \mathrm{k}^2}{2\times m^*_{n(p)}}$ being the kinetic energy of the electron (hole), and $\mathrm{V(r)}$ determined in Eq. (11), by using the two following integration methods, as developed in II, which strongly depend on $\mathrm{W_{n(p)}}\big(\nu_{\mathrm{n(p)}}, \mathrm{N^*}, \mathrm{r_{d(a)}}\big)$.

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

A. Kane integration method (KIM)

In heavily doped d(a)- GaAs systems, the effective Gaussian distribution probability is defined by

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

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

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

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

and using an identity:

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

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

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

B. Feynman path-integral method (FPIM)

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

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

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:

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

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 <u>$\mathbb{E} \geq 0$</u>, 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

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

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

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

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

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

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)-GaAs systems at T=0 K, in which $m^*_{n(p)}/m_o = m_{n(p)}/m_o = 0.066(0.291)$, as given in Section 2, using Eq. (13), for a=1, the density of states $\mathcal{D}(\mathbb{E})$ is defined by:

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

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 $\mathcal{H} = 0.48302632$ (1.58), respectively, 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:

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

(19)

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

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

where $\mathcal{D}(\mathbb{E} \leq 0)$ 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, $\beta(\mathrm{a}=1)=\frac{\sqrt{\pi}}{2^{\frac{3}{4}}\times\Gamma(5/4)}$.

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

$\mathrm{I}_{\mathrm{n(p)}}=\frac{1}{2^{5/4}\mathrm{A}_{\mathrm{n(p)}}}\times\int_{\mathrm{y}_{\mathrm{n(p)}}}^{\infty}\mathrm{t}^{\mathrm{b}-1}\,\mathrm{e}^{-\mathrm{t}}\mathrm{dt}\equiv\frac{\Gamma(\mathrm{b},\,\mathrm{y}_{\mathrm{n(p)}})}{2^{5/4}\times\mathrm{A}_{\mathrm{n(p)}}}$,

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

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

Finally, Eq. (20) now yields:

$$\mathrm{N}_{\mathrm{CDn(CDp)}}^{\mathrm{EBT}}[\mathrm{N}=\mathrm{N}_{\mathrm{CDn(NDp)}}(\mathrm{r}_{\mathrm{d(a)}}),\mathrm{r}_{\mathrm{d(a)}}]=\frac{\mathrm{g}_{\mathrm{c(v)}}\times(\mathrm{m}_{\mathrm{n(p)}})^{3/2}\sqrt{\eta_{\mathrm{n(p)}}}\times\mathbb{E}_{\mathrm{Fno(Fpo)}}}{2\pi^2\hbar^3}\times\left\{\int_0^{16}\beta(\mathrm{a}=1)\times\mathrm{F}_{\mathrm{n(p)}}(\nu_{\mathrm{n(p)}},\mathrm{r}_{\mathrm{d(a)}},\mathrm{a}=1)\,d\nu_{\mathrm{n(p)}}+\frac{\Gamma(\mathrm{b},\,\mathrm{y}_{\mathrm{n(p)}})}{2^{5/4}\times\mathrm{A}_{\mathrm{n(p)}}}\right\},\quad(21)$$

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

The numerical results of $\mathrm{N}_{\mathrm{CDn(CDp)}}^{\mathrm{EBT}}[\mathrm{N}=\mathrm{N}_{\mathrm{CDn(NDp)}}(\mathrm{r}_{\mathrm{d(a)}}),\mathrm{r}_{\mathrm{d(a)}}]\equiv\mathrm{N}_{\mathrm{CDn(CDp)}}^{\mathrm{EBT}}(\mathrm{r}_{\mathrm{d(a)}})$, for a simplicity of presentation, evaluated using Eq. (21), are given in Table 1, confirming thus those of $\mathrm{N}_{\mathrm{CDn(NDp)}}(\mathrm{r}_{\mathrm{d(a)}})$, calculated using Eq. (3), with a precision of the order of $2.35(0.361)\times10^{-3}$, respectively. In other word, this critical d(a)-density $\mathrm{N}_{\mathrm{CDn(NDp)}}(\mathrm{r}_{\mathrm{d(a)}})$ can thus be explained by the density of electrons(holes) localized in the EBT, $\mathrm{N}_{\mathrm{CDn(CDp)}}^{\mathrm{EBT}}(\mathrm{r}_{\mathrm{d(a)}})$, 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:

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

Then, if $\mathrm{N}^*=\mathrm{N}_{\mathrm{CDn(NDp)}}$, according to the Fermi energy, $\mathbb{E}_{\mathrm{Fno(Fpo)}}(\mathrm{N}^*=\mathrm{N}_{\mathrm{CDn(NDp)}})\equiv\frac{\hbar^2\times\mathrm{k}_{\mathrm{Fn(Fp)}}^2(\mathrm{N}^*)}{2\times\mathrm{m}_{\mathrm{n(p)}}^*}$, then the value of the density of electrons(holes), $\mathrm{N}_{\mathrm{CDn(CDp)}}^{\mathrm{EBT}}$, localized in the EBT for $\mathbb{E}\leq0$, is almost equal to $\mathrm{N}_{\mathrm{CDn(NDp)}}$, given in this parabolic conduction (valence) band, for $\mathbb{E}\geq0$. This can thus be expressed as:

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

5. Optical coefficients

Here, $\mathrm{m}_{\mathrm{n(p)}}^*/\mathrm{m}_{\mathrm{o}}$ is chosen as: $\mathrm{m}_{\mathrm{n(p)}}^*/\mathrm{m}_{\mathrm{o}}=\mathrm{m}_{\mathrm{r}}/\mathrm{m}_{\mathrm{o}}=0.0538$, as that used in Section 3, for determining the optical band gap in degenerate GaAs-crystals.

The optical properties of any medium can be described by the complex refraction index $\mathbb{N}$ and the complex dielectric function ε, $\mathbb{N}\equiv\mathrm{n}-\mathrm{i}\kappa$ and $\varepsilon\equiv\varepsilon_1-\mathrm{i}\varepsilon_2$, where $\mathrm{i}^2=-1$ 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]

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

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, $\varepsilon_{\text{free space}}$, 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 GaAs-transitions, for a=5/2, as discussed in I and III, one has:

at low values of E,

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

and at large values of E,

$$J_{n(p)}\left(E > \mathbb{E}_{gn(gp)}\right) = \frac{1}{2\pi^2} \times \left(\frac{2m_r}{\hbar^2}\right)^{3/2} \times \frac{(E - \mathbb{E}_{gn(gp)})^{a-(1/2)}}{E_{gni(gpi)}^{a-1}} = \frac{1}{2\pi^2} \times \left(\frac{2m_r}{\hbar^2}\right)^{3/2} \times \frac{(E - \mathbb{E}_{gn(gp)})^2}{E_{gni(gpi)}^{3/2}}, \text{ for a=5/2}. \quad (27)$$

Further, one notes that**,** as $E \to \infty$, Forouhi and Bloomer (FB) [11] claimed that $\kappa(E \to \infty) \to$ a constant, while the κ(E) -expressions, proposed by Jellison and Modine [12] and by Van Cong [3] quickly go to 0 as E^{-3}, and consequently, their numerical results of the optical functions such as: $\sigma_O(E)$ and α(E), given in Eq. (24), both go 0 as E^{-2}.

Now, an improved Forouhi-Bloomer parameterization model (FB-PM), used to determine the accurate expressions of the optical coefficients, obtained in the degenerate n(p) type GaAs-crystals, is proposed as follows.

If defining the band gap $\mathbb{E}_{gn(gp)}$, which can be equal to the optical band gap $\mathbb{E}_{gn1(gp1)}$, the effective intrinsic band gap $\mathbb{E}_{gnei(gpei)}$, or to the intrinsic band gap $\mathbb{E}_{gni(gpi)}$, and $f(E) \equiv \sum_{i=1}^{4} \frac{A_i}{E^2 \times (1 + 10^{-4} \times \frac{E}{6}) - B_i E + C_i}$, we propose:

$$\kappa(E^*) = f(E) \times \mathbb{E}_{gni(gpi)}^{3/2} \times \left(E^* \equiv E - \mathbb{E}_{gn(gp)}\right)^{1/2}, \text{ for } \mathbb{E}_{gni(gpi)} \le E \le 2.3 \text{ eV},$$

$$= f(E) \times \left(E^* \equiv E - \mathbb{E}_{gn(gp)}\right)^2, \text{ for } E \ge 2.3 \text{ eV}, \quad (28)$$

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 further,

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

going to a constant as $E \to \infty$, since $n(E \to \infty, r_{d(a)}) = n_\infty(r_{d(a)}) = \sqrt{\varepsilon(r_{d(a)})} \times \frac{\omega_T}{\omega_L}$, $\omega_T = 5.1 \times 10^{13}\ s^{-1}$ [5] and $\omega_L = 8.9755 \times 10^{13}\ s^{-1}$, according to $n_\infty(r_P) = 2.08$, obtained from the Lyddane-Sachs-Teller relation [5], from which T(L) represents the transverse (longitudinal) optical phonon mode, while in the FB-PM [11], $n_{\infty(FB)} = 2.156$ for the GaAs crystal.

Here, other parameters are determined by [11]: $B_{oi} = \frac{A_i}{Q_i} \times \left[-\frac{B_i^2}{2} + E_{gnei(gpei)} B_i - E_{gnei(gpei)}^2 + C_i\right]$, $C_{oi} = \frac{A_i}{Q_i} \times \left[\frac{B_i \times (E_{gnei(gpei)}^2 + C_i)}{2} - 2\mathbb{E}_{gnei(gpei)} C_i\right]$, $Q_i = \frac{\sqrt{4C_i - B_i^2}}{2}$, where, for i=(1, 2, 3, and 4), $A_i = 1.154 \times A_{i(FB)} = 4.7314 \times 10^{-4}$, $0.2314, 0.1118$ and 0.0116, $B_i \equiv B_{i(FB)} = 5.871, 6.154, 9.679$ and 13.232, and $C_i \equiv C_{i(FB)} = 8.619, 9.784, 23.803$, and 44.119.

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 compared with the corresponding ones, calculated using from FB-PM [11], and also the relative deviations (RDs) of those numerical results, calculated using the corresponding data given by Aspnes and Studna [9], suggesting that our obtained numerical results of these optical coefficients are found to be more accurate than the corresponding ones, obtained from the FB-PM, as observed in Table 3c.

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	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	↗	1519.8	1520	1520.7	1521.2	1521.8
$n_{MIT}(\mathbb{E}_{gni}, r_d)$	↘	3.4373	3.4161	3.3520	3.3133	3.2687
$\kappa_{MIT}(\mathbb{E}_{gni}, r_d)$		0	0	0	0	0
$\varepsilon_{1(MIT)}(\mathbb{E}_{gni}, r_d)$	↘	11.8152	11.6700	11.2358	10.9778	10.6843
$\varepsilon_{2(MIT)}(\mathbb{E}_{gni}, r_d)$		0	0	0	0	0
$\sigma_{O(MIT)}(\mathbb{E}_{gni}, r_d)$		0	0	0	0	0
$\propto_{MIT}(\mathbb{E}_{gni}, r_d)$		0	0	0	0	0
$R_{MIT}(\mathbb{E}_{gni}, r_d)$	↘	0.3017	0.2993	0.2921	0.2876	0.2825

Acceptor		B	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	↗	1503.7	1520	1522.7	1524.5
$n_{MIT}(\mathbb{E}_{gpi}, r_a)$	↘	4.173	3.4161	3.3580	3.3227

$\kappa_{MIT}(\mathbb{E}_{gpi}, r_a)$		0	0	0	0
$\varepsilon_{1(MIT)}(\mathbb{E}_{gpi}, r_a)$	↘	17.414	11.6700	11.2765	11.0401
$\varepsilon_{2(MIT)}(\mathbb{E}_{gpi}, r_a)$		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
$R_{MIT}(\mathbb{E}_{gpi}, r_a)$	↘	0.3762	0.2993	0.2928	0.2887

Table 2b. In d(a)-GaAs 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-GaAs systems	P	As	Te	Sb	Sn
$n^{ERI-T}(r_d)$ ↘	3.4373	3.4161	3.3520	3.3133	3.2687
$\kappa^{EEC-T}(r_d)$ ↗	0.2192	0.2193	0.2197	0.2199	0.2202
$\varepsilon_1^{EReD-T}(r_d)$ ↘	11.7671	11.6219	11.1876	10.9294	10.6358
$\varepsilon_2^{EImD-T}(r_d)$ ↘	1.5068	1.4982	1.4726	1.4573	1.4398
$\sigma_O^{EOC-T}(r_d)$ in $\Omega^{-1}cm^{-1}$ ↘	24.511	24.375	23.968	23.728	23.451
$\propto^{EOAC-T}(r_d)$ in $10^3\ cm^{-1}$ ↗	33.758	33.778	33.850	33.902	33.964
$R^{NIR-T}(r_d)$ ↘	0.303	0.301	0.294	0.289	0.284

a-GaAs systems	B	Ga(Al)	Mg	In
$n^{ERI-T}(r_a)$ ↘	4.1730	3.4161	3.3580	3.3227
$\kappa^{EEC-T}(r_a)$ ↗	0.2109	0.2193	0.2207	0.2217
$\varepsilon_1^{EReD-T}(r_a)$ ↘	17.3698	11.6219	11.2278	10.9910
$\varepsilon_2^{EImD-T}(r_a)$ ↘	1.7601	1.4982	1.4823	1.4730
$\sigma_O^{EOC-T}(r_a)$ in $\Omega^{-1}cm^{-1}$ ↘	28.329	24.375	24.158	24.035
$\propto^{EOAC-T}(r_a)$ in $10^3\ cm^{-1}$ ↗	32.137	33.778	34.057	34.245
$R^{NIR-T}(r_a)$ ↘	0.377	0.301	0.295	0.291

Table 2c. Here, the choice of the real refraction index: $n(E \to \infty, r_{d(a)}) = n_\infty(r_{d(a)}) = \sqrt{\varepsilon(r_{d(a)})} \times \frac{\omega_T}{\omega_L}$, $\omega_T = 5.1 \times 10^{13}\ s^{-1}$ [5] and $\omega_L = 8.9755 \times 10^{13}\ s^{-1}$, obtained from the Lyddane-Sachs-Teller relation [5], from which T(L) represents the transverse (longitudinal) optical phonon mode, giving rise to $n_\infty(r_P) = 2.08$, 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 $\sigma_O(E \to \infty, r_{d(a)})$ 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	As	Te	Sb	Sn
$\varepsilon(r_d)$	↘	13.40	13.13	12.33	11.86	11.33
$n_\infty(r_d)$	↘	2.08	2.0589	1.9952	1.9568	1.9126
$\kappa_\infty(r_d)$		0	0	0	0	0
$\varepsilon_{1,\infty}(r_d)$	↘	4.3264	4.2392	3.9809	3.8292	3.6581

$\varepsilon_{2,\infty}(\mathrm{r_d})$	0	0	0	0	0
$\sigma_{0,\infty}(\mathrm{r_d})$ in $\frac{10^5}{\Omega \times cm}$ ↘	9.4912	9.3951	9.1044	8.9292	8.7274
$\propto_{\infty}(\mathrm{r_d})$ in $(10^9 \times cm^{-1})$	2.1602	2.1602	2.1602	2.1602	2.1602
$R_{\infty}(\mathrm{r_d})$ ↘	0.123	0.120	0.110	0.105	0.098

Acceptor	B	Ga(Al)	Mg	In
$\varepsilon(\mathrm{r_a})$ ↘	24.3813	13.13	12.4205	11.9991
$n_{\infty}(\mathrm{r_a})$ ↘	2.8057	2.0589	2.0025	1.9683
$\kappa_{\infty}(\mathrm{r_a})$	0	0	0	0
$\varepsilon_{1,\infty}(\mathrm{r_a})$ ↘	7.8719	4.2392	4.0102	3.8741
$\varepsilon_{2,\infty}(\mathrm{r_a})$	0	0	0	0
$\sigma_{0,\infty}(\mathrm{r_a})$ in $\frac{10^5}{\Omega \times cm}$ ↘	12.803	9.3951	9.1377	8.9814
$\propto_{\infty}(\mathrm{r_a})$ in $(10^9 \times cm^{-1})$	2.1602	2.1602	2.1602	2.1602
$R_{\infty}(\mathrm{r_a})$ ↘	0.225	0.120	0.1115	0.106

Table 3a. In the P-GaAs 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 $\mathbb{E}_{\mathrm{gn}}(\mathrm{r_P}) = \mathbb{E}_{\mathrm{gni}}(\mathrm{r_P})[= 1.5198\ \mathrm{eV}]$, 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 $1.6 \leq \mathrm{E(eV)}$, using the Aspnes-and-Studna (AS)-data [9]. Here, as noted in above Table 2c, one obtains: $\kappa_{\infty}(\mathrm{E} \to \infty, \mathrm{r_P}) \to 0$ and $\varepsilon_{2,\infty}(\mathrm{E} \to \infty, \mathrm{r_P}) \to 0$, while, in the FB-model, $\kappa_{\infty(\mathrm{FB})}(\mathrm{E} \to \infty, \mathrm{r_P}) = 0.3079$ and $\varepsilon_{2,\infty(\mathrm{FB})}(\mathrm{E} \to \infty, \mathrm{r_P}) = 1.3275$.

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%
1.5198	**3.4373**	**0**	**11.8152**	**0**	**3.5230**	**0.0023709**	**12.4116**	**0.0167**
1.6	3.489 (5.7)	0.055 (39)	12.172 (11)	0.508 (24.9)	3.575 (3.4)	**0.006 (93.8)**	12.785 (6.6)	**0.040 (94.1)**
1.7	3.560 (4.9)	0.092 (17.4)	12.666 (9.5)	0.659 (21)	3.647 (2.5)	0.012 (89)	13.303 (4.9)	0.090 (89.2)
1.8	3.639 (3.9)	0.130 (13.7)	13.223 (7.6)	0.948 (16.9)	3.727 (1.54)	0.023 (84.7)	13.887 (2.9)	0.172 (84.9)
1.9	3.726 (2.6)	0.172 (12)	13.854 (5.2)	1.286 (6.0)	3.815 (0.3)	0.039 (78.1)	14.551 (0.4)	0.299 (78.2)
2	3.823 (1.4)	0.222 (5.3)	14.570 (2.8)	1.698 (3.7)	3.913 (0.9)	0.063 (70.3)	15.307 (2.1)	0.490 (70.1)
2.1	3.932 (0.2)	0.282 (17.4)	15.384 (0.5)	2.217 (17.1)	**4.022 (18.6)**	0.096 (59.9)	16.169 (4.6)	0.774 (59.1)
2.2	4.054 (1)	0.355 (28.7)	16.309 (1.7)	2.880 (30.2)	4.144 (3.3)	0.144 (47.9)	17.151 (7.0)	1.193 (46.1)
2.3	4.189 (2.2)	**0.446 (39.5)**	17.351 (3.8)	3.739 (42.6)	4.278 (4.3)	0.211 (34.1)	18.259 (9.3)	1.805 (31.2)
2.4	4.338 (3.2)	0.247 (33.5)	18.756 (6.9)	2.142 (31.4)	4.425 (5.2)	0.304 (17.9)	19.488 (11.1)	2.695 (13.7)
2.5	4.498 (3.8)	0.364 (17.5)	20.097(8.2)	3.272 (14.4)	4.581 (5.7)	0.434 (1.6)	20.798 (11.9)	3.977 (4.1)
2.6	4.663 (3.8)	0.526 (2.4)	21.464 (7.9)	4.907 (1.4)	4.740 (5.5)	0.611 (13.3)	22.091 (11.1)	5.791 (19.6)
2.7	4.823 (2.7)	0.747(7.3)	22.704 (5.4)	7.203 (10.2)	4.890 (4.2)	0.847 (21.7)	23.196 (7.6)	8.286 (26.78)
2.8	4.973 (0.3)	1.044 (5.3)	23.644 (0.2)	10.382 (5.6)	5.027 (1.4)	1.162 (17.3)	23.926 (1.4)	11.685 (18.9)
2.9	5.108 (1.1)	1.577 (8.4)	23.609 (4.7)	16.114 (7.3)	5.147 (1.9)	1.762 (2.4)	23.390 (3.7)	18.141 (4.4)
3	4.521 (0.2)	1.800 (7.6)	17.197 (4.0)	16.272 (7.4)	4.488 (0.5)	1.953 (0.3)	16.328 (1.3)	17.533 (0.2)
3.1	4.435 (1.4)	1.946 (9.3)	15.878 (9.4)	17.262 (8.0)	4.382 (0.2)	2.072 (3.4)	14.910 (2.7)	18.163 (3.2)
3.2	4.227 (7.3)	2.093 (8.5)	13.484 (31.3)	17.691 (1.8)	4.152 (5.4)	2.202 (3.7)	12.390 (20.6)	18.287 (1.5)
3.3	3.996 (7.7)	2.144 (0.8)	11.369 (25.1)	17.135 (6.8)	3.904 (5.3)	2.233 (3.3)	10.256 (12.9)	17.435 (8.7)
3.4	3.804 (5.8)	2.115 (1.9)	9.996 (15.9)	16.090 (7.8)	3.701 (2.9)	2.182 (5.1)	8.940 (3.6)	16.153 (8.2)
3.5	3.676 (4.1)	2.042 (1.4)	9.347 (11.1)	15.013 (5.6)	3.569 (1.1)	2.089(3.7)	8.373 (0.5)	14.906 (4.9)
3.6	3.615 (3.4)	1.958 (0.4)	9.236 (10.5)	14.156 (3.0)	3.505 (0.3)	1.987 (1.1)	8.336 (0.2)	13.930 (1.4)
3.7	3.611 (3.6)	1.886 (2.3)	9.479 (12.6)	13.619 (1.2)	3.499 (0.4)	1.901 (1.6)	8.633 (2.5)	13.303 (1.2)
3.8	3.651 (4.3)	1.840 (3.6)	9.941 (15.4)	13.437 (0.5)	3.539 (1.1)	1.843 (3.5)	9.127 (6.0)	13.043 (2.4)

3.9	3.724 (5.3)	1.830 (3.9)	10.523 (18.4)	13.631 (1.2)	3.611 (2.1)	1.822 (4.3)	9.722 (9.4)	13.157 (2.3)
4	3.822 (6.1)	1.862 (3.0)	11.140 (20.1)	14.232 (2.9)	3.706 (2.9)	1.844 (4.0)	10.338 (11.4)	13.667 (1.2)
4.1	3.933 (6.5)	1.943 (1.3)	11.690 (19.8)	15.287 (5.1)	3.814 (3.3)	1.915 (2.7)	10.879 (11.5)	14.607 (0.5)
4.2	4.045 (6.2)	2.082 (0.6)	12.029 (17.5)	16.845 (6.8)	3.922 (2.9)	2.042 (1.3)	11.211 (9.5)	16.021 (1.6)
4.3	4.142 (5.1)	2.285 (1.1)	11.934 (14.6)	18.928 (6.3)	4.014 (1.9)	2.232 (1.2)	11.128 (6.9)	17.922 (0.7)
4.4	4.199 (4.6)	2.556 (0.3)	11.095 (16.2)	21.465 (4.3)	4.067 (1.3)	2.488 (2.9)	10.345 (8.4)	20.239 (1.7)
4.5	4.183 (6.9)	2.890 (0.9)	9.143 (34.5)	24.178 (5.8)	4.049 (3.5)	2.804 (3.9)	8.527 (25.5)	22.709 (0.6)
4.6	4.058 (7.7)	3.263 (2.9)	**5.819 (39.8)**	26.482 (10.8)	3.926 (4.2)	3.157 (0.4)	5.445 (30.8)	24.787 (3.7)
4.7	3.796 (5.5)	3.626 (5.0)	1.263 (22.6)	27.533 (10.9)	3.672 (2.1)	3.499 (1.4)	1.245 (20.9)	25.699 (3.5)
4.8	3.401 (1.8)	3.912 (3.8)	−3.741 (22.8)	26.613 (5.6)	3.293 (1.5)	3.765 (0.1)	−3.335 (9.5)	24.795 (1.6)
4.9	2.918 (0.9)	4.061 (0.3)	−7.980 (0.5)	23.699 (1.3)	2.831 (2.0)	3.898 (3.7)	−7.180 (10.5)	22.071 (5.6)
5	2.422 (6.6)	4.049 (0.8)	−10.524 (8.6)	19.614 (5.7)	2.360 (3.8)	3.875 (5.1)	−9.449 (17.9)	18.294 (1.4)
5.1	1.986 (10.2)	3.898 (2.7)	−11.252 (0.8)	15.482 (13.2)	1.948 (8.1)	3.721 (1.9)	−10.053 (9.9)	14.497 (6)
5.2	1.648 (3.1)	3.660 (5.1)	−10.681 (11.5)	12.067 (8.3)	1.631 (2.0)	3.484 (0.01)	−9.480 (1.0)	11.368 (2)
5.3	1.416 (5.5)	3.387 (4.0)	−9.464 (13.3)	9.591 (1.7)	1.416 (5.6)	3.215 (1.2)	−8.333 (0.2)	9.103 (6.7)
5.4	1.275 (10.8)	3.114 (1.1)	−8.075 (8.6)	7.940(9.8)	1.286 (10)	2.949 (4.2)	−7.042 (5.3)	7.588 (13.8)
5.5	**1.203 (12.9)**	2.865 (2.4)	−6.762 (0.8)	6.896(15.1)	1.224 (11.5)	2.707 (7.8)	−5.828 (13.1)	6.625 (18.4)
5.6	1.182 (12.3)	2.649 (5.9)	−5.620 (7.9)	6.264 (17.5)	1.208 (10.4)	2.497 (11.3)	−4.773 (21.8)	6.033 (20.5)
5.7	1.195 (9.8)	2.469 (8.9)	−4.666 (16.5)	5.903 (17.8)	1.225 (7.6)	2.322 (14.3)	−3.891 (30.4)	5.687 (20.8)
5.8	1.231 (6.1)	2.324 (11.4)	−3.889 (24.8)	5.722 (16.9)	1.262 (3.8)	2.182 (16.9)	−3.168 (38.7)	5.506 (20.0)
5.9	1.279 (0.7)	2.215 (13.4)	−3.272 (32.9)	5.665 (14)	1.310 (1.7)	2.075 (18.8)	−2.591 (46.9)	5.438 (17.4)
6	1.331 (5.3)	2.140 (13.4)	−2.807 (37.8)	5.696 (8.8)	1.362 (7.8)	2.002 (19.0)	**−2.150 (52.3)**	5.454 (12.7)
…								
10^{21}	2.08	0	4.3264	0	2.156	0.3079	4.5536	1.3275
…								
10^{22}	2.08	0	4.3264	0	2.156	0.3079	4.5536	1.3275
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-GaAs 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 $\mathbb{E}_{gn}(r_P) = \mathbb{E}_{gni}(r_P)[= 1.5198\ eV]$, 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 $1.6 \le E(eV)$, using the Aspnes-and-Studna (AS)-data [9]. Here, as noted in above Table 2c, one obtains: $\propto_\infty(E \to \infty, r_P) = 2.1602 \times 10^9\ cm^{-1}$ and $\sigma_{0,\infty}(E \to \infty, r_P) = 9.4912 \times 10^5 \left(\frac{1}{\Omega \times cm}\right)$, while, in the FB-model, $\propto_{FB} \to \infty$, and $\sigma_{0(FB)} \to \infty$, which should be not correct.

E in eV	$\propto$ $(10^3 \times cm^{-1})$; RD%	R; RD%	$\sigma_0 \left(\frac{1}{\Omega \times cm}\right)$	$\sigma_{0(FB)} \left(\frac{1}{\Omega \times cm}\right)$	$\propto_{FB}(10^3 \times cm^{-1})$; RD%	R_{FB}; RD%
1.5198	**0**	**0.3017**	**0**	**0.2717**	**0.3651**	**0.3112**
1.6	**8.92; 39.9%**	0.308; 6.8%	6.572	0.6874	**0.910; 93.9%**	0.3169; 4.0%
1.7	15.93; 17.4%	0.3155; 5.8%	11.983	1.6385	2.127; 89.0 %	0.3245; 3.1%
1.8	23.76; 13.6%	0.3241; 4.4%	18.261	3.3091	4.203; 84.7 %	0.3328; 1.8%
1.9	33.22; 3.6%	0.3336; 3.0%	26.145	6.0735	7.537; 78.1 %	0.3418; 0.6%
2	45.01; 5.2%	0.3440; 1.4%	36.357	10.492	12.69; 70.3 %	0.3516; 0.7%
2.1	59.98; 17.3%	0.3556; 0.1%	49.827	17.407	20.49; 59.9 %	0.3624; 1.8%
2.2	79.19; 28.8%	0.3683; 1.4%	67.817	28.086	32.09; 47.8 %	0.3740; 3.0%
2.3	104.0; 39.5%	0.3823; 2.8%	92.056	44.427	49.16; 34.1 %	0.3867; 4.0%
2.4	60.03; 33.5%	0.3923; 2.7%	55.012	69.220	74.05; 18.0 %	0.4005; 4.8%
2.5	92.15; 17.5%	0.4074; 3.1%	87.552	106.41	109.96; 1.6 %	0.4152; 5.1%
2.6	138.6; 2.4%	0.4233; 3.2%	136.54	161.15	160.95; 13 %	0.4310; 5.1%
2.7	204.3; 7.2%	0.4402; 2.6%	208.14	239.47	231.82; 22 %	0.4476; 4.3%
2.8	296.2; 5.3%	0.4590; 0.6%	311.14	350.18	329.74; 17.2 %	0.4663; 2.3%

2.9	463.5; 8.3%	0.4866; 0.7%	500.18	563.08	517.86; 2.4 %	0.4965; 1.3%
3	547.1; 7.6%	0.4637; 1.8%	522.49	562.98	593.82; 0.2 %	0.4710; 0.2%
3.1	611.4; 9.3 %	0.4677; 1.9%	572.77	602.64	651.01; 3.4 %	0.4730; 0.8%
3.2	678.7; 8.6 %	0.4666; 0.3%	605.92	626.35	714.14; 3.8 %	0.4710; 0.6%
3.3	717.0; 0.8 %	0.4592; 2.7%	605.24	615.81	746.72; 3.3 %	0.4622; 3.3%
3.4	772.8; 8 %	0.4579; 5.5%	618.04	587.82	751.79; 5.1 %	0.4489; 3.4%
3.5	724.2; 1.4%	0.4352; 2.4 %	562.41	558.41	740.78; 3.7 %	0.4343; 2.2%
3.6	714.2; 0.4 %	0.4246; 1.3%	545.44	536.75	724.97; 1.1 %	0.4217; 0.6%
3.7	707.1; 2.3 %	0.4180; 0.7 %	539.32	526.4	712.70; 1.6 %	0.4133; 0.4%
3.8	708.7; 3.6 %	0.4163; 0.5 %	546.50	530.50	709.66; 3.5 %	0.4101; 0.9%
3.9	723.2; 3.9 %	0.4196; 0.9 %	568.99	549.23	719.99; 4.3 %	0.4124; 0.9%
4	754.7; 3.1 %	0.4278; 1.6 %	609.34	585.12	747.35; 4.0 %	0.4197; 0.3%
4.1	807.5; 1.3 %	0.4404; 2.4 %	670.84	641.02	795.66; 2.8 %	0.4316; 0.4%
4.2	886.2; 0.6 %	0.4568; 2.9 %	757.23	720.19	869.30; 1.3 %	0.4476; 0.8%
4.3	995.69; 1.1 %	0.4767; 2.3 %	871.16	824.86	972.81; 1.2 %	0.4670; 0.2%
4.4	1139.8; 0.3 %	0.4996; 1.1 %	1010.9	953.14	1109.6; 2.9 %	0.4895; 0.9%
4.5	1318.0; 0.9 %	0.5249; 0.7 %	1164.5	1093.8	1278.9; 3.9 %	0.5145; 1.3%
4.6	1521.1; 2.9 %	0.5520; 2.2 %	1303.8	1220.4	1471.7; 0.4 %	0.5412; 0.2%
4.7	1727.1; 5.0 %	0.5800; 2.6 %	1385.0	1292.8	1666.5; 1.3 %	0.5689; 0.7%
4.8	1903.1; 3.7 %	0.6077; 1.9 %	1367.3	1273.9	1831.5; 0.1 %	0.5960; 0.0%
4.9	2016.6; 0.3 %	0.6335; 0.07 %	1242.9	1157.5	1935.6; 3.7 %	0.6209; 1.9%
5	2051.4; 0.8 %	0.6552; 1.9 %	1049.7	979.03	1963.7; 5.1 %	0.6412; 4.0%
5.1	2014.7; 2.7 %	0.6706; 0.8 %	845.12	791.33	1923.2; 2.0 %	0.6543; 3.2%
5.2	1928.9; 5.0 %	0.6770; 2.4 %	671.59	632.74	1836.2; 0.001 %	0.6577; 0.5%
5.3	1818.9; 4.0 %	0.6727; 4.5 %	544.06	516.37	1726.9; 1.2 %	0.6499; 0.9%
5.4	1704.3; 1.1 %	0.6572; 4.6 %	458.90	438.59	1613.9; 4.2 %	0.6305; 0.4 %
5.5	1597.0; 2.4 %	0.6316; 3.0 %	405.97	389.98	1508.6; 7.8 %	0.6011; 1.9 %
5.6	1503.3; 5.9 %	0.5985; 0.08 %	375.47	361.63	1416.8; 11.3 %	0.5650; 5.7 %
5.7	1426.1; 8.9 %	0.5619; 3.8 %	360.14	347.00	1341.2; 14.3 %	0.5262; 9.9 %
5.8	1366.3; 11.5 %	0.5257; 7.9 %	355.20	341.78	1282.4; 16.9 %	0.4890; 14.4 %
5.9	1324.5; 13.4 %	0.4936; 12.2 %	357.72	343.42	1240.9; 18.8 %	0.4566; 18.7 %
6	1301.0; 13.4 %	**0.4682; 14.8 %**	365.79	350.27	1217.0; 19.0 %	**0.4316; 21.5 %**
…						
10^{21}	2.1602×10^6	0.123	9.4912×10^5	$\mathbf{1.4209 \times 10^{22}}$	$\mathbf{3.1198 \times 10^{22}}$	0.1423
…						
10^{22}	2.1602×10^6	0.123	9.4912×10^5	$\mathbf{1.4209 \times 10^{22}}$	$\mathbf{3.1198 \times 10^{22}}$	0.1423
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 $(\mathrm{MRD})_{\mathrm{FB}}$, calculated using the (AS)-data [9], 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	∝	R
E (eV)						
1.6					39.9%	
2.3		39.5%		**42.6%**		
4.6			39.8%			

5.5	12.9%					
6						14.8%

$(MRD)_{FB}$	n_{FB}	κ_{FB}	$\varepsilon_{1(FB)}$	$\varepsilon_{2(FB)}$	$\propto_{FB}$	R_{FB}
E (eV)						
1.6		93.8%		94.1%	**93.9%**	
2.1	18.6%					
6			52.3%			21.5%

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 $N = N_{CDn(CDp)} \cong N_{CDn(CDp)}^{EBT}$, vanishing the Fermi energy: $\mathbb{E}_{Fno(Fpo)}(N^*) \equiv \frac{\hbar^2 \times k_{Fn(Fp)}^2(N^*)}{2\times m_{n(p)}^*}$=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:

$$\kappa(E^* = 0) = f(E_{gni(gpi)}) \times \mathbb{E}_{gni(gpi)}^{3/2} \times \left(E^* \equiv E - E_{gni(gpi)} = 0\right)^{1/2} = 0, \tag{30}$$

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

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:

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

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:

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

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

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

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

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 $N = 10^{20} cm^{-3}$, 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-GaAs systems, and for two types of physical conditions such as: (T=0K and $N = N_{CDn}(r_d)$) and (T=20K, $N = 10^{20}$ 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 those extrema occur at the same E.

E in eV	2.5		**2.8**		3		**3.2**		3.9		**4**		**4.5**		**4.7**		**5.1**		100		10^{21}
In the P- GaAs system, at T=0K and $N = N_{CDn}(r_P) =$ 1.2538 x10^{16} cm^{-3}, $\mathbb{E}_{gn}(r_P) \equiv \mathbb{E}_{gni}(r_P)$[= 1.5198 eV]																					
$\varepsilon_1(E)$	20.10	↑	23.64	↓	17.20		13.48		10.52	↑	11.14	↓	9.14		1.26	↓	−11.25	↑	4.04		4.3264
$\varepsilon_2(E)$	3.27		10.38		16.27	↑	17.69	↓	13.63	↑	14.23		24.18	↑	27.53	↓	15.48		1.52		0
In the As-GaAs system, at T=0K and $N = N_{CDn}(r_{As}) =$ 1.333 x10^{16} cm^{-3}, $\mathbb{E}_{gn}(r_{As}) \equiv \mathbb{E}_{gni}(r_{As})$[= 1.52 eV]																					
$\varepsilon_1(E)$	19.90	↑	23.43	↓	17.01		13.31		10.37	↑	10.98	↓	8.97		1.11	↓	−11.33	↑	3.96		4.2392
$\varepsilon_2(E)$	3.25		10.33		16.19	↑	17.60	↓	13.55	↑	14.15		24.05	↑	27.38	↓	15.32		1.50		0
In the Te- GaAs system, at T=0K and $N = N_{CDn}(r_{Te}) =$ 1.6107x10^{16} cm^{-3}, $\mathbb{E}_{gn}(r_{Te}) \equiv \mathbb{E}_{gni}(r_{Te})$[= 1.5207eV]																					
$\varepsilon_1(E)$	19.32	↑	22.79	↓	16.43		12.78		9.90	↑	10.50	↓	8.45		0.64	↓	−11.56	↑	3.70		3.9809
$\varepsilon_2(E)$	3.20		10.19		15.94	↑	17.31	↓	13.31	↑	13.90		23.67	↑	26.90	↓	14.82		1.46		0
In the Sb- GaAs system, at T=0K and $N = N_{CDn}(r_{Sb}) =$ 1.8099 x10^{16} cm^{-3}, $\mathbb{E}_{gn}(r_{Sb}) \equiv \mathbb{E}_{gni}(r_{Sb})$[= 1.5212 eV]																					
$\varepsilon_1(E)$	18.98	↑	22.41	↓	16.09		12.46		9.63	↑	10.22	↓	8.14		0.36	↓	−11.70	↑	3.56		3.8292
$\varepsilon_2(E)$	3.17		10.09		15.79	↑	17.14	↓	13.16	↑	13.76		23.44	↑	26.61	↓	14.52		1.43		0
In the Sn- GaAs system, at T=0K and $N = N_{CDn}(r_{Sn}) =$ 2.0762x10^{16} cm^{-3}, $\mathbb{E}_{gn}(r_{Sn}) \equiv \mathbb{E}_{gni}(r_{Sn})$[= 1.5218 eV]																					
$\varepsilon_1(E)$	18.58	↑	21.97	↓	15.70		12.10		9.31	↑	9.89	↓	7.78		0.50	↓	−11.85	↑	3.39		3.6581
$\varepsilon_2(E)$	3.13		9.99		15.62	↑	16.94	↓	12.99	↑	13.58		23.17	↑	26.28	↓	14.17		1.39		0
E in eV	2.71		**2.8**		3		**3.2**		3.9		**4**		**4.5**		**4.7**		**5.1**		100		10^{21}
In the P- GaAs system, at T=20K and $N = 10^{20}$ cm^{-3}, $\mathbb{E}_{gn}(r_P) \equiv \mathbb{E}_{gn1}(r_P)$[= 2.7095 eV]																					
$\varepsilon_1(E)$	23.42	↑	24.75	↓	20.44		17.84	↓	13.66	↑	14.35	↑	16.41	↓	12.39	↓	0.92	↑	4.05		4.3264
$\varepsilon_2(E)$	1.58×10^{-6}		0.05		0.63		1.51		3.41		3.85		8.73	↑	10.78	↓	6.90		1.48		0
In the As- GaAs system, at T=20K and $N = 10^{20}$ cm^{-3}, $\mathbb{E}_{gn}(r_{As}) \equiv \mathbb{E}_{gn1}(r_{As})$[= 2.7059 eV]																					
$\varepsilon_1(E)$	23.21	↑	24.53	↓	20.25		17.65	↓	13.50	↑	14.19	↑	16.22	↓	12.22	↓	0.82	↑	3.97		4.2392
$\varepsilon_2(E)$	8.7×10^{-5}		0.056		0.64		1.52		3.41		3.85		8.72	↑	10.76	↓	6.85		1.47		0
In the Te- GaAs system, at T=20K and $N = 10^{20}$ cm^{-3}, $\mathbb{E}_{gn}(r_{Te}) \equiv \mathbb{E}_{gn1}(r_{Te})$[= 2.6948 eV]																					
$\varepsilon_1(E)$	22.59	↑	23.89	↓	19.67		17.12	↓	13.03	↑	13.70	↑	15.67	↓	11.70	↓	0.52	↑	3.71		3.9809
$\varepsilon_2(E)$	1.2×10^{-3}		0.069		0.68		1.57		3.41		3.85		8.69	↑	10.70	↓	6.69		1.42		0
In the Sb- GaAs system, at T=20K and $N = 10^{20}$ cm^{-3}, $\mathbb{E}_{gn}(r_{Sb}) \equiv \mathbb{E}_{gn1}(r_{Sb})$[= 2.6876 eV]																					
$\varepsilon_1(E)$	22.21	↑	23.50	↓	19.32		16.79	↓	12.74	↑	13.40	↑	15.33	↓	11.38	↓	0.34	↑	3.56		3.8292

$\varepsilon_2(E)$	2.6×10^{-3}	0.078	0.70	1.59	3.42	3.86	8.78 ↑	10.66 ↓	6.59	1.40	0
In the Sn- GaAs system, at T=20K and $\mathrm{N} = 10^{20}\ \mathrm{cm}^{-3}$, $\mathbb{E}_{gn}(r_{Sn}) \equiv \mathbb{E}_{gn1}(r_{Sn})[= 2.6789\ \mathrm{eV}]$											
$\varepsilon_1(E)$	21.79 ↑	23.06 ↓	18.92	16.42 ↓	12.42 ↑	13.07 ↑	14.95 ↓	11.02 ↓	0.13 ↑	3.39	3.6581
$\varepsilon_2(E)$	4.9×10^{-3}	0.09	0.74	1.63	4.43	3.86 ↑	8.66 ↓	10.63	6.49	1.36	0
E in eV	2.71	**2.8**	3	**3.2**	3.9	**4**	**4.5**	**4.7**	**5.1**	100	10^{21}

Table 4p. In a-GaAs systems, and for two types of physical conditions such as: (T=0K and $\mathrm{N} = \mathrm{N}_{CDp}(r_a)$) and (T=20K, $\mathrm{N} = 10^{20}\ \mathrm{cm}^{-3}$), 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	2.5	**2.8**	3	**3.2**	3.9	**4**	**4.5**	**4.7**	**5.1**	100	10^{21}
In the B- GaAs system, at T=0K and $\mathrm{N} = \mathrm{N}_{CDp}(r_B) =$ 1.7845 x10^{17} cm^{-3}, $\mathbb{E}_{gp}(r_B) \equiv \mathbb{E}_{gpi}(r_B)[= 1.5037\ \mathrm{eV}]$											
$\varepsilon_1(E)$	27.51 ↑	31.78 ↓	24.39	20.12	16.40 ↑	17.17 ↓	15.64	7.06 ↓	−8.19 ↑	7.54	7.8719
$\varepsilon_2(E)$	3.95	12.28	19.38 ↑	21.19 ↓	16.52 ↑	17.17	28.73 ↑	33.15 ↓	21.23	2.06	0
In the Ga- GaAs system, at T=0K and $\mathrm{N} = \mathrm{N}_{CDp}(r_{Ga}) =$ 1.1426 x10^{18} cm^{-3}, $\mathbb{E}_{gp}(r_{Ga}) \equiv \mathbb{E}_{gpi}(r_{Ga})[= 1.52\ \mathrm{eV}]$											
$\varepsilon_1(E)$	19.90 ↑	23.43 ↓	17.01	13.31	10.37 ↑	10.98 ↓	8.97	1.11 ↓	−11.33 ↑	3.96	4.2392
$\varepsilon_2(E)$	3.25	10.33	16.19 ↑	17.60 ↓	13.55 ↑	14.15	24.05 ↑	27.38 ↓	15.32	1.50	0
In the Mg- GaAs system, at T=0K and $N = \mathrm{N}_{CDp}(r_{Mg}) =$ 1.3497 x10^{18} cm^{-3}, $\mathbb{E}_{gp}(r_{Mg}) \equiv \mathbb{E}_{gpi}(r_{Mg})[= 1.5227\ eV]$											
$\varepsilon_1(E)$	19.35 ↑	22.82 ↓	16.49	12.84	9.96 ↑	10.56 ↓	8.52	0.72 ↓	−11.49 ↑	3.73	4.0102
$\varepsilon_2(E)$	3.19	10.16	15.91 ↑	17.29 ↓	13.31 ↑	13.91	23.68 ↑	26.92 ↓	14.87	1.46	0
In- GaAs system, at T=0K and $\mathrm{N} = \mathrm{N}_{CDp}(r_{In}) =$ 1.497 x10^{18} cm^{-3}, $\mathbb{E}_{gp}(r_{In}) \equiv \mathbb{E}_{gpi}(r_{In})[= 1.5245\ \mathrm{eV}]$											
$\varepsilon_1(E)$	19.02 ↑	22.45 ↓	16.18	12.56	9.72 ↑	10.31 ↓	8.25	0.50 ↓	−11.59 ↑	3.60	3.8741
$\varepsilon_2(E)$	3.15	10.05	15.74 ↑	17.11 ↓	13.16 ↑	13.76	23.44 ↑	26.63 ↓	14.60	1.44	0
E in eV	2.71	**2.8**	3	**3.2**	3.9	**4**	**4.5**	**4.7**	**5.1**	100	10^{21}
In the B- GaAs system, at T=20K and $\mathrm{N} = 10^{20}\ \mathrm{cm}^{-3}$, $\mathbb{E}_{gp}(r_B) \equiv \mathbb{E}_{gp1}(r_B)[= 2.7236\ \mathrm{eV}]$											
$\varepsilon_1(E)$	31.40 ↑	32.94 ↓	27.78	24.65 ↓	19.64 ↑	20.48 ↑	23.12 ↓	18.52 ↓	4.33 ↑	7.54	7.8719
$\varepsilon_2(E)$	1.1×10^{-3}	0.04	0.66	1.67	3.98	4.49	10.10 ↑	12.68 ↓	9.27	2.01	0
In the Ga- GaAs system, at T=20K and $\mathrm{N} = 10^{20}\ \mathrm{cm}^{-3}$, $\mathbb{E}_{gp}(r_{Ga}) \equiv \mathbb{E}_{gp1}(r_{Ga})[= 2.6231\ \mathrm{eV}]$											
$\varepsilon_1(E)$	23.21 ↑	24.53 ↓	20.24	17.63 ↓	13.44 ↑	14.12 ↑	16.01 ↓	11.86 ↓	0.38 ↑	3.96	4.2392
$\varepsilon_2(E)$	0.04	1.20	1.05	2.07	3.90	4.36	9.54 ↑	11.68 ↓	7.33	1.47	0
In the Mg- GaAs system, at T=20K and $\mathrm{N} = 10^{20}\ \mathrm{cm}^{-3}$, $\mathbb{E}_{gp}(r_{Mg}) \equiv \mathbb{E}_{gp1}(r_{Mg})[= 2.6118\ \mathrm{eV}]$											
$\varepsilon_1(E)$	22.61 ↑	23.91 ↓	19.70	17.13 ↓	13.01 ↑	13.67 ↑	15.50 ↓	11.38 ↓	0.10 ↑	3.74	4.0102
$\varepsilon_2(E)$	0.05	0.22	1.10	2.13	3.91	4.37	9.52 ↑	11.63 ↓	7.19	1.43	0
In the In- GaAs system, at T=20K and $\mathrm{N} = 10^{20}\ \mathrm{cm}^{-3}$, $\mathbb{E}_{gp}(r_{In}) \equiv \mathbb{E}_{gp1}(r_{In})[= 2.6045\ \mathrm{eV}]$											
$\varepsilon_1(E)$	22.25 ↑	23.54 ↓	19.37	16.83 ↓	12.75 ↑	13.41 ↑	15.19 ↓	11.09 ↓	−0.06 ↑	3.61	3.8741
$\varepsilon_2(E)$	0.057	0.24	1.13	2.16	3.916	4.372	9.51 ↑	11.60 ↓	7.11	1.40	0
E in eV	2.71	**2.8**	3	**3.2**	3.9	**4**	**4.5**	**4.7**	**5.1**	100	10^{21}

5.3. Variations of various optical coefficients as functions of N, typically for some d(a)-GaAs 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=3.2 eV and for some (P, Te, Sn)-GaAs systems and (Ga, In)-GaAs ones, being indicated by the arrows: ↗ and ↘ , as tabulated in following Tables 5n and 5p, in which the physical condition $N > N_{CDn(NDp)}$ (or $N^* > 0$) must be respected, and their variations thus depend on the ones of the optical band gap, $\mathbb{E}_{gn1(gp1)}(N^*, r_{d(a)})$.

Table 5n. In (P, Te, Sn)- GaAs systems, our numerical results of the following optical coefficients, expressed as functions of N, and calculated using Equations (31-36, 24), for E=3.2 eV and T=20K, present the variations by arrows, (↘ and ↗), since those of the optical gap $\mathbb{E}_{gn1}(N^*, r_d)$ increase with increasing N, at T=20 K.

$N\ (10^{18}\ cm^{-3})$ ↗	4	8.5	15	50	80	100
$\mathbb{E}_{gn1}(N^*, r_P, 20K)$ in eV ↗	1.6211	1.7078	1.8126	2.2400	2.5330	2.7095
$n(r_P)$=4.2271						
$\kappa(N, r_P)$ ↘	1.848	1.651	1.427	0.683	0.330	0.178
$\varepsilon_1(N, r_P)$ ↗	14.453	15.143	15.832	17.401	17.759	17.836
$\varepsilon_2(N, r_P)$ ↘	15.623	13.955	12.063	5.776	2.789	1.508
$\sigma_O(N, r_P)$ in $10^2\ \Omega^{-1}cm^{-1}$ ↘	5.351	4.780	4.132	1.978	0.955	0.517
$\propto (N, r_P)$ in $10^5\ cm^{-1}$ ↘	5.993	5.353	4.627	2.215	1.070	0.578
$R(N, r_P)$ ↘	0.450	0.437	0.424	0.392	0.384	0.382
$\mathbb{E}_{gn1}(N^*, r_{Te}, 20K)$ in eV ↗	1.6173	1.7025	1.8060	2.2290	2.5196	2.6948
$n(r_{Te})$=4.1415						
$\kappa(N, r_{Te})$ ↘	1.857	1.662	1.441	0.699	0.343	0.189
$\varepsilon_1(N, r_{Te})$ ↗	13.703	14.388	15.076	16.663	17.034	17.116
$\varepsilon_2(N, r_{Te})$ ↘	15.381	13.769	11.932	5.789	2.843	1.567
$\sigma_O(N, r_{Te})$ in $10^2\ \Omega^{-1}cm^{-1}$ ↘	5.268	4.716	4.087	1.983	0.974	0.537
$\propto (N, r_{Te})$ in $10^5\ cm^{-1}$ ↘	6.022	5.391	4.672	2.266	1.113	0.614
$R(N, r_{Te})$ ↘	0.446	0.433	0.419	0.385	0.376	0.374
$\mathbb{E}_{gn1}(N^*, r_{Sn}, 20K)$ in eV ↗	1.6132	1.6969	1.7988	2.2171	2.5051	2.6789
$n(r_{Sn})$=4.0578						
$\kappa(N, r_{Sn})$ ↘	1.867	1.675	1.455	0.716	0.358	0.201
$\varepsilon_1(N, r_{Sn})$ ↗	12.982	13.660	14.347	15.953	16.338	16.425
$\varepsilon_2(N, r_{Sn})$ ↘	15.149	13.593	11.812	5.812	2.905	1.634
$\sigma_O(N, r_{Sn})$ in $10^2\ \Omega^{-1}cm^{-1}$ ↘	5.189	4.656	4.046	1.991	0.995	0.560
$\propto (N, r_{Sn})$ in $10^5\ cm^{-1}$ ↘	6.053	5.432	4.720	2.322	1.161	0.653
$R(N, r_{Sn})$ ↘	0.442	0.428	0.414	0.378	0.369	0.366
$N\ (10^{18}\ cm^{-3})$	4	8.5	15	50	80	100

Table 5p. In (Ga, In)- GaAs systems, the numerical results of the following optical coefficients, expressed as functions of N, and calculated using Equations (31-36, 24), for E=3.2eV and T=20K, present the variations by arrows, (↘ or ↗), since those of the optical gap $\mathbb{E}_{gp1}(N^*, r_a)$ increase with increasing N, at T=20 K.

$N\ (10^{18}\ cm^{-3})$	15		26		60		100
$\mathbb{E}_{gp1}(N^*, r_{Ga}, 20K)$ in **eV**	1.7675	↗	1.9116	↗	2.2722	↗	2.6231
$n(r_{Ga})$=4.2058							
$\kappa(N, r_{Ga})$	1.5212	↘	1.2307	↘	0.6381	↘	0.247
$\varepsilon_1(N, r_{Ga})$	15.375	↗	16.175	↗	17.282	↗	17.628
$\varepsilon_2(N, r_{Ga})$	12.796	↘	10.352	↘	5.368	↘	2.075
$\sigma_O(N, r_{Ga})$ in $10^2\ \Omega^{-1}cm^{-1}$	4.3826	↘	3.5456	↘	1.838	↘	0.711
$\propto (N, r_{Ga})$ in $10^5\ cm^{-1}$	4.9330	↘	3.9908	↘	2.069	↘	0.800
$R(N, r_{Ga})$	0.428	↘	0.412	↘	0.388	↘	0.381
$\mathbb{E}_{gp1}(N^*, r_{In}, 20K)$ in eV	1.7580	↗	1.9003	↗	2.2571	↗	2.6045
$n(r_{In})$=4.1109							
$\kappa(N, r_{In})$	1.5416	↘	1.2522	↘	0.659	↘	0.263
$\varepsilon_1(N, r_{In})$	14.523	↗	15.332	↗	16.465	↗	16.831
$\varepsilon_2(N, r_{In})$	12.675	↘	10.295	↘	5.419	↘	2.161
$\sigma_O(N, r_{In})$ in $10^2\ \Omega^{-1}cm^{-1}$	4.341	↘	3.526	↘	1.856	↘	0.740
$\propto (N, r_{In})$ in $10^5\ cm^{-1}$	4.999	↘	4.061	↘	2.137	↘	0.852
$R(N, r_{In})$	0.423	↘	0.406	↘	0.381	↘	0.372
$N\ (10^{18}\ cm^{-3})$	15		26		60		100

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

Here, from Equations (24, 28, 29), we can determine the variations of various optical coefficients at $N = 1.5 \times 10^{19} cm^{-3}$, respectively, as functions of T, typically for E=3.2 eV and for some (P, Te, Sn)-GaAs systems and (Ga, In)-GaAs 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)-GaAs systems, our numerical results of the following optical coefficients, expressed as functions of T, and calculated using Equations (31-36, 24), for E=3.2 eV 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	↘	1.8126	1.8120	1.8100	1.8020	1.7769	1.7449
$n(r_P, T)$	↗	4.227	4.228	4.230	4.237	4.261	4.292
$\kappa(r_P, T)$	↗	1.427	1.428	1.432	1.449	1.501	1.570
$\varepsilon_1(r_P, T)$	↗	15.832	15.834	15.838	15.855	15.905	15.959
$\varepsilon_2(r_P, T)$	↗	12.063	12.076	12.116	12.279	12.796	13.474

$\sigma_O(\mathrm{r_P}, T)$ in $10^2\ \Omega^{-1}cm^{-1}$	↗	4.132	4.136	4.150	4.206	4.383	4.615
$\propto(\mathrm{r_P}, T)$ in $10^5\ cm^{-1}$	↗	4.627	4.631	4.645	4.699	4.869	5.090
$\mathrm{R}(\mathrm{r_P}, T)$	↗	0.424	0.424	0.424	0.426	0.431	0.437
$\mathbb{E}_{gn} \equiv \mathbb{E}_{gn1}(\mathrm{T}, \mathrm{r_{Te}})$ in eV	↘	1.8060	1.8053	1.8034	1.7953	1.7702	1.7382
$\mathrm{n}(\mathrm{r_{Te}}, T)$	↗	4.141	4.142	4.144	4.152	4.176	4.207
$\kappa(\mathrm{r_{Te}}, T)$	↗	1.441	1.442	1.446	1.463	1.515	1.584
$\varepsilon_1(\mathrm{r_{Te}}, T)$	↗	15.076	15.078	15.082	15.097	15.140	15.186
$\varepsilon_2(\mathrm{r_{Te}}, T)$	↗	11.932	11.946	11.985	12.146	12.656	13.327
$\sigma_O(\mathrm{r_{Te}}, T)$ in $10^2\ \Omega^{-1}cm^{-1}$	↗	4.087	4.091	4.105	4.160	4.335	4.564
$\propto(\mathrm{r_{Te}}, T)$ in $10^5\ cm^{-1}$	↗	4.672	4.676	4.689	4.744	4.914	5.137
$\mathrm{R}(\mathrm{r_{Te}}, T)$	↗	0.419	0.4191	0.4194	0.421	0.426	0.432
$\mathbb{E}_{gn} \equiv \mathbb{E}_{gn1}(\mathrm{T}, \mathrm{r_{Sn}})$ in eV	↘	1.7988	1.7981	1.7962	1.7881	1.7631	1.7311
$\mathrm{n}(\mathrm{r_{Sn}}, T)$	↗	4.058	4.058	4.060	4.068	4.092	4.123
$\kappa(\mathrm{r_{Sn}}, T)$	↗	1.455	1.457	1.461	1.478	1.531	1.600
$\varepsilon_1(\mathrm{r_{Sn}}, T)$	↗	14.347	14.348	14.352	14.365	14.402	14.440
$\varepsilon_2(\mathrm{r_{Sn}}, T)$	↗	11.812	11.825	11.864	12.024	12.528	13.191
$\sigma_O(\mathrm{r_{Sn}}, T)$ in $10^2\ \Omega^{-1}cm^{-1}$	↗	4.046	4.050	4.063	4.118	4.291	4.518
$\propto(\mathrm{r_{Sn}}, T)$ in $10^5\ cm^{-1}$	↗	4.720	4.724	4.738	4.792	4.964	5.187
$\mathrm{R}(\mathrm{r_{Sn}}, T)$	↗	0.414	0.4142	0.4145	0.4161	0.4211	0.4274
T in K		20	30	50	100	200	300

Table 6p. In (Ga, In)-GaAs systems, our numerical results of the following optical coefficients, expressed as functions of T, and calculated using Equations (31-36, 24), for E=3.2 eV and $\mathrm{N} = 1.5 \times 10^{19}\ \mathrm{cm}^{-3}$, increase with increasing T, since the optical band gap $\mathbb{E}_{gp1}(\mathrm{T}, \mathrm{r_a})$ decreases with increasing T.

T in K		20	30	50	100	200	300
$\mathbb{E}_{gp} \equiv \mathbb{E}_{gp1}(\mathrm{T}, \mathrm{r_{Ga}})$ in eV	↘	1.7675	1.7669	1.7649	1.7568	1.7318	1.6999
$\mathrm{n}(\mathrm{r_{Ga}}, T)$	↗	4.206	4.2065	4.208	4.216	4.240	4.271
$\kappa(\mathrm{r_{Ga}}, T)$	↗	1.521	1.523	1.527	1.544	1.598	1.668
$\varepsilon_1(\mathrm{r_{Ga}}, T)$	↗	15.375	15.376	15.379	15.391	15.425	15.458
$\varepsilon_2(\mathrm{r_{Ga}}, T)$	↗	12.796	12.809	12.851	13.019	13.551	14.250
$\sigma_O(\mathrm{r_{Ga}}, T)$ in $10^2\ \Omega^{-1}cm^{-1}$	↗	4.383	4.387	4.401	4.459	4.641	4.881
$\propto(\mathrm{r_{Ga}}, T)$ in $10^5\ cm^{-1}$	↗	4.933	4.938	4.951	5.007	5.182	5.410
$\mathrm{R}(\mathrm{r_{Ga}}, T)$	↗	0.428	0.4282	0.4286	0.430	0.435	0.441
$\mathbb{E}_{gp} \equiv \mathbb{E}_{gp1}(\mathrm{T}, \mathrm{r_{In}})$ in eV	↘	1.7580	1.7573	1.7553	1.7473	1.7223	1.6903
$\mathrm{n}(\mathrm{r_{In}}, T)$	↗	4.111	4.1116	4.113	4.121	4.145	4.176
$\kappa(\mathrm{r_{In}}, T)$	↗	1.542	1.543	1.547	1.564	1.619	1.689
$\varepsilon_1(\mathrm{r_{In}}, T)$	↗	14.523	14.524	14.527	14.536	14.563	14.585
$\varepsilon_2(\mathrm{r_{In}}, T)$	↗	12.675	12.688	12.729	12.895	13.421	14.111

$\sigma_O(\mathrm{r_{In}}, T)$ in $10^2\ \Omega^{-1}cm^{-1}$	↗	4.341	4.346	4.360	4.417	4.597	4.833
$\propto(\mathrm{r_{In}}, T)$ in $10^5\ cm^{-1}$	↗	4.999	5.004	5.017	5.073	5.250	5.479
$\mathrm{R}(\mathrm{r_{In}}, T)$	↗	0.423	0.4231	0.4235	0.425	0.430	0.436
T in K		20	30	50	100	200	300

6. Concluding remarks

In the n(p)-type degenerate GaAs-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, $\varepsilon(\mathrm{r_{d(a)}})$, due to the impurity size effect, determined by an effective Bohr model [1], and given in Eq. (2),

(ii) the critical donor(acceptor)-density, $\mathrm{N_{CDn(NDp)}}(\mathrm{r_{d(a)}})$, 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: $\mathrm{N^* \equiv N - N_{CDn(CDp)}(r_{d(a)})}$, which gives a physical condition, needed to define the metal-insulator transition (**MIT**) at T=0K, as: $\mathrm{N^* \equiv N - N_{CDn(CDp)}} = 0$ or $\mathrm{N = N_{CDn(CDp)}}$, noting that $\mathrm{N_{CDn(CDp)}}$ can also be explained as the density of electrons(holes) localized in the exponential conduction(valence)-band tails (EBT), $\mathrm{N^{EBT}_{CDn(CDp)}}$, as that determined in Eq. (21), with a precision of the order of 2.35×10^{-3}, as observed in Table 1,

(iii) the Fermi energy, $\mathbb{E}_{\mathrm{Fn(Fp)}}(\mathrm{N^*, T})$, 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 FB-PM [11].

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

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

(b) as discussed in Eq. (5), in the MIT, in which $\mathbb{E}_{\mathrm{gn1(gp1)}}\left(\mathrm{N^*} = 0, \mathrm{r_{d(a)}}, \mathrm{T} = 0\right) = \mathbb{E}_{\mathrm{gni(gpi)}}\left(\mathrm{r_{d(a)}}\right)$,

where $\mathbb{E}_{\mathrm{gn1(gp1)}}$ and $\mathbb{E}_{\mathrm{gni(Fgpi)}}$ 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 $\alpha(E^* = 0, r_{d(a)}) = 0$, 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 GaAs-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, and their numerical results are given in Table 1. It means that $N^* = 0$ at this transition.

First, 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, the values of $g_{c(v)}(=1)$, and $m^*_{n(p)}/m_o$, defined in Section 2, can be equal to : $m_{n(p)}/m_o = 0.066\ (0.291)$, and to $m_r/m_o = \frac{m_n \times m_p}{m_n + m_p} = 0.0538$. Then, in particular, as used in Section 3 for determining the optical band gap in degenerate GaAs-crystals, $m^*_{n(p)}/m_o = m_r/m_o = 0.0538$ was chosen. Then, the reduced Fermi energy in the n(p)-type GaAs 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 GaAs-crystals, we define the effective reduced Wigner-Seitz radius $r_{sn(sp)}$, characteristic of the interactions, by:

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

In particular, in the following, $m^*_{n(p)}/m_o = m_r/m_o$, 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]:

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

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

$$\Delta\mathbb{E}_{gn}(N^*, r_d) \simeq a_1 \times \frac{\varepsilon_o}{\varepsilon(r_d)} \times N_r^{1/3} + a_2 \times \frac{\varepsilon_o}{\varepsilon(r_d)} \times N_r^{\frac{1}{3}} \times (2.503 \times [-\mathbb{E}_{CE}(r_{sn}) \times r_{sn}]) + a_3 \times \left[\frac{\varepsilon_o}{\varepsilon(r_d)}\right]^{5/4} \times \sqrt{\frac{m_v}{m_r}} \times N_r^{1/4} + a_4 \times \sqrt{\frac{\varepsilon_o}{\varepsilon(r_d)}} \times N_r^{1/2} \times 2 + a_5 \times \left[\frac{\varepsilon_o}{\varepsilon(r_d)}\right]^{\frac{3}{2}} \times N_r^{\frac{1}{6}},\ N_r \equiv \frac{N^*=N-N_{CDn}(r_d)}{9.999\times10^{17}\,cm^{-3}}, \quad \text{(B3)}$$

where $\varepsilon_o = \varepsilon_{As} = 13.13$, $a_1 = 6.8256 \times 10^{-3}$(eV), $a_2 = 1.1681 \times 10^{-3}$(eV), $a_3 = 5.0316 \times 10^{-3}$(eV), $a_4 = 10.1 \times 10^{-3}$(eV) and $a_5 = 1.4556 \times 10^{-3}$(eV), and

$$\Delta\mathbb{E}_{gp}(N^*, r_a) \simeq a_1 \times \frac{\varepsilon_o}{\varepsilon(r_a)} \times N_r^{1/3} + a_2 \times \frac{\varepsilon_o}{\varepsilon(r_a)} \times N_r^{\frac{1}{3}} \times \left(2.503 \times [-\mathbb{E}_{CE}(r_{sp}) \times r_{sp}]\right) + a_3 \times \left[\frac{\varepsilon_o}{\varepsilon(r_a)}\right]^{5/4} \times \sqrt{\frac{m_c}{m_r}} \times N_r^{1/4} + 2a_4 \times \sqrt{\frac{\varepsilon_o}{\varepsilon(r_a)}} \times N_r^{1/2} + a_5 \times \left[\frac{\varepsilon_o}{\varepsilon(r_a)}\right]^{\frac{3}{2}} \times N_r^{\frac{1}{6}},\ N_r \equiv \left(\frac{N^*=N-N_{CDp}(r_a)}{9.999\times10^{17}\,cm^{-3}}\right), \quad \text{(B4)}$$

where $\varepsilon_o = \varepsilon_{Ga} = 13.13$, $a_1 = 9.3290 \times 10^{-3}$(eV), $a_2 = 1.5958 \times 10^{-3}$(eV), $a_3 = 6.874 \times 10^{-3}$(eV), $a_4 = 13.7 \times 10^{-3}$(eV) and $a_5 = 1.9886 \times 10^{-3}$(eV).

Therefore, in Equations (B3, B4), at T=0 K 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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