



# **Accurate expressions for optical coefficients, given in n(p)-type degenerate GaSb-crystals, due to the impurity-size effect, and obtained from an improved Forouhi-Bloomer parameterization model (FB-PM)**

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## **Abstract**

As given in Eq. (2) and Table 1, our analytical expression for the static dielectric constant,  $\epsilon(r_{d(a)})$ , given in the n(p)-type GaSb crystal, expressed as a function of the donor (acceptor) radius,  $r_{d(a)}$ , and determined from an effective Bohr model, decreases with increasing  $r_{d(a)}$ . It strongly affects the critical d(a)-density in the metal-insulator transition (MIT) at the temperature  $T (=0K)$ ,  $N_{CDn(CDp)}(r_{d(a)})$ , determined in Eq. (3), and all the expressions for optical coefficients, determined from Equations (24, 25, 28, 29) for the n(p)-type degenerate GaSb semiconductors.

In particular, in the P-GaSb system at  $T=0K$ , Table 3c shows that our obtained results for those optical coefficients are found to be more accurate than the corresponding ones, obtained from the FB-PM [11], suggesting that the present model, used here to study the optical properties of the n(p)-type degenerate GaSb -crystal, could be 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

Our new expression for the extrinsic static dielectric constant,  $\epsilon(r_{d(a)})$ ,  $r_{d(a)}$  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,  $\epsilon(r_{d(a)})$  decreases, affecting strongly: the critical impurity density in the metal-insulator transition [1], and also optical properties, defined in heavily doped semiconductors [2, 3].

In the following Sections 2-5 [4, 11], in the  $n(p)$ -type degenerate GaSb-crystals, our numerical results of the optical coefficients, due to such the impurity-size effect, and obtained from an improved Forouhi-Bloomer parameterization model (IFB-PM), are presented, and also compared with the corresponding experimental-and-theoretical ones [9, 11], suggesting that our present model is found to be a good IFB-PM, as that observed in Table 3c. Finally, some concluding remarks are discussed and reported in Section 6.

## 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 GaSbs -crystal, such as: (i) if denoting the free electron mass by  $m_0$ , the effective electron (hole) mass,  $m_{n(p)}^*/m_0$ , which is respectively equal to the relative effective mass,  $m_{n(p)}/m_0 = 0.047$  (0.3) [5], 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,  $m_r/m_0 = \frac{m_n \times m_p}{m_n + m_p} = 0.040634$ , as used in Sections 3 and 5 to determine the optical band gap and the optical coefficients given in the  $n(p)$ -type heavily doped InAs-crystals. Further,  $E_{go} = E_{gGaSb} = E_{gSb} = E_{gGa} = 0.81$  eV [2, 5] is the unperturbed intrinsic band gap,  $\epsilon_{GaSb} = \epsilon_{Ga} = \epsilon_{Sb} = \epsilon_0 = 15.69$  is the relative static intrinsic dielectric constant of the GaSb-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  $\epsilon(r_{d(a)})$  decreases, the functions:  $\mathbb{E}_{gni(gpi)}(r_{d(a)})$ ,  $N_{CDn(NDp)}(r_{d(a)})$  and  $N_{CDn(CDp)}^{EBT}(r_{d(a)})$  increase. The maximal relative deviations between the numerical results of  $N_{CDn(NDp)}(r_{d(a)})$  and  $N_{CDn(CDp)}^{EBT}(r_{d(a)})$ , in absolute values, calculated using Equations (3, 21), are found to be equal to: 7.8% (5.9)%, respectively, suggesting that  $N_{CDn(NDp)}(r_{d(a)})$  can be explained by  $N_{CDn}^{EBT}(r_d)$ , being localized in the EBT. So, in the  $n(p)$ -type GaSb- crystal, in which  $(m_{n(p)}/m_0) = 0.047$  (0.3) [5], all the numerical results for the energy-band-structure parameters and  $N_{CDn(CDp)}(r_{d(a)})$ , being expressed as functions of  $r_{d(a)}$ -radius, are obtained, by using Equations (3, 9, 10, 11, 12, 13, 21).

Donor		P	As	Te	Sb	Sn
$r_d$ (nm) [4]	↗	0.110	0.118	0.132	0.136	0.140
$\epsilon(r_d)$	↘	18.7494	16.9954	15.7505	15.69	15.6284
$E_d(r_d)$ in meV	↗	1.8183	2.2130	2.5766	2.5965	2.6170
$E_{gni}(r_d)$ in eV	↗	0.8092	0.8096	0.80998	0.81	0.81002
$N_{CDn}(r_d)$ in $10^{17} \text{ cm}^{-3}$	↗	4.6883	6.2949	7.9085	8	8.0954
$N_{CDn}^{EBT}(r_d)$ in $10^{17} \text{ cm}^{-3}$	↗	5.0549	6.2463	7.3636	7.4250	7.4890

RD		<b>7.8%</b>	0.77%	6.9%	7.2%	7.5%
$R_{sn} < 1$ , from Eq. (7),	$\searrow$	0.0134	0.0123	0.0115	0.0114	0.0114

Acceptor		Ge	Ga(Al, Mn)	Mg	In
$r_a$ (nm) [4]	$\nearrow$	0.122	0.126	0.140	0.144
$\epsilon(r_a)$	$\searrow$	15.7605	15.69	14.8422	14.3386
$E_a(r_a)$ in meV	$\nearrow$	16.48	16.57	18.52	19.84
$E_{gpi}(r_a)$ in eV	$\nearrow$	0.8098	0.81	0.8119	0.8133
$N_{CDp}(r_a)$ in $10^{17} \text{ cm}^{-3}$	$\nearrow$	7.8931	8	9.4507	10.4818
$N_{CDp}^{EBT}(r_a)$ in $10^{17} \text{ cm}^{-3}$	$\nearrow$	8.3576	8.4232	9.2832	9.8655
RD		<b>5.9%</b>	5.35%	1.8%	5.88%
$R_{sp} < 1$ , from Eq. (7),	$\searrow$	0.4581	0.4575	0.4490	0.4436

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

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

In the [d(a)-GaSb]-systems, since  $r_{d(a)}$ , given in tetrahedral covalent bonds, is usually either larger or smaller than  $r_{Sb(Ga)} = 0.136 \text{ nm}$  ( $0.126 \text{ nm}$ ), a local mechanical strain (or deformation potential energy) is induced, according to a compression (dilation) for:  $r_{d(a)} > r_{As(In)}$  ( $r_{d(a)} < r_{As(In)}$ ), 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,  $\epsilon(r_{d(a)})$ , 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  $E_{gni(gpi)}(r_{d(a)})$  and the effective donor(acceptor)-ionization energy  $E_{d(a)}(r_{d(a)})$  in absolute values, obtained in an effective Bohr model, as:

$$E_{gni(gpi)}(r_{d(a)}) - E_{go} = E_{d(a)}(r_{d(a)}) - E_{do(ao)} = E_{do(ao)} \times \left[ \left( \frac{\epsilon_0}{\epsilon(r_{d(a)})} \right)^2 - 1 \right], \quad (1)$$

where  $E_{do(ao)} \equiv \frac{13600 \text{ meV} \times (m_{n(p)}/m_0)}{\epsilon_0^2} = 2.5965 \text{ meV}$  ( $16.57 \text{ meV}$ ), and

$$\epsilon(r_{d(a)}) = \frac{\epsilon_0}{\sqrt{1 + \left[ \left( \frac{r_{d(a)}}{r_{Sb(Ga)}} \right)^3 - 1 \right] \times \ln \left( \frac{r_{d(a)}}{r_{Sb(Ga)}} \right)^3}} \leq \epsilon_0, \text{ for } r_{d(a)} \geq r_{Sb(Ga)},$$

$$\epsilon(r_{d(a)}) = \frac{\epsilon_0}{\sqrt{1 - \left[ \left( \frac{r_{d(a)}}{r_{Sb(Ga)}} \right)^3 - 1 \right] \times \ln \left( \frac{r_{d(a)}}{r_{Sb(Ga)}} \right)^3}} \geq \epsilon_0, \left[ \left( \frac{r_{d(a)}}{r_{Sb(Ga)}} \right)^3 - 1 \right] \times \ln \left( \frac{r_{d(a)}}{r_{Sb(Ga)}} \right)^3 < 1, \text{ for } r_{d(a)} \leq r_{Sb(Ga)}. \quad (2)$$

## 2.2. Our expressions for the critical density in the MIT

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

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

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

$$a_{Bn(Bp)}(r_{d(a)}) \equiv \frac{\varepsilon(r_{d(a)}) \times \hbar^2}{m_{n(p)}^* \times q^2} = 0.53 \times 10^{-8} \text{ cm} \times \frac{\varepsilon(r_{d(a)})}{(m_{n(p)}^*/m_0)}, \quad (4)$$

where  $-q$  is the electron charge,  $\varepsilon(r_{d(a)})$  is determined in Eq. (2), in which  $m_{n(p)}^*/m_0 = m_{n(p)}/m_0 = 0.047(0.3)$ . Here, we have chosen, in this work,  $y=1.6425(0.25732)$  so that we obtain:  $N_{CDn(NDp)}(r_{Sb(Ga)}) = 8 \times 10^{17} \text{ cm}^{-3}$  [5]. Then, 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), being localized in exponential conduction (valance)-band (EBT) tails,  $N_{CDn(CDp)}^{EBT}(r_{d(a)})$ , obtained using the next 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  $N_{CDn(CDp)}^{EBT}(r_{d(a)})$  are found to be equal to: 7.8% (5.9%), respectively. Thus, the numerical results of  $N_{CDn(NDp)}(r_{d(a)})$  are obtained, using Eq. (3), can be explained by the densities of electrons (holes) localized in exponential conduction (valance)-band (EBT) tails,  $N_{CDn(CDp)}^{EBT}(r_{d(a)})$ , being determined from Eq. (21).

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

### 3. Optical band gap

Here,  $m_{n(p)}^*/m_0$  is chosen as:  $m_{n(p)}^*/m_0 = m_r/m_0 = 0.040634$ , and then, if denoting  $N^* \equiv N - N_{CDn(NDp)}(r_{d(a)})$ , the optical band gap (**OBG**) is found to be given by:

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

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

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

Here, the effective intrinsic band gap  $E_{gnei(gpei)}$  is determined by:

$$E_{gnei(gpei)}(r_{d(a)}, T) \equiv E_{gni(gpi)}(r_{d(a)}) - 0.20251 \text{ eV} \times \left( \left[ 1 + \left( \frac{2T}{440.0613 \text{ K}} \right)^{2.201} \right]^{\frac{1}{2.201}} - 1 \right),$$

and the band gap narrowing,  $\Delta E_{gn(gp)}(N^*, r_{d(a)})$ , are determined in Equations (B3, B4) of the Appendix B and the values of  $E_{gni(gpi)}(r_{d(a)})$  are given in Table 1. In particular, in the n(p)-type Sb(Ga)-GaSb crystals, one gets:  $E_{gnei(gpei)}(r_{Sb(Ga)}, T = 300 \text{ K}) = 0.68 \text{ eV}$  [5].

Then, as noted in the Appendix A and B, at  $T=0\text{K}$ , as  $N^* = 0$ , one has:  $E_{Fn(Fp)}(N^*, T) = E_{Fno(Fpo)}(N^*) = 0$ , as given in Eq. (A4), and  $\Delta E_{gn(gp)}(N^*, r_{d(a)}) = 0$ , according to the MIT, as noted in Appendix A and B.

Therefore,  $E_{gn1(gp1)} = E_{gn2(gp2)} = E_{gnei(gpei)}(r_{d(a)}) = E_{gni(gpi)}(r_{d(a)})$  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 GaSb, 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

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

being proportional to  $N^{*-1/3}$ . Here,  $\gamma = (4/9\pi)^{1/3}$ ,  $k_{Fn(Fp)}^{-1}$  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

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

where the empirical parameters:  $a = 0.068$  (0.7615) and  $b = 0$  (0), respectively, were chosen so that the relative deviations between  $N_{CDn(NDp)}$  and  $N_{CDn(CDp)}^{EBT}$ , in absolute values, are minimized, as observed in Table 1. Here, 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  $R_{snTF(spTF)}(N^*, r_{d(a)})$  is reduced to

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

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

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

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

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

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

being needed to determine the expression for optical coefficients, as those investigated in Section 5. Here,  $R_{sn(sp)}$  is defined in Eq. (7).

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

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

where  $N$  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)- GaSb system, defined as

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

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  $\vec{k}$ -space is given by

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

where  $\Omega$  is the total GaSb -crystal volume.

Then, the effective auto-correlation function for potential fluctuations,  $W_{n(p)}(v_{n(p)}, N^*, r_d) \equiv \langle V(r)V(r') \rangle$ , was determined as [3] :

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

Here,  $\epsilon(r_{d(a)})$  is determined in Eq. (2),  $R_{sn(sp)}(N^*, r_{d(a)})$  in Eq. (7), the empirical Heisenberg parameter  $\mathcal{H} = 0.1$  (0.1), 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  $v_{n(p)} \equiv \frac{-\mathbb{E}}{\mathbb{E}_{Fno(Fpo)}}$ ,

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  $W_{n(p)}(v_{n(p)}, N^*, r_{d(a)})$ .

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

### A. Kane integration method (KIM)

In degenerate d(a)- GaSb 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

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

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

and using an identity:

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

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:

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

## 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

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

noting that as  $a=1$ ,  $(it)^{-\frac{3}{2}} \times \exp\left\{-\frac{(t\sqrt{W_{n(p)}})^2}{2\hbar^2}\right\}$  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:  $\langle \mathbb{E}_k^{a-\frac{1}{2}} \rangle_{\text{FPIM}} \equiv \langle \mathbb{E}_k^{a-\frac{1}{2}} \rangle_{\text{KIM}}$ ,  $\langle \mathbb{E}_k^{a-\frac{1}{2}} \rangle_{\text{KIM}}$  being determined in Eq. (13).

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

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

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

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

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

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

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

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

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

(ii)  $\mathbb{E} \leq 0$  – case.

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

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

$$\beta(1) = \frac{\sqrt{\pi}}{2^{\frac{3}{4}} \Gamma(5/4)} \text{ and } \beta(5/2) = \frac{\sqrt{\pi}}{2^{3/2}}.$$

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

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

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

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

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

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

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

such that:  $F_{n(p)}(v_{n(p)}, r_{d(a)}, a) \rightarrow H_{n(p)}(v_{n(p)}, r_{d(a)}, a)$  for  $0 \leq v_n \leq 16$ , and  $F_{n(p)}(v_{n(p)}, r_{d(a)}, a) \rightarrow K_{n(p)}(v_{n(p)}, r_{d(a)}, a)$  for  $v_{n(p)} \geq 16$ . 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),  $N_{\text{CDn(CDp)}}^{\text{EBT}}(N, r_{d(a)})$ , in the following.

### C. Critical impurity density in the MIT

In degenerate d(a)- GaSb systems at  $T=0$  K, in which  $m_{n(p)}^*/m_0 = m_{n(p)}/m_0 = 0.047$  (0.3), as given in Section 2, using Eq. (13), for  $a=1$ , the density of states  $\mathcal{D}(\mathbb{E})$  is defined by:

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

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

Here,  $E_{\text{Fno}}$  is determined in Eq. (A4) of the Appendix A, with  $m_{n(p)}^*/m_0 = m_{n(p)}/m_0$  and  $\mathcal{H} = 0.1$  (0.1), respectively, being chosen such that the following determination of  $N_{\text{CDn(CDp)}}^{\text{EBT}}(N, r_{d(a)})$  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

$\frac{1}{f(a=1)} \langle \mathbb{E}_k^2 \rangle_{\text{KIM}}$  is now replaced by:

$$\frac{1}{f(a=1)} \langle \mathbb{E}_k^2 \rangle_{\text{KIM}} = \frac{\mathcal{D}(\mathbb{E} \leq 0)}{\mathcal{D}_0} = F_{n(p)}(v_{n(p)}, r_{d(a)}, a = 1), \quad \mathcal{D}_0 = \frac{g_c(v) \times (m_{n(p)} \times m_o)^{3/2} \times \sqrt{\eta_{n(p)}}}{2\pi^2 \hbar^3} \times \beta(a = 1), \quad \beta(a = 1) = \frac{\sqrt{\pi}}{2^4 \times \Gamma(5/4)}. \quad (19)$$

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

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

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

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

where

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

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

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

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

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

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

Finally, Eq. (20) now yields:

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

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

The numerical results of  $N_{\text{CDn(CDp)}}^{\text{EBT}}[N = N_{\text{CDn(NDp)}}(r_{d(a)})] \equiv N_{\text{CDn(CDp)}}^{\text{EBT}}(r_{d(a)})$ , for a simplicity of presentation, evaluated using Eq. (21), are given in Table 1, confirming thus those of  $N_{\text{CDn(NDp)}}(r_{d(a)})$ , calculated using Eq. (3), with a precision of the order of 7.8% (5.9%), respectively. In other words, this critical d(a)-density  $N_{\text{CDn(NDp)}}(r_{d(a)})$  can thus be explained by the density of electrons(holes) localized in the EBT,  $N_{\text{CDn(CDp)}}^{\text{EBT}}(r_{d(a)})$ .

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

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

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

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

## 5. Optical coefficients

Here,  $m_{\text{n(p)}}^*/m_0$  is chosen as:  $m_{\text{n(p)}}^*/m_0 = m_r/m_0 = 0.040634$ , as that used in Section 3, for determining the optical band gap in degenerate GaSb-crystals.

The optical properties of any medium can be described by the complex refraction index  $\mathbb{N}$  and the complex dielectric function  $\varepsilon$ ,  $\mathbb{N} \equiv n - i\kappa$  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  $\varepsilon$  denoted by  $\varepsilon_1$  and  $\varepsilon_2$  can thus be expressed in terms of the refraction index  $n$  and the extinction coefficient  $\kappa$  as:  $\varepsilon_1 \equiv n^2 - \kappa^2$  and  $\varepsilon_2 \equiv 2n\kappa$ . One notes that the optical absorption coefficient  $\alpha$  is related to  $\varepsilon_2$ ,  $n$ ,  $\kappa$ , and the optical conductivity  $\sigma_0$  by [3]

$$\alpha(E) \equiv \frac{\hbar q^2 \times |v(E)|^2}{n(E) \times \varepsilon_{\text{free space}} \times c E} \times J(E^*) = \frac{E \times \varepsilon_2(E)}{\hbar c n(E)} \equiv \frac{2E \times \kappa(E)}{\hbar c} \equiv \frac{4\pi\sigma_0(E)}{c n(E) \times \varepsilon_{\text{free space}}}, \quad \varepsilon_1 \equiv n^2 - \kappa^2 \text{ and } \varepsilon_2 \equiv 2n\kappa, \quad (24)$$

where the effective photon energy:  $E^* = E - E_{\text{gn(gp)}}$  is the reduced photon energy, the band gap  $E_{\text{gn(gp)}}$  can be equal to the optical band gap  $E_{\text{gn1(gp1)}}$ , the effective intrinsic band gap  $E_{\text{gnei(gpei)}}$ , or to the intrinsic band gap  $E_{\text{gni(gpi)}}$ , determined in Eq. (5). Here,  $E \equiv \hbar\omega$ ,  $-q$ ,  $\hbar$ ,  $|v(E)|$ ,  $\omega$ ,  $\varepsilon_{\text{free space}}$ ,  $c$  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 GaSb -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  $\kappa(E)$  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,  $\varepsilon_1$  and  $\varepsilon_2$ , (or  $n$  and  $\kappa$ ), are both known, the other ones defined above can thus be determined.

Then, using a transformation for the joint density of states,  $J(E^*)$ , given in allowed direct InAs -transitions, one obtains: at low values of  $E$ ,  $E_{\text{gni(gpi)}} \leq E \leq 1.6 \text{ eV}$ , and for  $a = \left(\frac{1}{2} + 10^{-21}\right)$ ,

$$J_{\text{n(p)}}(E^*) = \frac{1}{2\pi^2} \times \left(\frac{2m_r}{\hbar^2}\right)^{3/2} \times E_{\text{gni(gpi)}}^{1-a} \times (E - E_{\text{gn(gp)}})^{a-(1/2)} = \frac{1}{2\pi^2} \times \left(\frac{2m_r}{\hbar^2}\right)^{3/2} \times E_{\text{gni(gpi)}}^{\left(\frac{1}{2}-10^{-21}\right)} \times (E - E_{\text{gn(gp)}})^{10^{-21}} \quad (26)$$

and, at large values of E,  $E \geq 1.6$  eV and for  $a=5/2$ ,

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

Further, one notes that, as  $E \rightarrow \infty$ , Forouhi and Bloomer (FB) [11] claimed that  $\kappa(E \rightarrow \infty) \rightarrow$  a constant, while the  $\kappa(E)$  -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:  $\sigma_0(E)$  and  $\alpha(E)$ , given in Eq. (24), both go 0 as  $E^{-2}$ .

Now, taking into account Equations (26, 27) and also those remarks, an improved Forouhi-Bloomer parameterization model (IFB-PM), used to determine the accurate expressions of the optical coefficients, obtained in the degenerate  $n(p)$  type GaSb -crystals, is proposed as follows.

If, defining the band gap  $E_{gn(gp)}$ , which can be equal to the optical band gap  $E_{gn1(gp1)}$ , the effective intrinsic band gap  $E_{gnei(gpei)}$ , or to the intrinsic band gap  $E_{gni(gpi)}$ , determined in Equations (1, 5), and defining the function:  $f(E) \equiv \sum_{i=1}^4 \frac{A_i}{g(E)-B_iE+C_i}$ , where  $g(E)=E^2 \times \left(1 + 10^{-4} \times \frac{E}{6}\right)$ , we propose:

$$\begin{aligned} \kappa(E^*) &= f(E) \times E_{gni(gpi)}^{(2-10^{-21})} \times (E^* \equiv E - E_{gn1(gp1)})^{10^{-21}}, \text{ for } E_{gni(gpi)} \leq E \leq 1.6 \text{ eV}, \\ &= f(E) \times (E^* \equiv E - E_{gn1(gp1)})^2, \text{ for } E \geq 1.6 \text{ eV}, \end{aligned} \quad (28)$$

being equal to 0 for  $E^* = 0$  (or for  $E = E_{gn1(gp1)}$ ), and also going to 0 as  $E^{-1}$  as  $E \rightarrow \infty$ . Further,

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

going to a constant, as  $E \rightarrow \infty$ ,  $n(E \rightarrow \infty, r_{d(a)}) = n_{\infty}(r_{d(a)}) = \sqrt{\varepsilon(r_{d(a)})} \times \frac{\omega_T}{\omega_L}$ ,  $\omega_T = 4.3 \times 10^{13} \text{ s}^{-1}$  [5]

and  $\omega_L = 1.00819 \times 10^{14} \text{ s}^{-1}$ , obtained from the Lyddane-Sachs-Teller relation [5], from which  $T(L)$

represents the transverse (longitudinal) optical phonon mode, so that, in the P-GaSb system, in which

$E_{gni(r_p)} = 0.8092 \text{ eV}$ , we obtain:  $n_{\infty}(r_p) = 1.846799$ . One also notes that in the FB-PM [11],

$n_{\infty(\text{FB-PM})} = 1.914$  and the band gap  $E_{g(\text{FM-PM})} = 0.65 \text{ eV} < E_{gni(r_p)} = 0.8092 \text{ eV}$ , as observed in Table

1. Here,  $B_{oi}(E_{gnei(gpei)}) = \frac{A_i}{Q_i} \times \left[-\frac{B_i^2}{2} + E_{gnei(gpei)}B_i - E_{gnei(gpei)}^2 + C_i\right]$ ,  $C_{oi}(E_{gnei(gpei)}) = \frac{A_i}{Q_i} \times$

$\left[\frac{B_i \times (E_{gnei(gpei)}^2 + C_i)}{2} - 2E_{gnei(gpei)}C_i\right]$ ,  $Q_i = \frac{\sqrt{4C_i - B_i^2}}{2}$ , where, for  $i=(1, 2, 3, \text{ and } 4)$ , the numerical values of the

parameters for the GaSb-crystal, are chosen as:  $A_i = A_{i(\text{FB})}$ ,  $B_i = B_{i(\text{FB})}$ , and  $C_i = C_{i(\text{FB})}$ . Here, the values of  $A_{i(\text{FB})}$ ,  $B_{i(\text{FB})}$ , and  $C_{i(\text{FB})}$  are given in Ref. [11].

The important numerical results of the above optical functions, at  $T=0\text{K}$ ,  $N = N_{\text{CDn}(\text{CDp})}$ , and for  $E = E_{gni(gi)}$ , 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  $E_{CPE} = E = E_{gni(gpi)}(r_{d(a)})$ ,  $\kappa_{MIT}(E_{gni(gpi)}, r_{d(a)}) = 0$ ,  $\varepsilon_{2(MIT)}(E_{gni(gpi)}, r_{d(a)}) = 0$ ,  $\sigma_{O(MIT)}(E_{gni(gpi)}, r_{d(a)}) = 0$  and  $\alpha_{MIT}(E, r_{d(a)}) = 0$ , and the other functions such as :  $n_{MIT}(E_{gni(gpi)}, r_{d(a)})$ ,  $\varepsilon_{1(MIT)}(E_{gni(gpi)}, r_{d(a)})$ , and  $R_{MIT}(E_{gni(gpi)}, r_{d(a)})$  decrease, with increasing  $r_{d(a)}$  and  $E_{gni}(r_{d(a)})$ .

Donor		P	As	Te	Sb	Sn
At the MIT, $T=0K$ , $N=N_{CDn}(r_d)$ , and the critical photon energy $E_{CPE} = E = E_{gni}(r_a)$ , one has :						
$E_{gni}(r_d)$ in eV	↗	0.8092	0.8096	0.80998	0.81	0.81002
$n_{MIT}(E_{gni}, r_d)$	↘	3.2051	3.1164	3.0505	3.0472	3.0439
$\kappa_{MIT}(E_{gni}, r_d)$		0	0	0	0	0
$\varepsilon_{1(MIT)}(E_{gni}, r_d)$	↘	10.272828	9.711691	9.305541	9.285606	9.265294
$\varepsilon_{2(MIT)}(E_{gni}, r_d)$		0	0	0	0	0
$\sigma_{O(MIT)}(E_{gni}, r_d)$		0	0	0	0	0
$\alpha_{MIT}(E_{gni}, r_d)$		0	0	0	0	0
$R_{MIT}(E_{gni}, r_d)$	↘	0.2750	0.2643	0.2563	0.2559	0.2554

  

Acceptor		Ge	Ga(Al, Mn)	Mg	In
At the MIT, $T=0K$ , $N=N_{CDp}(r_a)$ , and the critical photon energy $E_{CPE} = E = E_{gpi}(r_a)$ , one has :					
$E_{gpi}(r_a)$ in eV	↗	0.8098	0.81	0.8119	0.8133
$n_{MIT}(E_{gpi}, r_a)$	↘	3.0512	3.0472	2.9997	2.9707
$\kappa_{MIT}(E_{gpi}, r_a)$		0	0	0	0
$\varepsilon_{1(MIT)}(E_{gpi}, r_a)$	↘	9.3095	9.2856	8.9979	8.8248
$\varepsilon_{2(MIT)}(E_{gpi}, r_a)$		0	0	0	0
$\sigma_{O(MIT)}(E_{gpi}, r_a)$		0	0	0	0
$\alpha_{MIT}(E_{gpi}, r_a)$		0	0	0	0
$R_{MIT}(E_{gpi}, r_a)$	↘	0.2563	0.2559	0.2499	0.2463

**Table 2b.** In d(a)-GaSb systems, the values of the following optical coefficients at the total carrier energy  $E \leq 0$ , as that given in Section 4, being expressed as functions of  $r_{d(a)}$ , and calculated using Equations (31-36, 24), for  $E^* = E_{gni(gpi)}(r_{d(a)})$ , present the exponential tail-states for  $\kappa^{EEC-T}$ ,  $\varepsilon_2^{ElmD-T}$ ,  $\sigma_0^{EOC-T}$ ,  $\sigma_0^{EOC-T}$ ,  $\alpha^{EOAC-T}$  and  $R^{NIR-T}$ , and their variations with increasing  $r_{d(a)}$  are represented by the arrows: ↗ and ↘, suggesting that the obtained results of  $n^{ERI-T}$ ,  $\varepsilon_1^{EReD-T}$ , and  $R^{NIR-T}$  are almost equal to the corresponding ones given in the above Table 2a.

d- GaSb systems		P	As	Te	Sb	Sn
$n^{ERI-T}(r_d)$	↘	3.2051	3.1164	3.0505	3.0472	3.0439
$\kappa^{EEC-T}(r_d)$ in $10^{-3}$	↗	0.0848	0.0849	0.0850	0.08504	0.08505
$\varepsilon_1^{EReD-T}(r_d)$	↘	10.2656	9.7045	9.2983	9.2784	9.2581
$\varepsilon_2^{ElmD-T}(r_d)$	↘	0.5436	0.5293	0.5188	0.5183	0.5177
$\sigma_0^{EOC-T}(r_d)$ in $\Omega^{-1}cm^{-1}$	↘	4.7086	4.5868	4.4976	4.4932	4.4888
$\alpha^{EOAC-T}(r_d)$ in $10^3 cm^{-1}$	↗	6.9548	6.9678	6.9798	6.9805	6.9811
$R^{NIR-T}(r_d)$	↘	0.2753	0.2646	0.2566	0.2562	0.2558

a- GaSb systems		Ge	Ga(Al, Mn)	Mg	In
$n^{\text{ERI-T}}(r_a)$	$\searrow$	3.0511	3.0472	2.9997	2.9707
$\kappa^{\text{EEC-T}}(r_a)$	in $10^{-3}$ $\nearrow$	0.0850	0.08504	0.0856	0.0860
$\varepsilon_1^{\text{EReD-T}}(r_a)$	$\searrow$	9.3023	9.2784	8.9906	8.8174
$\varepsilon_2^{\text{ElmD-T}}(r_a)$	$\searrow$	0.5186	0.5183	0.5137	0.5111
$\sigma_0^{\text{EOC-T}}(r_a)$	in $\Omega^{-1}\text{cm}^{-1}$ $\searrow$	4.4947	4.4932	4.4641	4.4487
$\alpha^{\text{EOAC-T}}(r_a)$	in $10^3 \text{ cm}^{-1}$ $\nearrow$	6.9738	6.9804	7.0451	7.0894
$R^{\text{NIR-T}}(r_a)$	$\searrow$	0.2566	0.2562	0.2503	0.2467

**Table 2c.** Here, the choice of the real refraction index:  $n(E \rightarrow \infty, r_{d(a)}) = n_\infty(r_{d(a)}) = \sqrt{\varepsilon(r_{d(a)})} \times \frac{\omega_T}{\omega_L}$ ,  $\omega_T = 4.3 \times 10^{13} \text{ s}^{-1}$  [5] and  $\omega_L = 1.00819 \times 10^{14} \text{ s}^{-1}$ , obtained from the Lyddane-Sachs-Teller relation [5], from which T(L) represents the transverse (longitudinal) optical phonon mode, giving rise to  $n_\infty(r_p) = 1.8468$ , and further, that of the asymptotic behavior, given for the extinction coefficient:  $\kappa_\infty(E \rightarrow \infty, r_{d(a)}) \rightarrow 0$ , as  $E^{-1}$ , so that  $\sigma_0(E \rightarrow \infty, r_{d(a)})$  and  $\alpha(E \rightarrow \infty, r_{d(a)})$  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
$\varepsilon(r_d)$	$\searrow$	18.7494	16.9954	15.7505	15.69	15.6284
$n_\infty(r_d)$	$\searrow$	1.8468	1.7583	1.6927	1.6894	1.6861
$\kappa_\infty(r_d)$		0	0	0	0	0
$\varepsilon_{1,\infty}(r_d) = n_\infty(r_d)^2$	$\searrow$	3.410668	3.091599	2.865151	2.854139	2.84293
$\varepsilon_{2,\infty}(r_d)$		0	0	0	0	0
$\sigma_{0,\infty}(r_d)$	in $\frac{10^5}{\Omega \times \text{cm}}$ $\searrow$	10.8204	10.3019	9.9174	9.8983	9.8789
$\alpha_\infty(r_d)$	in $(10^9 \times \text{cm}^{-1})$	2.7737	2.7737	2.7737	2.7737	2.7737
$R_\infty(r_d)$	$\searrow$	0.08848	0.07558	0.06617	0.06571	0.06524

  

Acceptor		Ge	Ga(Al, Mn)	Mg	In
$\varepsilon(r_a)$	$\searrow$	15.7605	15.69	14.8422	14.3386
$n_\infty(r_a)$	$\searrow$	1.6932	1.6894	1.6431	1.6150
$\kappa_\infty(r_a)$		0	0	0	0
$\varepsilon_{1,\infty}(r_a)$	$\searrow$	2.8670	2.8541	2.6999	2.6083
$\varepsilon_{2,\infty}(r_a)$		0	0	0	0
$\sigma_{0,\infty}(r_a)$	in $\frac{10^5}{\Omega \times \text{cm}}$ $\searrow$	9.9205	9.8983	9.6272	9.4625
$\alpha_\infty(r_a)$	in $(10^9 \times \text{cm}^{-1})$	2.7737	2.7737	2.7737	2.7737
$R_\infty(r_a)$	$\searrow$	0.0662	0.0657	0.0592	0.0553

**Table 3a.** In the P-GaSb 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  $E_{\text{gnt}}(r_p) [= 0.8092 \text{ eV}]$ , and the corresponding ones, obtained from the FB-model [11], are reported in this Table 3a, in which the relative deviations (RDs) of those are also given and calculated, using the Aspnes-and-Studna (AS)-data [9]. Here, as repoted in above Table 2c, we obtain here:  $\kappa_{\infty}(E \rightarrow \infty, r_p) \rightarrow 0$  and  $\epsilon_{2,\infty}(E \rightarrow \infty, r_p) \rightarrow 0$ , while, in this Table 3a,  $\kappa_{\infty(\text{FB})}(E \rightarrow \infty, r_p) = 0.45617$  and  $\epsilon_{2,\infty(\text{FB})}(E \rightarrow \infty, r_p) = 1.746219$ .

E in eV	n (RD%)	$\kappa$ (RD%)	$\epsilon_1$ (RD%)	$\epsilon_2$ (RD%)	$n_{\text{FB}}$ (RD%)	$\kappa_{\text{FB}}$ (RD%)	$\epsilon_{1(\text{FB})}$ (RD%)	$\epsilon_{2(\text{FB})}$ (RD%)
$E_{\text{gnt}}(r_p)$	3.2051	0	10.272828	0	3.491711	0.0032833	12.192034	0.022929
<b>1.5</b>	3.863 ( <b>11.9</b> )	0.195 (43.4)	14.888 (22.2)	1.5039 (50.2)	4.245 (3.3)	0.215 ( <b>37.6</b> )	17.971 (6.1)	1.823 ( <b>39.7</b> )
<b>1.6</b>	4.000 (11.2)	0.224 ( <b>46.2</b> )	15.954 (20.8)	1.791 ( <b>52.3</b> )	4.399 (2.4)	0.308 (25.8)	19.25 (4.4)	2.714 (27.6)
1.7	4.150 (10.6)	0.314 (35.3)	17.122 (19.7)	2.604 (42.1)	4.566 (1.6)	0.436 (10.1)	20.657 (3.1)	3.982 (11.6)
1.8	4.312 (10.5)	0.454 (25.7)	18.386 (19.4)	3.916 (33.5)	4.746 (1.5)	0.612 (0.1)	22.154 (2.9)	5.809 (1.3)
1.9	4.489 (11.1)	0.665 (19.8)	19.708 (20.6)	5.970 (28.7)	4.943 (2.2)	0.874 (5.4)	23.668 (4.7)	8.638 (3.2)
2	4.624 (11.7)	1.055 (23.4)	20.267 (20.7)	9.756 (32.4)	5.082 (3.0)	1.360 (1.3)	23.974 (6.1)	13.822 (4.3)
2.1	4.316 (8.3)	1.411 (21.7)	16.634 (11.9)	12.182 (28.1)	4.661 (0.9)	1.789 (0.7)	18.522 (1.9)	16.681 (1.7)
2.2	4.216 (6.7)	1.404 (19.6)	15.801 (9.1)	11.842 (25)	4.516 (0.1)	1.746 (0.03)	17.341 (0.2)	15.772 (0.1)
2.3	4.204 (6.4)	1.536 (14.1)	15.311 (9.8)	12.918 (19.6)	4.484 (0.2)	1.883 (5.3)	16.564 (2.4)	16.890 (5.1)
2.4	4.131 (8.5)	1.697 (13.5)	14.186 (14.1)	14.024 (20.8)	4.382 (2.9)	2.055 (4.7)	14.982 (9.3)	18.012 (1.7)
<b>2.5</b>	4.014 (6.9)	1.829 (19.9)	12.764 (4.5)	14.686 (25.5)	4.230 ( <b>18.9</b> )	2.191 (4.1)	13.097 (2.0)	18.539 (5.9)
2.6	3.880 (2.6)	1.915 (15.9)	11.388 (6.7)	14.864 (18.2)	4.063 (2.0)	2.272 (0.3)	11.349 (6.3)	18.465 (1.6)
2.7	3.755 (2.1)	1.957 (11.5)	10.269 (4.5)	14.699 (13.4)	3.910 (1.9)	2.302 (4.1)	9.988 (1.6)	18.000 (6.1)
2.8	3.654 (2.8)	1.967 (8.8)	9.486 (0.02)	14.376 (11.3)	3.788 (0.3)	2.295 (6.4)	9.081 (4.2)	17.388 (7.2)
2.9	3.586 (3.8)	1.959 (7.6)	9.024 (3.9)	14.052 (11.1)	3.706 (0.6)	2.270 (7.0)	8.581 (8.7)	16.823 (6.4)
3	3.552 (4.8)	1.948 (7.6)	8.825 (6.9)	13.839 (12)	3.664 (1.8)	2.242 (6.3)	8.398 (11.4)	16.432 (4.4)
3.1	3.550 (5.7)	1.945 (8.8)	8.817 (8.4)	13.811 (14)	3.659 (2.8)	2.226 (4.3)	8.435 (12.4)	16.291 (1.4)
3.2	3.574 (5.9)	1.961 (11.2)	8.928 (6.6)	14.022 (16.5)	3.685 (3.0)	2.232 (1.0)	8.597 (10)	16.454 (2.0)
3.3	3.619 (4.9)	2.006 (13.5)	9.078 (0.5)	14.519 (17.8)	3.735 (1.9)	2.271 (2.0)	8.788 (3.6)	16.965 (3.9)
3.4	3.677 (3.1)	2.086 (14.1)	9.168 (7.9)	15.344 (16.8)	3.798 (0.1)	2.352 (3.2)	8.890 (4.7)	17.864 (3.1)
3.5	3.736 (1.3)	2.212 (13.1)	9.062 (15.4)	16.526 (14.2)	3.861 (2.0)	2.483 (2.4)	8.744 (11.3)	19.175 (0.5)
3.6	3.778 (0.1)	2.388 (11.2)	8.570 (22.2)	18.049 (11.1)	3.907 (3.5)	2.671 (0.7)	8.129 (15.9)	20.870 (2.8)
3.7	3.782 (0.9)	2.617 (8.5)	7.454 (27.4)	19.796 (7.7)	3.909 (4.3)	2.916 (1.9)	6.774 (15.7)	22.798 (6.3)
3.8	3.718 (0.5)	2.887 (5.9)	5.488 (28.2)	21.470 (5.5)	3.836 (3.6)	3.207 (4.5)	4.429 (3.5)	24.604 (8.3)
<b>3.9</b>	3.560 (1.7)	3.170 (4.6)	2.621 (27.3)	22.573 (6.2)	3.659 (1.1)	3.511 (5.7)	1.061 ( <b>48.4</b> )	25.697 (6.8)
<b>4</b>	3.297 (4.4)	3.420 (6.1)	-0.826 ( <b>39.9</b> )	22.546 (10.3)	3.368 (2.3)	3.777 (3.7)	-2.920 ( <b>112.5</b> )	25.441 (1.2)
4.1	2.949 (4.9)	3.582 (9.9)	-4.136 (33.3)	21.129 (14.3)	2.986 (3.7)	3.946 (0.7)	-6.655 (7.3)	23.566 (4.4)
4.2	2.568 (1.8)	3.626 (12.2)	-6.553 (38.7)	18.628 (10.6)	2.570 (1.9)	3.984 (3.5)	-9.268 (13.4)	20.476 (1.7)
4.3	2.214 (11.3)	3.555 (9.4)	-7.738 (32.3)	15.478 (0.9)	2.185 (9.8)	3.896 (0.7)	-10.406 (9.0)	17.024 (9.1)
4.4	1.929 (11.8)	3.404 (6.2)	-7.867 (22.8)	13.133 (5.1)	1.876 (8.9)	3.721 (2.5)	-10.323 (1.2)	13.961 (11.7)
4.5	1.725 (8.8)	3.214 (5.2)	-7.357 (18.1)	11.093 (3.1)	1.658 (4.5)	3.505 (3.3)	-9.534 (6.1)	11.622 (8.0)
4.6	1.597 (6.2)	3.022 (5.8)	-6.581 (18.0)	9.649 (0.08)	1.522 (1.3)	3.287 (2.4)	-8.485 (5.6)	10.005 (3.8)
4.7	1.526 (5.7)	2.847 (6.8)	-5.778 (20.3)	8.691 (1.5)	1.450 (0.4)	3.090 (1.1)	-7.446 (2.7)	8.959 (1.5)
4.8	1.496 (6.2)	2.702 (7.7)	-5.065 (23.2)	8.086 (1.9)	1.421 (0.9)	2.927 (0.05)	-6.546 (0.7)	8.318 (0.9)
4.9	1.490 (7.4)	2.591 (8.4)	-4.493 (26.1)	7.722 (1.6)	1.418 (2.3)	2.800 (1.0)	-5.831 (4.0)	7.945 (1.3)
5	1.495 (9.2)	2.513 (8.6)	-4.080 (28.3)	7.513 (0.2)	1.427 (4.2)	2.711 (1.4)	-5.313 (6.7)	7.739 (2.8)
5.1	1.500 (10.4)	2.465 (8.2)	-3.826 (28.6)	7.389 (1.3)	1.435 (5.7)	2.655 (1.1)	-4.990 (7.0)	7.619 (4.5)
5.2	1.492 (10)	2.442 (7.7)	-3.736 (27.5)	7.286 (1.6)	1.431 (5.5)	2.626 (0.7)	-4.848 (6.0)	7.515 (4.8)
5.3	1.467 (9.0)	2.435 (7.7)	-3.778 (26.6)	7.144 (0.6)	1.407 (4.6)	2.615 (0.8)	-4.860 (5.6)	7.360 (3.7)
5.4	1.419 (9.2)	2.435 (8.2)	-3.915 (26.9)	6.910 (0.3)	1.359 (4.6)	2.612 (1.5)	-4.975 (7.1)	7.097 (3.0)
5.5	1.349 (11.3)	2.429 (8.2)	-4.081 (26.2)	6.552 (2.2)	1.286 (6.1)	2.602 (1.6)	-5.117 (7.4)	6.693 (4.4)
5.6	1.261 (11.8)	2.407 (7.5)	-4.204 (23.5)	6.074 (3.5)	1.195 (6.0)	2.576 (1.0)	-5.207 (5.3)	6.158 (5.0)
5.7	1.167 (9.9)	2.364 (6.7)	-4.226 (20.2)	5.518 (2.5)	1.097 (3.3)	2.526 (0.3)	-5.179 (2.2)	5.542 (2.9)

5.8	1.076 (5.3)	2.298 (7.3)	-4.121 (19.2)	4.945 (2.4)	1.002 (1.9)	2.452 (1.1)	-5.010 (1.8)	4.916 (3.0)
5.9	0.997 (1.2)	2.213 (9.4)	-3.903 (21.9)	4.414 (8.3)	0.921 (6.5)	2.359 (3.5)	-4.718 (5.7)	4.344 (9.8)
6	0.935 (0.05)	2.117 (12.4)	-3.606 (27.3)	3.961 (12.4)	0.857 (8.2)	2.254 (6.7)	-4.344 (12.4)	3.865 (14.5)
...								
10 <sup>21</sup>	1.8468	0	1.8468 <sup>2</sup> = 3.410668	0	1.914	0.45617	3.455305	1.746219
...								
10 <sup>30</sup>	1.8468	0	1.8468 <sup>2</sup> = 3.410668	0	1.914	0.45617	3.455305	1.746219

E in eV	n (RD%)	$\kappa$ (RD%)	$\epsilon_1$ (RD%)	$\epsilon_2$ (RD%)	$n_{FB}$ (RD%)	$\kappa_{FB}$ (RD%)	$\epsilon_{1(FB)}$ (RD%)	$\epsilon_{2(FB)}$ (RD%)
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**Table 3b.** In the P-GaSb 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  $E_{gn}(r_p) = E_{gni}(r_p)[ = 0.8092 \text{ eV}]$ , and the corresponding ones, obtained from the FB-model [11], are reported in this Table 3b, in which the relative deviations (RDs) of those are also given and calculated, using the AS-data [9]. Here, as reported in above Table 2c, we obtain here:  $\alpha_\infty(E \rightarrow \infty, r_p) = 2.7737 \times 10^9 \text{ cm}^{-1}$ ,  $\sigma_{0\infty}(E \rightarrow \infty, r_p) = 1.082043 \times 10^6 \left(\frac{1}{\Omega \times \text{cm}}\right)$  and  $R_\infty(E \rightarrow \infty, r_p) = 0.08848$ , while, in the FB-model,  $\alpha_{FB} \rightarrow \infty$ ,  $\sigma_{0(FB)} \rightarrow \infty$  and  $R_{FB}(E \rightarrow \infty, r_p) = 0.119948$ .

E in eV	$\alpha (10^3 \times \text{cm}^{-1})$ ; RD%	R; RD%	$\sigma_0 \left(\frac{1}{\Omega \times \text{cm}}\right)$	$\sigma_{0(FB)} \left(\frac{1}{\Omega \times \text{cm}}\right)$	$\alpha_{FB} (10^3 \times \text{cm}^{-1})$ ; RD%	$R_{FB}$ ; RD%
0.8092	0	0.274985	0	0.198592	0.269249	0.307732
<b>1.5</b>	29.586; 43.5	0.348; <b>12.6</b>	24.145	29.270	32.644; <b>37.7</b>	0.384; 3.6
<b>1.6</b>	36.296; <b>46.2</b>	0.361; 11.6	30.672	46.486	50.026; 25.9	0.398; 2.6
1.7	54.064; 35.3	0.376; 10.6	47.391	72.459	75.127; 10.1	0.414; 1.6
<b>1.8</b>	82.837; 25.7	0.393; 10.0	75.451	111.91	111.62; 0.08	0.431; <b>12.6</b>
1.9	128.04; 19.8	0.413; 9.9	121.41	175.67	168.25; 5.4	0.452; 1.3
2	213.83; 23.5	0.435; 10.6	208.85	295.89	275.65; 1.3	0.477; 2.1
2.1	300.36; 2.2	0.429; 9.4	273.82	374.93	380.81; 0.8	0.471; 0.6
2.2	313.12; 8.4	0.422; 8.4	278.85	371.40	389.36; 0.05	0.460; 0.1
2.3	358.12; 14.1	0.429; 7.0	318.02	415.79	438.93; 5.3	0.466; 1.2
2.4	412.81; 13.5	0.434; 8.2	360.24	462.69	499.81; 4.7	0.472; 0.2
2.5	463.47; 19.9	0.436; 9.8	392.96	496.08	555.12; 4.1	0.474; 2.1
2.6	504.66; 16	0.435; 7.4	413.64	513.86	598.66; 0.4	0.472; 0.5
2.7	535.54; 11.5	0.432; 5.5	424.79	520.17	629.83; 4.1	0.468; 2.4
2.8	558.11; 8.8	0.427; 4.8	430.84	521.11	651.25; 6.4	0.462; 3.0
2.9	575.75; 7.6	0.423; 4.9	436.18	522.19	667.07; 7.0	0.457; 2.7
3	592.19; 9.4	0.420; 5.3	444.37	527.63	681.68; 25.9	0.453; 2.0
3.1	611.11; 8.8	0.420; 6.2	458.24	540.25	699.31; 4.3	0.451; 0.7
3.2	636.09; 11.1	0.423; 7.3	480.26	563.57	723.95; 1.1	0.453; 0.7
3.3	670.75; 13.5	0.429; 7.7	512.83	599.23	759.59; 2.1	0.458; 1.4
3.4	718.90; 14.1	0.439; 7.5	558.41	650.11	810.40; 3.2	0.468; 1.4
3.5	784.56; 13.1	0.453; 6.6	619.10	718.34	880.70; 2.4	0.482; 0.7
3.6	871.39; 11.2	0.470; 5.3	695.47	804.15	974.41; 0.7	0.499; 0.5
3.7	981.29; 8.6	0.491; 4.1	783.95	902.85	1093.5; 1.9	0.520; 1.6
3.8	1111.8; 5.9	0.514; 3.0	873.24	1000.7	1235.0; 4.5	0.544; 2.7
3.9	1253.0; 4.6	0.538; 2.6	942.25	1072.7	1387.7; 5.6	0.570; 3.1
4	1386.2; 6.2	0.562; 3.5	965.28	1089.2	1530.9; 3.6	0.596; 2.2
4.1	1488.4; 9.9	0.585; 5.6	927.22	1034.1	1639.5; 0.8	0.620; 0.05
4.2	1543.4; 12.2	0.603; 8.3	837.39	920.46	1695.7; 3.6	0.641; 2.6
4.3	1549.4; 9.4	0.614; 8.7	724.77	783.54	1697.8; 0.7	0.655; 2.7
4.4	1517.9; 6.2	0.617; 7.1	618.47	657.49	1659.0; 2.5	0.661; 0.6
4.5	1465.9; 5.2	0.611; 6.1	534.28	559.80	1598.2; 3.3	0.657; 0.9
4.6	1408.6; 5.8	0.598; 6.1	475.09	492.62	1532.1; 2.4	0.645; 1.3
4.7	1356.2; 6.8	0.579; 7.1	437.23	450.71	1471.7; 1.1	0.627; 0.6

4.8	1314.6; 7.7	0.558; 8.2	415.45	427.33	1423.6; 0.08	0.606; 0.3
4.9	1286.6; 8.4	0.538; 9.5	405.02	416.68	1390.6; 1.0	0.586; 1.6
5	1273.3; 8.7	0.523; 10.6	402.09	414.16	1373.7; 1.4	0.569; 2.7
5.1	1274.0; 8.2	0.513; 10.7	403.34	415.91	1372.2; 1.1	0.558; 3.0
5.2	1286.7; 7.6	0.510; 10.3	405.53	418.27	1383.8; 0.7	0.553; 2.6
5.3	1307.9; 7.7	0.512; 9.9	405.28	417.51	1404.7; 0.9	0.554; 2.4
5.4	1332.4; 8.2	0.518; 10.3	399.40	410.17	1429.2; 1.6	0.561; 2.9
5.5	1353.9; 8.1	0.527; 10.9	385.73	394.03	1450.4; 1.6	0.571; 3.5
5.6	1366.2; 7.5	0.537; 10.6	364.09	369.13	1461.9; 1.0	0.582; 3.1
5.7	1365.5; 6.8	0.546; 9.3	336.65	338.12	1459.2; 0.4	0.593; 1.5
5.8	1350.5; 7.3	0.551; 8.3	307.01	305.17	1441.4; 1.1	0.600; 0.2
5.9	1323.2; 9.5	0.551; 8.6	278.77	274.32	1410.5; 3.5	0.602; 0.1
6	1287.2; 12.4	0.545; 10.6	254.35	248.18	1370.3; 6.7	0.598; 2.0
...						
$10^{21}$	$2.7737 \times 10^6$	0.08848	$1.082043 \times 10^6$	$1.869027 \times 10^{22}$	$4.622779 \times 10^{22}$	0.119948
...						
$10^{30}$	$2.7737 \times 10^6$	0.08848	$1.082043 \times 10^6$	$1.869027 \times 10^{31}$	$4.622779 \times 10^{31}$	0.119948
E in eV	$\alpha$ ( $10^3 \times \text{cm}^{-1}$ ); RD%	R; RD%	$\sigma_0 \left( \frac{1}{\Omega \times \text{cm}} \right)$	$\sigma_{0(\text{FB})} \left( \frac{1}{\Omega \times \text{cm}} \right)$	$\alpha_{\text{FB}} (10^3 \times \text{cm}^{-1}); \text{RD}\%$	$R_{\text{FB}}; \text{RD}\%$

**Table 3c.** Here, our highest relative deviation (HRD)-values and those of  $(\text{HRD})_{\text{FB}}$ , 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-PM.

HRD	n	$\kappa$	$\epsilon_1$	$\epsilon_2$	$\alpha$	R
E (eV)						
-----						
1.5	11.9%					12.6%
1.6		46.2%		52.3%	46.2%	
4			39.9%			
-----						
$(\text{HRD})_{\text{FB}}$	$n_{\text{FB}}$	$\kappa_{\text{FB}}$	$\epsilon_{1(\text{FB})}$	$\epsilon_{2(\text{FB})}$	$\alpha_{\text{FB}}$	$R_{\text{FB}}$
E (eV)						
-----						
1.5		37.6%		39.7%	37.7%	
1.8						12.6%
2.5	18.9%					
4			112.5%			

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:

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

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

$\kappa(E^*, r_{d(a)}) = 0$ ,  $\varepsilon_2(E^*, r_{d(a)}) = 0$ ,  $\sigma_0(E^*, r_{d(a)}) = 0$  and  $\alpha(E^*, r_{d(a)}) = 0$ , corresponding also to the MIT.

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

$$\kappa(E^* = 0) = f(E) \times E_{gni(gpi)}^{(2-10^{-21})} \times (E^* \equiv E - E_{gn1(gp1)} = 0)^{10^{-21}}, \text{ for } E = E_{CPE}(r_{d(a)}) = E_{gni(gpi)}, \quad (30)$$

where  $E_{CPE}$  is the critical photon energy, and

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

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

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

Now, replacing Equations (31, 32) into Equations (24, 25), one obtains for  $E \leq 0$  the expressions, given for the following exponential tail-states of  $\varepsilon_2$ ,  $\sigma_0(E)$ ,  $\alpha$ , and  $R$  as:

$$\varepsilon_2^{ElmD-T}(E_{gni(gpi)}) = 2 \times \kappa^{EEC-T}(E_{gni(gpi)}) \times n^{ERI-T}(E = E_{gni(gpi)}), \quad (33)$$

$$\sigma_0^{EOC-T}(E_{gni(gpi)}) = \frac{\varepsilon_{free\ space} \times E_{gni(gpi)} \times \varepsilon_2^{ElmD-T}(E_{gni(gpi)})}{4\pi\hbar}, \quad (34)$$

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

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

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  $N = 10^{19}cm^{-3}$ , respectively, as given in following Tables 4n and 4p, in which the arrows ( $\uparrow \downarrow$ ) indicates the maximum, and ( $\downarrow \uparrow$ ) the minimum, and the extrema-values of those occur at the same corresponding photon energy  $E$ .

**Table 4n.** In d-GaSb systems, and for two types of physical conditions such as:  $[T=0K \text{ and } N = N_{CDn}(r_d)]$  and  $[T=20K, N = 10^{19} \text{ cm}^{-3}]$ , 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:  $\uparrow$  or  $\downarrow$ , suggesting that their extrema occur at the same E.

E in eV	1.5	2	2.1	2.2	2.3	2.6	3.1	3.4	3.9	4.4	5.2	10	$10^{21}$
In the P- GaSb system, at T=0K and $N = N_{CDn}(r_P) = 4.6883 \times 10^{17} \text{ cm}^{-3}$ , $E_{gni}(r_P) = 0.8092 \text{ eV}$													
$\varepsilon_1(E)$	14.89	$\uparrow$ 20.27	$\downarrow$ 16.63	15.80	15.31	11.39	8.82	$\uparrow$ 9.17	$\downarrow$ 2.62	$\downarrow$ -7.87	$\uparrow$ -3.74	1.21	3.410668
$\varepsilon_2(E)$	1.50	9.7	$\uparrow$ 12.18	$\downarrow$ 11.84	$\uparrow$ 12.92	$\uparrow$ 14.86	$\downarrow$ 13.8	$\uparrow$ 15.34	$\uparrow$ 22.57	$\downarrow$ 13.1	7.29	2.19	$\downarrow$ 0
In the As- GaSb system, at T=0K and $N = N_{CDn}(r_{As}) = 6.2949 \times 10^{17} \text{ cm}^{-3}$ , $E_{gni}(r_{As}) = 0.8096 \text{ eV}$													
$\varepsilon_1(E)$	14.20	$\uparrow$ 19.45	$\downarrow$ 15.87	15.06	14.57	10.71	8.20	$\uparrow$ 8.53	$\downarrow$ 2.00	$\downarrow$ -8.19	$\uparrow$ -3.99	0.97	3.091599
$\varepsilon_2(E)$	1.47	9.56	$\uparrow$ 11.92	$\downarrow$ 11.58	$\uparrow$ 12.64	$\uparrow$ 14.52	$\downarrow$ 13.5	$\uparrow$ 14.97	$\uparrow$ 22.00	$\downarrow$ 12.5	6.85	2.05	$\downarrow$ 0
In the Te- GaSb system, at T=0K and $N = N_{CDn}(r_{Te}) = 7.9085 \times 10^{17} \text{ cm}^{-3}$ , $E_{gni}(r_{Te}) = 0.80998 \text{ eV}$													
$\varepsilon_1(E)$	13.71	$\uparrow$ 18.85	$\downarrow$ 15.32	14.52	14.03	10.22	7.75	$\uparrow$ 8.06	$\downarrow$ 1.56	$\downarrow$ -8.43	$\uparrow$ -4.16	0.81	2.865151
$\varepsilon_2(E)$	1.45	9.41	$\uparrow$ 11.73	$\downarrow$ 11.39	$\uparrow$ 12.43	$\uparrow$ 14.26	$\downarrow$ 13.2	$\uparrow$ 14.69	$\uparrow$ 21.58	$\downarrow$ 12.08	6.53	1.95	$\downarrow$ 0
In the Sb- GaSb system, at T=0K and $N = N_{CDn}(r_{Sb}) = 8 \times 10^{17} \text{ cm}^{-3}$ , $E_{gni}(r_{Sb}) = 0.81 \text{ eV}$													
$\varepsilon_1(E)$	13.68	$\uparrow$ 18.82	$\downarrow$ 15.29	14.49	14.00	10.19	7.73	$\uparrow$ 8.04	$\downarrow$ 1.53	$\downarrow$ -8.44	$\uparrow$ -4.17	0.80	2.854139
$\varepsilon_2(E)$	1.44	9.41	$\uparrow$ 11.72	$\downarrow$ 11.38	$\uparrow$ 12.42	$\uparrow$ 14.25	$\downarrow$ 13.19	$\uparrow$ 14.68	$\uparrow$ 21.56	$\downarrow$ 12.06	6.52	1.94	$\downarrow$ 0
In the Sn- GaSb system, at T=0K and $N = N_{CDn}(r_{Sn}) = 8.0954 \times 10^{17} \text{ cm}^{-3}$ , $E_{gni}(r_{Sn}) = 0.81002 \text{ eV}$													
$\varepsilon_1(E)$	13.66	$\uparrow$ 18.79	$\downarrow$ 15.27	14.47	13.98	10.17	7.70	$\uparrow$ 8.01	$\downarrow$ 1.51	$\downarrow$ -8.45	$\uparrow$ -4.18	0.80	2.84293
$\varepsilon_2(E)$	1.44	9.40	$\uparrow$ 11.71	$\downarrow$ 11.37	$\uparrow$ 12.41	$\uparrow$ 14.23	$\downarrow$ 13.17	$\uparrow$ 14.66	$\uparrow$ 21.54	$\downarrow$ 12.04	6.50	1.94	$\downarrow$ 0
E in eV	1.5	2	2.1	2.2	2.3	2.6	3.1	3.4	3.9	4.4	5.2	10	$10^{21}$
In the P- GaSb system, at T=20K and $N = 10^{19} \text{ cm}^{-3}$ , $E_{gn1}(r_P) = 1.16185 \text{ eV}$													
$\varepsilon_1(E)$	14.89	$\uparrow$ 21.12	$\downarrow$ 18.08	17.17	16.87	13.53	10.66	$\uparrow$ 11.09	$\downarrow$ 6.48	$\downarrow$ -3.94	$\uparrow$ -2.04	1.3	3.410668
$\varepsilon_2(E)$	1.50	4.83	6.44	6.60	7.53	9.59	9.89	11.45	$\uparrow$ 17.72	$\downarrow$ 10.68	6.16	2.03	$\downarrow$ 0
In the As- GaSb system, at T=20K and $N = 10^{19} \text{ cm}^{-3}$ , $E_{gn1}(r_{As}) = 1.154209 \text{ eV}$													
$\varepsilon_1(E)$	14.21	$\uparrow$ 20.29	$\downarrow$ 17.30	16.40	16.11	12.82	10.01	$\uparrow$ 10.42	$\downarrow$ 5.79	$\downarrow$ -4.35	$\uparrow$ -2.33	1.07	3.091599
$\varepsilon_2(E)$	1.47	4.82	6.41	6.55	7.47	9.47	9.71	11.25	$\uparrow$ 17.37	$\downarrow$ 10.24	5.82	1.90	$\downarrow$ 0
In the Te- GaSb system, at T=20K and $N = 10^{19} \text{ cm}^{-3}$ , $E_{gn1}(r_{Te}) = 1.147162 \text{ eV}$													
$\varepsilon_1(E)$	13.72	$\uparrow$ 19.68	$\downarrow$ 16.72	15.85	15.55	12.29	9.53	$\uparrow$ 9.92	$\downarrow$ 5.27	$\downarrow$ -4.65	$\uparrow$ -2.54	0.90	2.865151
$\varepsilon_2(E)$	1.44	4.84	6.40	6.54	7.44	9.34	9.60	11.11	$\uparrow$ 17.13	$\downarrow$ 9.92	5.57	1.81	$\downarrow$ 0
In the Sb- GaSb system, at T=20K and $N = 10^{19} \text{ cm}^{-3}$ , $E_{gn1}(r_{Sb}) = 1.146776 \text{ eV}$													
$\varepsilon_1(E)$	13.69	$\uparrow$ 19.65	$\downarrow$ 16.69	15.82	15.52	12.27	9.51	$\uparrow$ 9.90	$\downarrow$ 5.25	$\downarrow$ -4.67	$\uparrow$ -2.55	0.89	2.854139
$\varepsilon_2(E)$	1.44	4.84	6.40	6.54	7.44	9.39	9.59	11.11	$\uparrow$ 17.12	$\downarrow$ 9.90	5.55	1.80	$\downarrow$ 0
In the Sn- GaSb system, at T=20K and $N = 10^{19} \text{ cm}^{-3}$ , $E_{gn1}(r_{Sn}) = 1.146377 \text{ eV}$													
$\varepsilon_1(E)$	13.66	$\uparrow$ 19.62	$\downarrow$ 16.67	15.79	15.50	12.24	9.48	$\uparrow$ 9.87	$\downarrow$ 5.22	$\downarrow$ -4.68	$\uparrow$ -2.56	0.89	2.84293
$\varepsilon_2(E)$	1.44	4.84	6.40	6.54	7.44	9.39	9.59	11.10	$\uparrow$ 17.11	$\downarrow$ 9.88	5.54	1.80	$\downarrow$ 0
E in eV	1.5	2	2.1	2.2	2.3	2.6	3.1	3.4	3.9	4.4	5.2	10	$10^{21}$

**Table 4p.** In a-GaSb systems, and for two types of physical conditions such as: (T=0K and  $N = N_{CDP}(r_a)$ ) and (T=20K,  $N = 10^{19} \text{ cm}^{-3}$ ), 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:  $\uparrow$  or  $\downarrow$ , suggesting that their extrema occur at the same E.

E in eV	1.5	2	2.1	2.2	2.3	2.6	3.1	3.4	3.9	4.4	5.2	10	$10^{21}$
In the Ge- GaSb system, at T=0K and $N = N_{CDn}(r_{Ge}) = 7.8931 \times 10^{17} \text{ cm}^{-3}$ , $E_{gpi}(r_{Ge}) = 0.8098 \text{ eV}$													
$\varepsilon_1(E)$	13.72	$\uparrow$ 18.86	$\downarrow$ 15.33	14.52	14.04	10.22	7.75	$\uparrow$ 8.06	$\downarrow$ 1.56	$\downarrow$ -8.43	$\uparrow$ -4.17	0.81	2.866963
$\varepsilon_2(E)$	1.44	9.4	$\uparrow$ 11.73	$\downarrow$ 11.40	$\uparrow$ 12.43	$\uparrow$ 14.26	$\downarrow$ 13.2	$\uparrow$ 14.7	$\uparrow$ 21.59	$\downarrow$ 12.1	6.54	1.95	$\downarrow$ 0
In the Ga- GaSb system, at T=0K and $N = N_{CDp}(r_{Ga}) = 8 \times 10^{17} \text{ cm}^{-3}$ , $E_{gpi}(r_{Ga}) = 0.81 \text{ eV}$													
$\varepsilon_1(E)$	13.68	$\uparrow$ 18.82	$\downarrow$ 15.29	14.49	14.01	10.19	7.73	$\uparrow$ 8.04	$\downarrow$ 1.53	$\downarrow$ -8.44	$\uparrow$ -4.17	0.80	2.854139
$\varepsilon_2(E)$	1.44	9.4	$\uparrow$ 11.72	$\downarrow$ 11.38	$\uparrow$ 12.42	$\uparrow$ 14.25	$\downarrow$ 13.2	$\uparrow$ 14.7	$\uparrow$ 21.56	$\downarrow$ 12.06	6.52	1.94	$\downarrow$ 0
In the Mg- GaSb system, at T=0K and $N = N_{CDp}(r_{Mg}) = 9.4507 \times 10^{17} \text{ cm}^{-3}$ , $E_{gpi}(r_{Mg}) = 0.8119 \text{ eV}$													
$\varepsilon_1(E)$	13.32	$\uparrow$ 18.38	$\downarrow$ 14.89	14.11	13.63	9.85	7.42	$\uparrow$ 7.72	$\downarrow$ 1.24	$\downarrow$ -8.57	$\uparrow$ -4.28	0.70	2.699917
$\varepsilon_2(E)$	1.43	9.3	$\uparrow$ 11.54	$\downarrow$ 11.21	$\uparrow$ 12.24	$\uparrow$ 14.00	$\downarrow$ 12.98	$\uparrow$ 14.5	$\uparrow$ 21.24	$\downarrow$ 11.74	6.29	1.87	$\downarrow$ 0
In the In- GaSb system, at T=0K and $N = N_{CDp}(r_{In}) = 1.0482 \times 10^{18} \text{ cm}^{-3}$ , $E_{gpi}(r_{In}) = 0.8133 \text{ eV}$													
$\varepsilon_1(E)$	13.09	$\uparrow$ 18.11	$\downarrow$ 14.65	13.88	13.40	9.65	7.24	$\uparrow$ 7.53	$\downarrow$ 1.07	$\downarrow$ -8.64	$\uparrow$ -4.34	0.63	2.608312
$\varepsilon_2(E)$	1.42	9.2	$\uparrow$ 11.44	$\downarrow$ 11.11	$\uparrow$ 12.12	$\uparrow$ 13.9	$\downarrow$ 12.86	$\uparrow$ 14.3	$\uparrow$ 21.04	$\downarrow$ 11.55	6.16	1.82	$\downarrow$ 0
E in eV	1.5	2	2.1	2.2	2.3	2.6	3.1	3.4	3.9	4.4	5.2	10	$10^{21}$
In the Ge- GaSb s system, at T=20K and $N = 10^{19} \text{ cm}^{-3}$ , $E_{gpi}(r_{Ge}) = 1.1551 \text{ eV}$													
$\varepsilon_1(E)$	13.72	$\uparrow$ 19.70	$\downarrow$ 16.75	15.87	15.58	12.33	9.57	$\uparrow$ 9.96	$\downarrow$ 5.35	$\downarrow$ -4.57	$\uparrow$ -2.50	0.90	2.866963
$\varepsilon_2(E)$	1.44	4.7	6.29	6.44	7.34	9.29	9.52	11.04	$\uparrow$ 17.03	$\downarrow$ 9.87	5.55	1.80	$\downarrow$ 0
In the Ga- GaSb system, at T=20K and $N = 10^{19} \text{ cm}^{-3}$ , $E_{gpi}(r_{Ga}) = 1.1549 \text{ eV}$													
$\varepsilon_1(E)$	13.69	$\uparrow$ 19.66	$\downarrow$ 16.71	15.84	15.55	12.30	9.54	$\uparrow$ 9.93	$\downarrow$ 5.32	$\downarrow$ -4.59	$\uparrow$ -2.51	0.90	2.854139
$\varepsilon_2(E)$	1.44	4.7	6.29	6.44	7.33	9.28	9.51	11.03	$\uparrow$ 17.02	$\downarrow$ 9.85	5.53	1.80	$\downarrow$ 0
In the Mg- GaSb system, at T=20K and $N = 10^{19} \text{ cm}^{-3}$ , $E_{gpi}(r_{Mg}) = 1.1511 \text{ eV}$													
$\varepsilon_1(E)$	13.32	$\uparrow$ 19.20	$\downarrow$ 16.30	15.43	15.14	11.93	9.21	$\uparrow$ 9.59	$\downarrow$ 4.97	$\downarrow$ -4.78	$\uparrow$ -2.65	0.79	2.699917
$\varepsilon_2(E)$	1.43	4.7	6.27	6.40	7.29	9.21	9.42	10.92	$\uparrow$ 16.83	$\downarrow$ 9.62	5.36	1.73	$\downarrow$ 0
In the In- GaSb system, at T=20K and $N = 10^{19} \text{ cm}^{-3}$ , $E_{gpi}(r_{In}) = 1.1485 \text{ eV}$													
$\varepsilon_1(E)$	13.10	$\uparrow$ 18.92	$\downarrow$ 16.04	15.19	14.90	11.71	9.01	$\uparrow$ 9.38	$\downarrow$ 4.76	$\downarrow$ -4.90	$\uparrow$ -2.73	0.72	2.608312
$\varepsilon_2(E)$	1.42	4.7	6.25	6.39	7.27	9.17	9.36	10.85	$\uparrow$ 16.72	$\downarrow$ 9.49	5.25	1.69	$\downarrow$ 0
E in eV	1.5	2	2.1	2.2	2.3	2.6	3.1	3.4	3.9	4.4	5.2	10	$10^{21}$

### 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, at E=3.3 eV, for example, and for some (P, Te, Sn)-GaSb systems and for some (Ga, In)-

GaSb 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,  $E_{gn1(gp1)}(N^*, r_{d(a)})$ .

**Table 5n.** In (P, Te, Sn)- degenerate GaSb systems ( $\frac{E_{Fn}(N^*, r_d)}{k_B T} \gg 1$ ), our numerical results of the following optical coefficients, expressed as functions of N, and calculated using Equations (31-36, 24), for E=3.3 eV and T=20K, present the variations by arrows, (↘ and ↗), since those of the optical gap  $E_{gn1}(N^*, r_d)$  increase with increasing N, at T=20 K.

(↘ and ↗), since those of the optical gap $E_{gn1}(N^*, r_d)$ increase with increasing N, at T=20 K.						$\frac{E_{Fn(Fp)}(u)}{k_B T}$
N ( $10^{18} \text{ cm}^{-3}$ )	↗	4	8.5	15	50	
$\frac{E_{Fn}(N^*, r_p)}{k_B T} \gg 1$	↗	131	217	316	706	
$E_{gn1}(N^*, r_p)$ in eV	↗	0.983398	1.121791	1.283068	1.917333	
n ( $r_p$ )=3.619629						
$\kappa(N, r_p)$	↘	1.7350	1.5339	1.3152	0.6181	
$\varepsilon_1(N, r_p)$	↗	10.0914	10.7488	11.3720	12.7197	
$\varepsilon_2(N, r_p)$	↘	12.560	11.104	9.521	4.474	
$\sigma_O(N, r_p)$ in $10^2 \Omega^{-1} cm^{-1}$	↘	4.436	3.922	3.363	1.580	
$\alpha(N, r_p)$ in $10^5 cm^{-1}$	↘	5.802	5.130	4.398	2.067	
R ( $N, r_p$ )	↘	0.405	0.389	0.372	0.333	
$\frac{E_{Fn}(N^*, r_{Te})}{k_B T} \gg 1$	↗	131	217	316	706	
$E_{gn1}(N^*, r_{Te})$ in eV	↗	0.967738	1.107065	1.26824	1.899986	
n ( $r_{Te}$ )=3.465253						
$\kappa(N, r_{Te})$	↘	1.7586	1.5547	1.3346	0.6337	
$\varepsilon_1(N, r_{Te})$	↗	8.9155	9.5908	10.2269	11.6064	
$\varepsilon_2(N, r_{Te})$	↘	12.188	10.775	9.249	4.392	
$\sigma_O(N, r_{Te})$ in $10^2 \Omega^{-1} cm^{-1}$	↘	4.305	3.806	3.267	1.551	
$\alpha(N, r_{Te})$ in $10^5 cm^{-1}$	↘	5.881	5.199	4.463	2.119	
R ( $N, r_{Te}$ )	↘	0.398	0.380	0.362	0.318	
$\frac{E_{Fn}(N^*, r_{Sn})}{k_B T} \gg 1$	↗	131	217	316	706	
$E_{gn1}(N^*, r_{Sn})$ in eV	↗	0.966871	1.106273	1.26746	1.899107	
n ( $r_{Sn}$ )=3.458663						
$\kappa(N, r_{Sn})$	↘	1.7599	1.5558	1.3356	0.6345	
$\varepsilon_1(N, r_{Sn})$	↗	8.8652	9.5417	10.1785	11.5598	
$\varepsilon_2(N, r_{Sn})$	↘	12.173	10.762	9.239	4.389	
$\sigma_O(N, r_{Sn})$ in $10^2 \Omega^{-1} cm^{-1}$	↘	4.300	3.801	3.263	1.550	
$\alpha(N, r_{Sn})$ in $10^5 cm^{-1}$	↘	5.885	5.203	4.466	2.122	
R ( $N, r_{Sn}$ )	↘	0.398	0.380	0.361	0.318	
N ( $10^{18} \text{ cm}^{-3}$ )		4	8.5	15	50	

**Table 5p.** In (Ga, In)- degenerate GaSb systems ( $\frac{E_{Fp}(N^*, r_a)}{k_B T} \gg 1$ ), the numerical results of the following optical coefficients, expressed as functions of N, and calculated using Equations (31-36, 24), for E=3.3 eV and T=20K, present the variations by arrows, ( $\searrow$  or  $\nearrow$ ), since those of the optical gap  $E_{gp1}(N^*, r_a)$  increase with increasing N.

N ( $10^{18} \text{ cm}^{-3}$ )	$\nearrow$	15	26	60
$\frac{E_{Fp}(N^*, r_{Ga})}{k_B T} \gg 1$	$\nearrow$	305	447	791
$E_{gp1}(N^*, r_{Ga})$ in eV	$\nearrow$	1.2769	1.5050	2.0612
$n(r_{Ga})=3.46199$				
$\kappa(N, r_{Ga})$	$\searrow$	1.323	1.042	0.496
$\varepsilon_1(N, r_{Ga})$	$\nearrow$	10.234	10.900	11.739
$\varepsilon_2(N, r_{Ga})$	$\searrow$	9.162	7.212	3.435
$\sigma_0(N, r_{Ga})$ in $10^2 \Omega^{-1} \text{ cm}^{-1}$	$\searrow$	3.236	2.547	1.213
$\alpha(N, r_{Ga})$ in $10^5 \text{ cm}^{-1}$	$\searrow$	4.425	3.483	1.659
$R(N, r_{Ga})$	$\searrow$	0.361	0.340	0.313
$\frac{E_{Fp}(N^*, r_{In})}{k_B T}$	$\nearrow$	301	444	788
$E_{gp1}(N^*, r_{In})$ in eV	$\nearrow$	1.2708	1.4989	2.0542
$n(r_{In})=3.386507$				
$\kappa(N, r_{In})$	$\searrow$	1.331	1.049	0.502
$\varepsilon_1(N, r_{In})$	$\nearrow$	9.696	10.368	11.217
$\varepsilon_2(N, r_{In})$	$\searrow$	9.016	7.103	3.398
$\sigma_0(N, r_{In})$ in $10^2 \Omega^{-1} \text{ cm}^{-1}$	$\searrow$	3.184	2.509	1.200
$\alpha(N, r_{In})$ in $10^5 \text{ cm}^{-1}$	$\searrow$	4.452	3.507	1.678
$R(N, r_{In})$	$\searrow$	0.355	0.334	0.305
N ( $10^{18} \text{ cm}^{-3}$ )		15	26	60

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

Here, from Equations (24, 28, 29), we can determine the variations of various optical coefficients for  $N = 1.5 \times 10^{19} \text{ cm}^{-3}$ , respectively, as functions of T, at E=3.3 eV, for example, and for some (P, Te, Sn)- GaSb systems and for some (Ga, In)- GaSb ones, being indicated by the arrows:  $\nearrow$  and  $\searrow$ , as given in following Tables 6n and 6p, in which their variations thus depend on the ones of the optical band gap,  $E_{gn1(gp1)}(N^*, r_{d(a)})$ .

**Table 6n.** In (P, Te, Sn)- degenerate GaSb systems ( $\frac{E_{Fn}(N^*, r_d)}{k_B T} \gg 1$ ), our numerical results of the following optical coefficients, expressed as functions of T, and calculated using Equations (31-36, 24), for E=3.3 eV and  $N = 1.5 \times 10^{19} \text{ cm}^{-3}$ , increase with increasing T, since the optical band gap  $E_{gn1}(T, r_d)$  decreases with increasing T.

T in K	20	30	50	100	200	300
$\frac{E_{Fp}(N^*, r_P)}{k_B T} \gg 1$	$\searrow$	309	206	124	62	31
		21				

$E_{\text{gn1}}(T, r_p)$ in eV $\searrow$	1.28307	1.28240	1.2801	1.2682	1.2215	1.1551
$n(r_p, T)$ $\nearrow$	3.6196	3.6198	3.6206	3.6246	3.6395	3.6593
$\kappa(r_p, T)$ $\nearrow$	1.315	1.316	1.319	1.335	1.3966	1.4874
$\varepsilon_1(r_p, T)$ $\searrow$	11.3720	11.3714	11.3690	11.3563	11.2956	11.1786
$\varepsilon_2(r_p, T)$ $\nearrow$	9.521	9.528	9.552	9.675	10.160	10.886
$\sigma_O(r_p, T)$ in $10^2 \Omega^{-1} \text{cm}^{-1}$ $\nearrow$	3.363	3.365	3.374	3.417	3.591	3.845
$\alpha(r_p, T)$ in $10^5 \text{cm}^{-1}$ $\nearrow$	4.398	4.401	4.411	4.463	4.671	4.974
$R(r_p, T)$ $\nearrow$	0.372	0.3725	0.3728	0.3742	0.3799	0.3881
$\frac{E_{\text{FP}}(N^*, r_{\text{Te}})}{k_B T} \gg 1$ $\searrow$	305	203	122	61	30	20
$E_{\text{gn1}}(T, r_{\text{Te}})$ in eV $\searrow$	1.26824	1.2676	1.2652	1.2534	1.2067	1.1403
$n(r_{\text{Te}}, T)$ $\nearrow$	3.4652	3.4655	3.4662	3.4702	3.4852	3.5050
$\kappa(r_{\text{Te}}, T)$ $\nearrow$	1.334	1.335	1.338	1.354	1.417	1.508
$\varepsilon_1(r_{\text{Te}}, T)$ $\searrow$	10.2269	10.2261	10.2233	10.2085	10.140	10.011
$\varepsilon_2(r_{\text{Te}}, T)$ $\nearrow$	9.249	9.256	9.279	9.399	9.874	10.571
$\sigma_O(r_{\text{Te}}, T)$ in $10^2 \Omega^{-1} \text{cm}^{-1}$ $\nearrow$	3.267	3.269	3.277	3.320	3.488	3.734
$\alpha(r_{\text{Te}}, T)$ in $10^5 \text{cm}^{-1}$ $\nearrow$	4.460	4.466	4.476	4.529	4.737	5.043
$R(r_{\text{Te}}, T)$ $\nearrow$	0.3618	0.3619	0.3622	0.3637	0.3699	0.3788
$\frac{E_{\text{FP}}(N^*, r_{\text{Sn}})}{k_B T} \gg 1$ $\searrow$	305	203	122	61	30	20
$E_{\text{gn1}}(T, r_{\text{Sn}})$ in eV $\searrow$	1.2674	1.2668	1.2645	1.2526	1.2059	1.1395
$n(r_{\text{Sn}}, T)$ $\nearrow$	3.4587	3.4589	3.4597	3.4636	3.4786	3.4984
$\kappa(r_{\text{Sn}}, T)$ $\nearrow$	1.336	1.3365	1.339	1.355	1.418	1.509
$\varepsilon_1(r_{\text{Sn}}, T)$ $\searrow$	10.1785	10.1777	10.1749	10.1600	10.091	9.962
$\varepsilon_2(r_{\text{Sn}}, T)$ $\nearrow$	9.239	9.245	9.269	9.388	9.863	10.559
$\sigma_O(r_{\text{Sn}}, T)$ in $10^2 \Omega^{-1} \text{cm}^{-1}$ $\nearrow$	3.263	3.265	3.274	3.316	3.484	3.729
$\alpha(r_{\text{Sn}}, T)$ in $10^5 \text{cm}^{-1}$ $\nearrow$	4.466	4.469	4.479	4.532	4.741	5.047
$R(r_{\text{Sn}}, T)$ $\nearrow$	0.3614	0.3615	0.3618	0.3633	0.3695	0.3784
T in K	20	30	50	100	200	300

**Table 6p.** In (Ga, In)- degenerate GaSb systems ( $\frac{E_{\text{FP}}(N^*, r_a)}{k_B T} \gg 1$ ), our numerical results of the following optical coefficients, expressed as functions of T, and calculated using Equations (31-36, 24), for  $E=3.3$  eV and  $N = 1.5 \times 10^{19} \text{cm}^{-3}$ , increase with increasing T, since the optical band gap  $E_{\text{gp1}}(T, r_a)$  decreases with increasing T.

T in K	20	30	50	100
$\frac{E_{\text{FP}}(N^*, r_{\text{Ga}})}{k_B T} \gg 1$ $\searrow$	305	203	122	61
$E_{\text{gn1}}(T, r_{\text{Ga}})$ in eV $\searrow$	1.2769	1.2763	1.2739	1.2621
$n(r_{\text{Ga}}, T)$ $\nearrow$	3.4620	3.4622	3.4630	3.4669
$\kappa(r_{\text{Ga}}, T)$ $\nearrow$	1.3232	1.3240	1.3271	1.3427
$\varepsilon_1(r_{\text{Ga}}, T)$ $\searrow$	10.2346	10.2338	10.2312	10.2169
$\varepsilon_2(r_{\text{Ga}}, T)$ $\nearrow$	9.162	9.168	9.191	9.310

$\sigma_O(r_{Ga}, T)$ in $10^2 \Omega^{-1}cm^{-1}$	$\nearrow$	3.236	3.238	3.246	3.288
$\alpha(r_{Ga}, T)$ in $10^5 cm^{-1}$	$\nearrow$	4.425	4.428	4.438	4.490
$R(r_{Ga}, T)$	$\nearrow$	0.3606	0.3607	0.3610	0.3626
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$\frac{E_{Fp}(N^*, r_{In})}{k_B T} \gg 1$	$\searrow$	301	201	121	60
$E_{gn1}(T, r_{In})$ in eV	$\searrow$	1.2708	1.2701	1.2678	1.2559
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$n(r_{In}, T)$	$\nearrow$	3.3865	3.3867	3.3875	3.3915
$\kappa(r_{In}, T)$	$\nearrow$	1.3312	1.3320	1.3351	1.3507
$\varepsilon_1(r_{In}, T)$	$\searrow$	9.6963	9.6955	9.6927	9.6776
$\varepsilon_2(r_{In}, T)$	$\nearrow$	9.016	9.022	9.045	9.162
$\sigma_O(r_{In}, T)$ in $10^2 \Omega^{-1}cm^{-1}$	$\nearrow$	3.184	3.186	3.194	3.236
$\alpha(r_{In}, T)$ in $10^5 cm^{-1}$	$\nearrow$	4.452	4.454	4.464	4.517
$R(r_{In}, T)$	$\nearrow$	0.3554	0.35545	0.3557	0.3574
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T in K		20	30	50	100
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## 6. Concluding remarks

In the n(p)-type degenerate GaSb -crystal, by using the same physical model, as that given in Eq. (7), and same mathematical methods, as those proposed Refs. [1-3], 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  $\kappa$ , as the photon energy  $E(\rightarrow \infty)$ , all the numerical results, obtained in [3], are now revised and performed.

Then, by basing on our following basic expressions, such 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 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),  $N_{CDn(CDp)}^{EBT}$ , as that determined in Eq. (21), with a precision of the order of 7.8%, as observed in Table 1,
- (iii) the Fermi energy,  $E_{Fn(Fp)}(N^*, T)$ , determined in Eq. (A3) of the Appendix A, with a precision of the order of  $2.11 \times 10^{-4}$  [3], and finally,
- (iv) the refraction index  $n$  and the extinction coefficient  $\kappa$ , 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)  $E_{Fno(Fpo)}(N^* = 0, T = 0) = 0$ , 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  $E_{gn1(gp1)}(N^* = 0, r_{d(a)}, T = 0) = E_{gni(gpi)}(r_{d(a)})$ , where  $E_{gn1(gp1)}$  and  $E_{gni(gpi)}$  are the optical band gap and intrinsic band gap, respectively, and

c) as discussed in Section 5.1, as  $E = E_{CPE}(r_{d(a)}) \equiv E_{gni(gpi)}(r_{d(a)})$  or the effective photon energy  $E^* \equiv E - E_{gni(gpi)}(r_{d(a)}) = 0$ , one has:  $\kappa(E^* = 0, r_{d(a)}) = 0$ ,  $\varepsilon_2(E^* = 0, r_{d(a)}) = 0$ ,  $\sigma_0(E^* = 0, r_{d(a)}) = 0$  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 [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 GaSb -crystals, the Fermi energy  $E_{Fn(Fp)} \equiv [E_{fn} - E_c](E_{Fp} \equiv [E_v - E_{fp}])$ ,  $E_{c(v)}$  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  $2.11 \times 10^{-4}$  [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, being characteristic of the MIT-phenomenon, and their numerical results are given in Table 1, meaning that  $N^* = 0$  at this transition.

First, we define the reduced electron density by:

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

where  $N_{c(v)}(T)$  is the conduction (valence)-band density of states, the values of  $g_{c(v)} = 1(1)$ , and  $m_{n(p)}^*/m_0$ , defined in Section 2, can be equal to :  $m_{n(p)}/m_0 = 0.047 (0.3)$ , and to  $m_r/m_0 = \frac{m_n \times m_p}{m_n + m_p} = 0.040634$ . In particular, here, as used in Sections 3 and 5 for determining the optical band gap in degenerate GaSb-crystals,  $m_{n(p)}^*/m_0 = m_r/m_0$  was chosen.

Then, the reduced Fermi energy in the n(p)-type GaSb crystals is determined by :

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

where  $F(N^*, T) = au^{\frac{2}{3}} \left( 1 + bu^{-\frac{4}{3}} + cu^{-\frac{8}{3}} \right)^{-\frac{2}{3}}$ , 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  $G(u) \simeq \text{Ln}(u) + 2^{-\frac{3}{2}} \times u \times e^{-du}$  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 degenerate case ( $u \gg 1$ ), one has:

$$E_{Fn(Fp)}(N^*, T) = E_{Fn(Fpo)}(u) \times \left(1 + bu^{-\frac{4}{3}} + cu^{-\frac{8}{3}}\right)^{-\frac{2}{3}}. \quad (A3)$$

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

$$E_{Fn(Fpo)}(N^*) \equiv \frac{\hbar^2 \times k_{Fn(Fp)}^2(N^*)}{2 \times m_r}, \quad (A4)$$

being proportional to  $(N^*)^{2/3}$ , and equal to 0,  $E_{Fn(Fpo)}(N^* = 0) = 0$ , 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 GaSb-crystals, we define the effective reduced Wigner-Seitz radius  $r_{sn(sp)}$ , characteristic of the interactions, by:

$$r_{sn(sp)}(N^*, r_{d(a)}) \equiv \left(\frac{3g_c(v)}{4\pi N^*}\right)^{1/3} \times \frac{1}{a_{Bn(Bp)}(r_{d(a)})} = 1.1723 \times 10^8 \times \left(\frac{g_c(v)}{N^*}\right)^{1/3} \times \frac{m_{n(p)}^*/m_0}{\epsilon(r_{d(a)})}. \quad (B1)$$

In particular, in the following,  $m_{n(p)}^*/m_0 = m_r/m_0$ , is taken to calculate the band gap narrowing (BGN), as used in Sections 3 and 5. Therefore, the correlation energy of an effective electron gas,  $E_{CE}(r_{sn(sp)})$ , is found to be given by [1]:

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

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

$$\Delta E_{gn}(N^*, r_d) \simeq a_1 \times \frac{\epsilon_0}{\epsilon(r_d)} \times N_r^{1/3} + a_2 \times \frac{\epsilon_0}{\epsilon(r_d)} \times N_r^{\frac{1}{3}} \times (2.503 \times [-E_{CE}(r_{sn}) \times r_{sn}]) + a_3 \times \left[\frac{\epsilon_0}{\epsilon(r_d)}\right]^{5/4} \times \sqrt{\frac{m_p}{m_r}} \times N_r^{1/4} + a_4 \times \sqrt{\frac{\epsilon_0}{\epsilon(r_d)}} \times N_r^{1/2} \times 2 + a_5 \times \left[\frac{\epsilon_0}{\epsilon(r_d)}\right]^{\frac{3}{2}} \times N_r^{\frac{1}{6}}, \quad N_r \equiv \frac{N^* = N - N_{CDn}(r_d)}{9.999 \times 10^{17} \text{ cm}^{-3}}, \quad (B3)$$

and

$$\Delta E_{gp}(N^*, r_a) \simeq a_1 \times \frac{\epsilon_0}{\epsilon(r_a)} \times N_r^{1/3} + a_2 \times \frac{\epsilon_0}{\epsilon(r_a)} \times N_r^{\frac{1}{3}} \times (2.503 \times [-E_{CE}(r_{sp}) \times r_{sp}]) + a_3 \times \left[\frac{\epsilon_0}{\epsilon(r_a)}\right]^{5/4} \times \sqrt{\frac{m_n}{m_r}} \times N_r^{1/4} + 2a_4 \times \sqrt{\frac{\epsilon_0}{\epsilon(r_a)}} \times N_r^{1/2} + a_5 \times \left[\frac{\epsilon_0}{\epsilon(r_a)}\right]^{\frac{3}{2}} \times N_r^{\frac{1}{6}}, \quad N_r \equiv \left(\frac{N^* = N - N_{CDp}(r_a)}{9.999 \times 10^{17} \text{ cm}^{-3}}\right), \quad (B4)$$

Here,  $\epsilon_0 = 15.69$ ,  $a_1 = 3.80 \times 10^{-3}(\text{eV})$ ,  $a_2 = 6.5 \times 10^{-4}(\text{eV})$ ,  $a_3 = 2.85 \times 10^{-3}(\text{eV})$ ,  $a_4 = 5.597 \times 10^{-3}(\text{eV})$  and  $a_5 = 8.1 \times 10^{-4}(\text{eV})$ .

Therefore, in Equations (B3, B4), at  $T=0 K$  and  $N^* = 0$ , and for any  $r_{d(a)}$ ,  $\Delta E_{gn(gp)}(N^* = 0, r_{d(a)}) = 0$ , according to the metal-insulator transition (MIT).

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