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NEW CRITICAL IMPURITY DENSITY IN METAL-INSULATOR TRANSITION, OBTAINED IN VARIOUS N(P)- TYPE DEGENERATE ALKALI METALS, BEING JUST THAT OF THE CARIERS, LOCALIZED IN EXPONENTIAL BAND TAILS. (I)

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ABTRACT

By basing on the same physical model and treatment method, as used in our recent works (Van Cong, 2023), we will investigate the critical impurity densities in the metal-insulator transition (MIT), obtained in various n(p)-type degenerate [Li, Na, Mg, Ca, and Sr]- alkali metals, being due to the effects of the size of donor (acceptor) d(a)-radius, $r_{d(a)}$, and the high d(a)-density, N, assuming that all the impurities are ionized even at T=0 K. In such n(p)-type degenerate metals, we will determine:

(i)-the critical impurity density $N_{CDn(CDp)}(r_{d(a)})$ in the MIT, as that given in Eq. (8), by using an empirical Mott parameter $M_{n(p)} = 0.25$, and

(ii)-the density of electrons (holes) localized in the exponential conduction (valence)-band tails (EBT), $N^{EBT}_{CDn(CDp)}(r_{d(a)}, x)$, as that given in Eq. (26), by using our empirical Heisenberg parameter, $\mathcal{H}_{n(p)} = 0.47137$, as given in Eq. (15), according to: for a given $r_{d(a)}$, $N^{EBT}_{CDn(CDp)}(r_{d(a)}) \cong N_{CDn(CDp)}(r_{d(a)})$, with a precision of the order of 3.4931×10^{-7}, as observed in Tables 2-6.

In other words, such the critical d(a)-density $N_{CDn(NDp)}(r_{d(a))}$, is just the density of electrons (holes) localized in the EBT, $N^{EBT}_{CDn(CDp)}(r_{d(a)})$, respectively.

KEYWORS: n(p)-type degenerate alkali metals, critical impurity density in the metal-insulator transition (MIT).

INTRODUCTION

By basing on the same intrinsic energy-band-structure parameters, physical model and treatment method, as used in our recent works (Van Cong, 2023; 2023; 2023), and also other works (Green, 2022; Kitell, 1976; Moon et al., 2016; Van Cong et al., 2014; Van Cong & Debiais, 1993; Van Cong et al., 1984), we will investigate the critical impurity density in the metal-insulator transition (MIT), obtained in various n(p)-type degenerate **X ≡ [Li, Na, Mg, Ca, and Sr]- alkali metals**, being due to the effects of the size of donor (acceptor) d(a)-radius, $r_{d(a)}$ and the high d(a)-density, N, assuming that all the impurities are ionized even at T=0 K. In such alkali metals, we will determine:

(i)-the critical impurity densities $N_{CDn(CDp)}(r_{d(a)})$ in the MIT, as that given in Eq. (8), by using an empirical Mott parameter $M_{n(p)} = 0.25$, and

(ii)-the density of electrons (holes) localized in the exponential conduction(valence)-band tails (EBT), $N^{EBT}_{CDn(CDp)}(r_{d(a)})$, as that given in Eq. (26), by using the empirical Heisenberg parameter, $\mathcal{H}_{n(p)} = 0.47137$, as that given in Eq. (15), according to: for given $r_{d(a)}$ and x, $N^{EBT}_{CDn(CDp)}(r_{d(a)}) \cong N_{CDn(CDp)}(r_{d(a)})$, with a precision of the order of 3.4931×10^{-7}, as observed in Tables 2-6. In other words, such the critical d(a)-density $N_{CDn(NDp)}(r_{d(a))}$, is just the density of electrons (holes) localized in the EBT, $N^{EBT}_{CDn(CDp)}(r_{d(a)})$, respectively.

In the following, we will determine those functions: $N_{CDn(CDp)}(r_{d(a)})$ and $N^{EBT}_{CDn(CDp)}(r_{d(a)})$.

CRITICAL DENSITY IN THE MOTT MIT

Such the critical impurity density $N_{CDn(CDp)}(r_{d(a)})$, expressed as a function of $r_{d(a)}$, is determined as follows.

Here, the values of the intrinsic energy-band-structure parameters (So and Wang, 1977), such as: the reduced effective electron (hole) mass in conduction (valence) bands, $m_{c(v)}/m_o$, m_o ($= 9.109558 \times 10^{-28}$ g) being the free electron mass and the static dielectric constant ε_o are given in **Table 1 in Appendix 1**.

Therefore, the effective donor (acceptor)-ionization energy, $E_{do(ao)}$, is given by:

$$E_{do(ao)} = \frac{13600\times[m_{c(v)}/m_o]}{[\varepsilon_o]^2}\ meV, \quad (1)$$

and the isothermal bulk modulus $B_{do(ao)}$, at $r_{d(a)} = r_{do(ao)}$, by:

$$B_{do(ao)} \equiv \frac{E_{do(ao)}}{(4\pi/3)\times(r_{do(ao)})^3}\left(\frac{N}{m^2}\right) \quad (2)$$

Effects of impurity size

Here, one shows that the effect of the size of donor (acceptor) d(a)-radius, $r_{d(a)}$, strongly affects the changes in all the energy-band-structure parameters, which can be represented by the effective relative static dielectric constant $\varepsilon(r_{d(a)})$ (Van Cong, 2023; Van Cong et al., 1984), in the following.

At $r_{d(a)} = r_{do(ao)}$, the needed boundary conditions are found to be, for the impurity-atom volume $V = (4\pi/3)\times(r_{d(a)})^3$, $V_{do(ao)} = (4\pi/3)\times(r_{do(ao)})^3$, for the pressure p, as: $p_o = 0$, and for the deformation potential energy (or the strain energy) σ, as: $\sigma_o = 0$. Further, the two important equations, used to determine the σ-variation: $\Delta\sigma \equiv \sigma - \sigma_o = \sigma$, are defined by: $\frac{dp}{dV} = -\frac{B}{V}$ and $p = -\frac{d\sigma}{dV}$. giving: $\frac{d}{dV}\left(\frac{d\sigma}{dV}\right) = \frac{B}{V}$. Then, by an integration, one gets:

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

Furthermore, we also shown that, as $r_{d(a)} > r_{do(ao)}$ ($r_{d(a)} < r_{do(ao)}$), the compression (dilatation) gives rise to: the increase (the decrease) in the effective donor (acceptor)-ionization energy $E_{d(a)}(r_{d(a)})$ in the absolute values, being obtained from the effective Bohr model, and then such the compression (dilatation) is represented respectively by: $\pm[\Delta\sigma(r_{d(a)})]_{n(p)}$,

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

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

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

Therefore, from above Equations (3) and (4), one obtains the expressions for $\varepsilon(r_{d(a)})$ and $E_{d(a)}(r_{d(a)})$ as:

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

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

according to the increase in $E_{d(a)}(r_{d(a)})$, and

(ii)-for $r_{d(a)} \leq r_{do(ao)}$, since $\varepsilon(r_{d(a)}) = \frac{\varepsilon_o}{\sqrt{1-\left[\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3-1\right]\times\ln\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3}} \geq \varepsilon_o$, with a condition, given by: $\left[\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 - 1\right] \times \ln\left(\frac{r_{d(a)}}{r_{do(ao)}}\right)^3 < 1$, and

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

corresponding to the decrease in $E_{d(a)}(r_{d(a)})$.

Furthermore, the effective Bohr radius $a_{Bn(Bp)}(r_{d(a)})$ is defined by:

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

where $-q$ is the electron charge; $q > 0$.

Then, the critical donor (acceptor)-density in the Mott MIT, $N_{CDn(NDp)}(r_{d(a)})$, is determined, using an empirical Mott parameter, $M_{n(p)} = 0.25$, for each the conduction (valence) band, as:

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

Noting that $M_{n(p)}$ could be chosen in general case so that the obtained numerical $N_{CDn(NDp)}(r_{d(a)})$-results, being found to be in good agreement with the corresponding experimental ones.

In the following, these obtained numerical results can also be justified by calculating the numerical results of the density of electrons (holes) localized in exponential conduction (valence)-band (EBT) tails, $N^{EBT}_{CDn(CDp)}(r_{d(a)})$.

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

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

Physical model

In n(p)-type degenerate X-alkali metals, if denoting the Fermi wave number by: $k_{Fn(Fp)}(N) \equiv (3\pi^2 N)^{1/3}$, N being the total impurity density, assuming that all the impurities are ionized even at 0 K, the effective reduced Wigner-Seitz radius $r_{sn(sp)}$, characteristic of interactions, is defined by:

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

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

$$R_{sn(sp)}\left(N, r_{d(a)}\right) \equiv \frac{k_{sn(sp)}}{k_{Fn(Fp)}} = \frac{k_{Fn(Fp)}^{-1}}{k_{sn(sp)}^{-1}} =$$

$$R_{snWS(spWS)} + \left[R_{snTF(spTF)} - R_{snWS(spWS)}\right]e^{-r_{sn(sp)}} < 1. \quad (10)$$

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

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

$$R_{snTF(spTF)}\left(N, r_{d(a)}\right) \equiv \frac{k_{snTF(spTF)}}{k_{Fn(Fp)}} = \frac{k_{Fn(Fp)}^{-1}}{k_{snTF(spTF)}^{-1}} = \sqrt{\frac{4\gamma r_{sn(sp)}\left(N, r_{d(a)}\right)}{\pi}} \ll 1, \ \gamma \equiv \left(\frac{4}{9\pi}\right)^{\frac{1}{3}}, \quad (11)$$

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

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

$$R_{snWS(spWS)}\left(N, r_{d(a)}\right) \equiv \frac{k_{snWS(spWS)}}{k_{Fn(Fp)}} = \left(\frac{3}{2\pi} - \gamma \frac{d\left[r_{sn(sp)}^2 \times E_{CE}\left(N, r_{d(a)}\right)\right]}{dr_{sn(sp)}}\right) \times 0.5\,, \quad (12)$$

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

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

So, n(p)-type degenerate X- alkali metals, the physical conditions are found to be given by :

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

(13)

Here, $\pm E_{Fno(Fpo)}$ is the Fermi energy at 0 K, and $\eta_{n(p)}$ is defined in next Eq. (15), as: $\pm E_{Fno(Fpo)}(N) = \frac{\hbar^2 \times k_{Fn(Fp)}(N)^2}{2 \times m_{c(v)}} \geq 0, \eta_{n(p)}(N, r_{d(a)}) = \frac{\sqrt{2\pi N}}{\varepsilon(r_{d(a)})} \times q^2 k_{sn(sp)}^{-1/2}$.

Then, the total screened Coulomb impurity potential energy due to the attractive interaction between an electron (hole) charge, $-q(+q)$, at position $\vec{r}$, and an ionized donor (ionized acceptor) charge: $+q(-q)$ at position $\overrightarrow{R_j}$, randomly distributed throughout X(x)- crystalline alloys, is defined by:

$$V(r) \equiv \sum_{j=1}^{\mathbb{N}} v_j(r) + V_o, \qquad (14)$$

where $\mathbb{N}$ is the total number of ionized donors (acceptors), V_o is a constant potential energy, and the screened Coulomb potential energy $v_j(r)$ is defined as:

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

where $k_{sn(sp)}$ is the inverse screening length determined in Eq. (11).

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

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

where Ω is the total X- alkali metal volume.

Then, the effective auto-correlation function for potential fluctuations, $W_{n(p)}(\nu_{n(p)}, N, r_{d(a)}) \equiv \langle V(r)V(r') \rangle$, was determined, [4, 5] as :

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

$$\nu_{n(p)}(E, N) \equiv \frac{\mp E}{\pm E_{Fno(Fpo)}(N)}, \ \mathcal{H}_{n(p)} = 0.47137 . \qquad (15)$$

Here, E is the total electron energy, and the empirical Heisenberg parameter $\mathcal{H}_{n(p)} = 0.47137$ was chosen above such that the determination of the density of electrons localized in the conduction(valence)-band tails will be accurate, noting that as $E \to \pm\infty$, $|\nu_{n(p)}| \to \infty$, and therefore, $W_{n(p)} \to \eta_{n(p)}^2$.

In the following, we will calculate the ensemble average of the function: $(E-V)^{a-\frac{1}{2}} \equiv E_k^{a-\frac{1}{2}}$, for $a \geq 1$, $E_k \equiv \frac{\hbar^2 \times k^2}{2 \times m_{c(v)}}$ being the kinetic energy of the electron (hole), and V(r) determined in Eq. (16), by using the two following integration methods, which strongly depend on $W_{n(p)}\left(\nu_{n(p)}, N, r_{d(a)}\right)$.

Mathematical Methods

Kane integration method (KIM)

Here, the effective Gaussian distribution probability is defined by:

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

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

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

Then, by variable changes: $s = (E-V)/\sqrt{W_{n(p)}}$ and $y = \mp E/\sqrt{W_{n(p)}} \equiv \frac{\pm E_{Fno(Fpo)}}{\eta_{n(p)}} \times \nu_{n(p)} \times \exp\left(\frac{\mathcal{H}_{n(p)} \times R_{sn(sp)}}{4 \times \sqrt{|\nu_{n(p)}|}}\right)$, and using an identity:

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

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

$$\langle E_k^{a-\frac{1}{2}} \rangle_{KIM} = \frac{\exp(-y^2/4) \times W_{n(p)}^{\frac{2a-1}{4}}}{\sqrt{2\pi}} \times \Gamma(a+\tfrac{1}{2}) \times D_{-a-\frac{1}{2}}(y) =$$

$$\frac{\exp(-y^2/4) \times \eta_{n(p)}^{a-\frac{1}{2}}}{\sqrt{2\pi}} \times \exp\left(-\frac{\mathcal{H}_{n(p)} \times R_{sn(sp)} \times (2a-1)}{8 \times \sqrt{|\nu_{n(p)}|}}\right) \times \Gamma(a+\tfrac{1}{2}) \times D_{-a-\frac{1}{2}}(y). \qquad (16)$$

Feynman path-integral method (FPIM)

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

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

noting that as a=1, $(it)^{-\frac{3}{2}} \times \exp\left\{-\frac{(t\sqrt{W_p})^2}{2\hbar^2}\right\}$ is found to be proportional to the averaged Feynman propagator given the dense donors (acceptors). Then, by variable changes: $t = \frac{\hbar}{\sqrt{W_{n(p)}}}$ and $y = \mp E/\sqrt{W_{n(p)}} \equiv \frac{\pm E_{Fno(Fpo)}}{\eta_{n(p)}} \times \nu_{n(p)} \times \exp\left(\frac{\mathcal{H}_{n(p)} \times R_{sn(sp)}}{4\times\sqrt{|\nu_{n(p)}|}}\right)$, for n(p)-type respectively, and then using an identity:

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

one finally obtains: $\langle E_k^{a-\frac{1}{2}}\rangle_{FPIM} \equiv \langle E_k^{a-\frac{1}{2}}\rangle_{KIM}$, $\langle E_k^{a-\frac{1}{2}}\rangle_{KIM}$ being determined in Eq. (16).

In the following, with the use of asymptotic forms for $D_{-a-\frac{1}{2}}(y)$, those given for $\langle (E-V)^{a-\frac{1}{2}}\rangle_{KIM}$ can be obtained in the two following cases.

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

As $E \to \pm\infty$, one has: $\nu_{n(p)} \to \mp\infty$ and $y \to \mp\infty$. In this case, one gets: $D_{-a-\frac{1}{2}}(y \to \mp\infty) \approx \frac{\sqrt{2\pi}}{\Gamma(a+\frac{1}{2})} \times e^{\frac{y^2}{4}} \times (\mp y)^{a-\frac{1}{2}}$, and therefore from Eq. (16), one gets:

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

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

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

(18)

Therefore, as $E \to \pm 0$, from Eq. (16), one gets: $\langle E_k^{a-\frac{1}{2}}\rangle_{KIM} \to 0$.

Thus, in this case, one gets:

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

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

As $E \to \mp 0$, one has: $(y, \nu_{n(p)}) \to \pm 0$, and by putting $f(a) \equiv \frac{\eta_{n(p)}^{a-\frac{1}{2}}}{\sqrt{2\pi}} \times \Gamma(a+\frac{1}{2}) \times \beta(a)$, Eq. (18) yields:

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

Further, as $E \to \mp\infty$, one has: $(y, \nu_{n(p)}) \to \pm\infty$. Thus, one gets: $D_{-a-\frac{1}{2}}(y \to \pm\infty) \approx y^{-a-\frac{1}{2}} \times e^{-\frac{y^2}{4}} \to 0.$

Therefore, from Eq. (16), one gets:

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

noting that $\beta(a) = \frac{\sqrt{\pi}}{2^{\frac{2a+1}{4}}\Gamma(\frac{a}{2}+\frac{3}{4})]}$, being equal to: $\frac{\sqrt{\pi}}{2^{\frac{3}{4}}\times\Gamma(5/4)}$ for a=1, and $\frac{\sqrt{\pi}}{2^{3/2}}$ for $a = 5/2$.

It should be noted that those ratios: $\frac{\langle E_k^{a-\frac{1}{2}}\rangle_{KIM}}{f(a)}$, obtained in Equations (20) and (21), can be taken in an approximate form as:

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

So that: $F_{n(p)}(\nu_{n(p)}, N, r_{d(a)}, a) \to H_{n(p)}(\nu_{n(p)}, N, r_{d(a)}, a)$ for $0 \le \nu_n \le 16$, and $F_{n(p)}(\nu_{n(p)}, N, r_{d(a)}, a) \to K_{n(p)}(\nu_{n(p)}, N, r_{d(a)}, a)$ for $\nu_{n(p)} \ge 16$. Here, the constants c_1 and c_2 may be respectively chosen as: $c_1 = 10^{-40}$ and $c_2 = 80$, as $a = 1$, being used to determine the critical density of electrons (holes) localized in the exponential conduction(valence) band-tails (EBT), $N_{CDn(CDp)}^{EBT}(N, r_{d(a)})$, given in the following.

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

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

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

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

$$\mathcal{D}_o(N, r_{d(a)}, a=1) = \frac{g_{c(v)}\times\left(m_{c(v)}\times m_o\right)^{3/2}\times\sqrt{\eta_{n(p)}}}{2\pi^2\hbar^3}\times\beta(a),\ \beta(a=1) = \frac{\sqrt{\pi}}{2^{\frac{3}{4}}\times\Gamma(5/4)}. \quad (24)$$

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

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

where

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

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

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

Finally, Eq. (25) now yields

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

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

In n(p)-type degenerate X - alkali metals, the numerical results of $N_{CDn(CDp)}^{EBT}[N = N_{CDn(NDp)}(r_{d(a)}, x), r_{d(a)}] \equiv N_{CDn(CDp)}^{EBT}(r_{d(a)})$, for a simplicity of presentation, evaluated using Eq. (26), are given in following Tables 2-6 in Appendix 1, in which those of other functions such as: $B_{do(ao)}$, ε, and $N_{CDn(CDp)}$ are also computed, using Equations (2), (5), (6),

and (8), respectively, noting that the relative deviations in absolute values are defined by: $|RD| \equiv \left|1 - \frac{N^{EBT}_{CDn(CDp)}}{N_{CDn(CDp)}}\right|$.

CONCLUSION

In those Tables 2-6, some concluding remarks are given and discussed in the following.

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

(2)- In those Tables 2-6, one notes that the maximal value of |RD| is found to be given by: $\mathbf{3.4931 \times 10^{-7}}$, meaning that $N^{EBT}_{CDn} \cong N_{CDn}$. In other words, such the critical d(a)-density $N_{CDn(NDp)}(r_{d(a))})$, is just the density of electrons (holes), being localized in the EBT, $N^{EBT}_{CDn(CDp)}(r_{d(a)})$, respectively.

(3) Finally, once $N_{CDn(CDp)}$ is determined, the effective density of free electrons (holes), N^*, given in the parabolic conduction (valence) bands of the n(p)-type degenerate X- alkali metals, can thus be defined by:

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

being equivalent to the "compensation effect".

REFERENCES

1. So, C.B. & Wang, S. Electronic Structure of Metals : V. Density of States Effective Masses of Alkali Metals. *J. Phys. F : Met. Phys.*, 1977; 7(8): 1453-1465.
2. Kittel, C. Introduction to Solid State Physics, Wiley, New York, 1976; 84-100.
3. Moon S. et al.. Highly efficient single GaAs thin-film solar cell on flexible substrate. *Sci. Rep.*, 2016; 6: 30107.
4. Van Cong, H. (43.82 %, or 44.05 %)- Limiting Highest Efficiencies, Obtained Respectively in $n^+(p^+) - p(n)$ Crystalline CdS-Junction Solar Cells at T=300 K, Due to the Effects of Impurity Size, Temperature, Heavy Doping, and Photovoltaic Conversion. *European Journal of Theoretical and Applied Sciences*, 2023; 1: 229-245.
5. Van Cong, H. (26.552 %, or 23.69 %)- Limiting Highest Efficiencies, Obtained Respectively in $n^+(p^+) - p(n)$ Crystalline $(X \equiv CdTe, \text{or } CdSe)$-Junction Solar Cells, Due to the Effects of Impurity Size, Temperature, Heavy Doping, and Photovoltaic Conversion. *European Journal of Theoretical and Applied Sciences*, 2023; 1: 249-268.

6. Van Cong, H. 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). *SCIREA J. Phys.*, 2023; 8: 172-197.
7. Van Cong, H. et al. Optical bandgap in various impurity-Si systems from the metal-insulator transition study. *Physica B.*, 2014; 436: 130-139.
8. Van Cong, H. & Debiais, G. A simple accurate expression of the reduced Fermi energy for any reduced carrier density. *J. Appl. Phys.*, 1993; 73: 1545-1546.
9. Van Cong, H. et al. Size effect on different impurity levels in semiconductors. *Solid State Communications*, 1984; 49: 697-699.

APPENDIX 1

Table 1: The values of the energy-band-structure parameters are given in various Alkali Metals in the following (So and Wang, 1977).

In the $n(p)\ type\ degenerate\ Lithium\ (Li) - Metal$, in which $r_{do(ao)} = r_{Li}$ =0.128 nm, we have: $m_{c(v)}/m_o = 1.59$, $\varepsilon_o = 1$.

In the $n(p)\ type\ degenerate\ Sodium\ (Na) - Metal$, in which $r_{do(ao)} = r_{Na}$ =0.166 nm, we have: $m_{c(v)}/m_o = 1.06$, $\varepsilon_o = 1$.

In the $n(p)\ type\ degenerate\ Magnesium\ (Mg) - Metal$, in which $r_{do(ao)} = r_{Rb}$ =0.141 nm, we have: $m_{c(v)}/m_o = 1$, $\varepsilon_o = 1$.

In the $n(p)\ type\ degenerate\ Calcium\ (Ca) - Metal$, in which $r_{do(ao)} = r_{Cs}$ =0.176 nm, we have: $m_{c(v)}/m_o = 1$, $\varepsilon_o = 1$.

In the $n(p)\ type\ degenerate\ Strontium\ (Sr) - Metal$, in which $r_{do(ao)} = r_{Be}$ =0.195 nm, we have: $m_{c(v)}/m_o = 1$, $\varepsilon_o = 1$.

Table 2: In the n(p) type degenerate **Li** – Metal, the numerical results of $B_{do(ao)} = 3.9434835 \times 10^{11}\ (\frac{N}{m^2})$, ε, $N_{CDn(CDp)}$, and $N^{EBT}_{CDn(CDp)}$ are computed, using Equations (2), (5), (6), (8), and (26), respectively, noting that the relative deviations in absolute values are defined by: $|RD| \equiv \left|1 - \frac{N^{EBT}_{CDn(CDp)}}{N_{CDn(Cdp)}}\right|$, giving rise to their maximal value equal to $\mathbf{3.4704} \times \mathbf{10^{-7}}$. It means that such the critical d(a)-density $N_{CDn(NDp)}(r_{d(a)})$, determined in Eq. (8), is just the density of electrons (holes) localized in the EBT, $N^{EBT}_{CDn(CDp)}(r_{d(a)})$, determined in Eq. (26), respectively.

Donor	P	As	**Li**	Sb	Sn
r_d (nm) ↗	0.110	0.118	**0.128**	0.136	0.140
$\varepsilon(r_d)$ ↘	1.0951	1.0275	1	0.9823	0.9609
$N_{CDn}(r_d)$ in 10^{23} cm^{-3} ↗	3.2126248	3.8888301	4.2187787	4 .4504158	4.7542438
$N^{EBT}_{CDn}(r_d)$ in 10^{23} cm^{-3} ↗	3.2126240	3.8888289	4.2187776	4.4504147	4.7542422
$\|RD\|$ in 10^{-7}	2.3529	3.1053	2.6521	2.5536	**3.4704**

Acceptor	Ga	**Li**	Mg	In	Cd
r_a (nm) ↗	0.126	**0.128**	0.141	0.144	0.148
$\varepsilon(r_a)$ ↘	1.0011	1	0.9609	0.9326	0.8988
$N_{CDp}(r_a)$ in 10^{23} cm^{-3} ↗	4.2049896	4.2187787	4.7542438	5.2011232	5.8092822
$N^{EBT}_{CDp}(r_a)$ in 10^{23} cm^{-3} ↗	4.2049884	4.2187776	4.7542422	5.2011219	5.8092806
$\|RD\|$ in 10^{-7}	2.9719	2.6505	3.4688	2.4160	2.7404

Table 3: In the n(p) type degenerate **Na** – Metal, the numerical results of $B_{do(ao)} = 1.2052979 \times 10^{11}$ $(\frac{N}{m^2})$, ε, $N_{CDn(CDp)}$, and $N^{EBT}_{CDn(CDp)}$ are computed, using Equations (2), (5), (6), (8), and (26), respectively, noting that the relative deviations in absolute values are defined by: $|RD| \equiv \left|1 - \frac{N^{EBT}_{CDn(CDp)}}{N_{CDn(Cdp)}}\right|$, giving rise to their maximal value equal to $\mathbf{3.4931 \times 10^{-7}}$. It means that such the critical d(a)-density $N_{CDn(NDp)}(r_{d(a)})$, determined in Eq. (8), is just the density of electrons (holes) localized in the EBT, $N^{EBT}_{CDn(CDp)}(r_{d(a)})$, determined in Eq. (26), respectively.

Donor		P	As	Sb	Sn	**Na**
r_d (nm)	↗	0.110	0.118	0.136	0.140	**0.166**
$\varepsilon(r_d)$	↘	2.8319	1.7053	1.1697	1.1212	1
$N_{CDn}(r_d)$ in 10^{21} cm^{-3}	↗	5.5038570	25.205638	78.100359	88.693230	125.00085
$N^{EBT}_{CDn}(r_d)$ in 10^{21} cm^{-3}	↗	5.5038554	25.205631	78.100343	88.693201	125.00082
$\|RD\|$ in 10^{-7}		2.8489	2.8590	2.0438	3.2447	2.6347

Acceptor		Ga	Mg	In	Cd	**Na**
r_a (nm)	↗	0.126	0.141	0.144	0.148	**0.166**
$\varepsilon(r_a)$	↘	1.3677	1.1212	1.0834	1.0543	1
$N_{CDp}(r_a)$ in 10^{22} cm^{-3}	↗	4.8858614	8.8693230	9.8286993	10.667367	42.187787
$N^{EBT}_{CDp}(r_a)$ in 10^{22} cm^{-3}	↗	4.8858598	8.8693201	9.8286972	10.667363	42.187776
$\|RD\|$ in 10^{-7}		3.3206	3.2431	2.1367	**3.4931**	2.6505

Table 4. In the n(p) type degenerate **Mg** – Metal, the numerical results of $B_{do(ao)} = 1.8554766 \times 10^{11}$ $(\frac{N}{m^2})$, ε, $N_{CDn(CDp)}$, and $N^{EBT}_{CDn(CDp)}$ are computed, using Equations (2), (5), (6), (8), and (26), respectively, noting that the relative deviations in absolute values are defined by: $|RD| \equiv \left|1 - \frac{N^{EBT}_{CDn(CDp)}}{N_{CDn(Cdp)}}\right|$, giving rise to their maximal value equal to $\mathbf{3.2028 \times 10^{-7}}$. It means that such the critical d(a)-density $N_{CDn(NDp)}(r_{d(a)})$, determined in Eq. (8), is just the density of electrons (holes) localized in the EBT, $N^{EBT}_{CDn(CDp)}(r_{d(a)})$, determined in Eq. (26), respectively.

Donor		P	As	Sb	Sn	**Mg**
r_d (nm)	↗	0.110	0.118	0.136	0.140	**0.141**
$\varepsilon(r_d)$	↘	1.2816	1.1331	1.0056	1.0002	1
$N_{CDn}(r_d)$ in 10^{22} cm^{-3}	↗	4.9857167	7.2146410	10.320752	10.488212	10.495313
$N^{EBT}_{CDn}(r_d)$ in 10^{22} cm^{-3}	↗	4.9857154	7.2146387	10.320750	10.488209	10.495310
$\|RD\|$ in 10^{-7}		2.5092	**3.2028**	1.6640	2.4201	2.9654

Acceptor		Ga	**Mg**	In	Cd
r_a (nm)	↗	0.126	**0.141**	0.144	0.148
$\varepsilon(r_a)$	↘	1.0521	1	0.9979	0.9888
$N_{CDp}(r_a)$ in 10^{23} cm^{-3}	↗	0.9011263	1.0495313	1.0560207	1.0855359
$N^{EBT}_{CDp}(r_a)$ in 10^{23} cm^{-3}	↗	0.9011261	1.0495310	1.0560204	1.0855356
$\|RD\|$ in 10^{-7}		2.4709	2.9668	2.8218	2.8911

Table 5. In the n(p) type degenerate **Ca** – Metal, the numerical results of $B_{do(ao)} = 9.5405807 \times 10^{10}$ $(\frac{N}{m^2})$, ε, $N_{CDn(CDp)}$, and $N^{EBT}_{CDn(CDp)}$ are computed, using Equations (2), (5), (6), (8), and (26), respectively, noting that the relative deviations in absolute values are defined by: $|RD| \equiv \left|1 - \frac{N^{EBT}_{CDn(CDp)}}{N_{CDn(Cdp)}}\right|$, giving rise to their maximal value equal to $\mathbf{3.2253} \times \mathbf{10^{-7}}$. It means that such the critical d(a)-density $N_{CDn(NDp)}(r_{d(a)})$, determined in Eq. (8), is just the density of electrons (holes) localized in the EBT, $N^{EBT}_{CDn(CDp)}(r_{d(a)})$, determined in Eq. (26), respectively.

Donor		As	Sb	Sn	**Ca**
r_d (nm)	↗	0.118	0.136	0.140	**0.176**
$\varepsilon(r_d)$	↘	2.4840	1.3092	1.2318	1
$N_{CDn}(r_d)$ in 10^{22} cm^{-3}	↗	0.68478457	4.6767671	5.6148959	10.495313
$N^{EBT}_{CDn}(r_d)$ in 10^{22} cm^{-3}	↗	0.68478439	4.6767658	5.6148941	10.495310
$\|RD\|$ in 10^{-7}		2.5669	2.7507	**3.2253**	2.9684

Acceptor		Ga	Mg	In	Cd	**Ca**
r_a (nm)	↗	0.126	0.141	0.144	0.148	**0.176**
$\varepsilon(r_a)$	↘	1.6546	1.2155	1.1722	1.1256	1
$N_{CDp}(r_a)$ in 10^{22} cm^{-3}	↗	2.3169669	5.8443109	6.5153448	7.3594320	10.495313
$N^{EBT}_{CDp}(r_a)$ in 10^{22} cm^{-3}	↗	2.3169664	5.8443090	6.5153433	7.3594298	10.495310
$\|RD\|$ in 10^{-7}		2.3028	3.2202	2.3519	2.9345	2.9669

Table 6. In the n(p) type degenerate **Sr** – Metal, the numerical results of $B_{do(ao)} = 7.014698 \times 10^{10}$ $(\frac{N}{m^2})$, ε, $N_{CDn(CDp)}$, and $N^{EBT}_{CDn(CDp)}$ are computed, using Equations (2), (5), (6), (8), and (26), respectively, noting that the relative deviations in absolute values are defined by: $|RD| \equiv \left|1 - \frac{N^{EBT}_{CDn(CDp)}}{N_{CDn(Cdp)}}\right|$, giving rise to their maximal value equal to $\mathbf{3.3270} \times \mathbf{10^{-7}}$. It means that such the critical d(a)-density $N_{CDn(NDp)}(r_{d(a)})$, determined in Eq. (8), is just the density of electrons (holes) localized in the EBT, $N^{EBT}_{CDn(CDp)}(r_{d(a)})$, determined in Eq. (26), respectively.

Donor		Te	Sb	Sn	**Sr**
r_d (nm)	↗	0.132	0.136	0.140	**0.195**
$\varepsilon(r_d)$	↘	2.2792	1.8709	1.6356	1
$N_{CDn}(r_d)$ in 10^{22} cm^{-3}	↗	0.88645906	1.6027389	2.3985955	10.495313
$N^{EBT}_{CDn}(r_d)$ in 10^{22} cm^{-3}	↗	0.88645884	1.6027384	2.3985947	10.495310
$\|RD\|$ in 10^{-7}		2.4824	**3.3270**	3.1684	2.9684

Acceptor		Ga	Mg	In	Cd	**Sr**
r_a (nm)	↗	0.126	0.141	0.144	0.148	**0.195**
$\varepsilon(r_a)$	↘	4.8058	1.5911	1.4797	1.3680	1
$N_{CDp}(r_a)$ in 10^{22} cm^{-3}	↗	0.094559463	2.6057077	3.2394674	4.0996650	10.495313
$N^{EBT}_{CDp}(r_a)$ in 10^{22} cm^{-3}	↗	0.094559437	2.6057071	3.2394667	4.0996642	10.495310
$\|RD\|$ in 10^{-7}		2.7645	2.4801	2.2158	2.0682	2.9668