Double exponential density of states and modified charge carrier transport in organic semiconductors

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Abstract
This paper discusses the use of an approximated charge carrier density to model an organic thin-film transistor (OTFT) using a double exponential density of states. Traditionally, published work employs a single exponential density of states and Gaussian density of states. On the contrary, this paper employs a double exponential density of states in the Fermi integral to evaluate the charge carrier density for the OTFT. We consider two exponential density of states, one rateled to the tail region and one to a deep region, in addition to various associated parameters. The distribution of localized trap states between the highest and lowest orbital is expressed as a density of states, one for the tail states and one for the deep states. Tail states are better described by the Gaussian function, while deep states are better described by the exponential density of states. Therefore, if we require that the two regions be defined by a single function, then the function should be a sum of the two, the exponential and the Gaussian, to more accurately describe the complete region. The double exponential density of states is employed to evaluate and approximate the Fermi integral using various mathematical methods, so that the error is lower for various parameters.

Keywords Organic thin film transistor (OTFT) · Double exponential density of states · Charge carrier density · Fermi–Dirac-type integral

1 Introduction

The concentration of electrons at various energy levels in a semiconductor is a very important parameter to determine the characteristics of devices manufactured using the semiconductor. To determine the concentration of the electrons, we need to know the probability of an electron residing at that particular energy level, which would tell us what the chances are of finding an electron possessing said amount of energy. Also, the electrons cannot occupy all the energy values in a continuum; i.e., there are only predefined states or energy levels which are allowed for an electron to possess. These states are the actual energy levels that are occupied by the electrons. So, in addition to the probability of number of electrons at a particular energy, we also need to know the number of states that are allowed in a particular range of energy, which is called the density of states (number of states per unit volume of semiconductor material).

Traditionally, the probability of an electron in a particular energy level is given by the Fermi–Dirac function [1]:

\[ f(E, T) = \frac{1}{1 + e^{\frac{E-E_F}{k_B T}}} \]

Here, \( E \) is the energy of the electron and \( T \) is the temperature at which this energy is attained, \( k_B \) is the Boltzmann constant and \( E_F \) is the energy associated with the Fermi level of the semiconductor.

The Fermi level in semiconductor engineering is the energy level which has a 50% chance of occupation at finite temperatures. This is historically given by a Gaussian density of states [2–5] or by an exponential density of states [1,
A double exponential density of states function will be used as stated in [6] and [9] and given by
\[
g(E) = \frac{N_{\text{Deep}}}{\Phi_{\text{Deep}}} \cdot e^{\frac{E}{\Phi_{\text{Deep}}}} + \frac{N_{\text{Tail}}}{\Phi_{\text{Tail}}} \cdot e^{\frac{E}{\Phi_{\text{Tail}}}}
\]

To bolster this claim, it can be seen in [10–12] that the current for a thin film transistor (TFT) is modeled using a double exponential density of states because it has a greater resemblance to the actual experimental data than when a single exponential density of states is used.

Currently, the calculation of charge carrier density, which is basically the integral of \( f(E, T) \) and \( g(E) \) over all the energies from \(-\infty\) to 0, has been done by taking \( g(E) \) as the Gaussian density of states and the exponential density of states, as shown in [13], and by the single exponential density of states, as shown in [1].

Since we are developing a double exponential density of states, the focus will be kept on Hart [1], in which they have taken the Fermi function \( f(E, T) = \frac{1}{1 + e^{\frac{E - E_F}{k_B T}}} \) and the single exponential density of states function as \( g(E) = \frac{N}{E_0} e^{\frac{E}{E_0}} \). This depiction is correct, but this might be made more accurate if we consider it to be a summation of two exponentials [14] with different \( E_0 \)s to characterize both deep and tail states, as deep and tail states have different associated \( E_0 \). We will then calculate the charge carrier density by integrating the Electronic Density Of States (EDOS) and Fermi–Dirac function [2]. A double exponential density of states yields a more accurate description of the density of states.

## 2 The VM model [5]

The VM model begins with an assumed exponential density of states of the form where \( E_0 = k_B T_0 \). The single DOS is given by the following equation and is defined for \(-\infty < E \leq 0\).

\[
D(E, T_0) = \frac{N}{E_0} e^{\frac{E}{E_0}}
\]

### 2.1 Approximate charge carrier density

The actual charge density function can be written as the following equation, which integrates the product of the density of states and Fermi–Dirac function:

\[
\delta = \frac{1}{N} \int_{-\infty}^{0} D(E, T_0) f_c(E, T, E_c) \, dE
\]

Here, \( f_c \) is the Fermi–Dirac function for an electron defined as

\[
f_c = \frac{1}{1 + e^{\frac{E_c - E}{k_B T}}}
\]

Also, \( N \) is the number of energetic states per unit volume, \( k_B \) is Boltzmann’s constant, and \( T_0 > 0 \) is the representative width of exponential distribution that can be considered a measure of the disorder of the system in question. The energy, \( E_0 \), in the denominator of the equation is a normalizing factor used to ensure that the total charge carrier density resulting from integration over all energy states is \( N \). The EDOS is considered to be zero for all energies \( E > 0 \). Refer to Fig. 1.

### 2.2 Double exponential density of states

As introduced in the earlier sections, a double exponential function is a better approximation for the density of states. The equation for this double-EDOS is considered from [9] (Fig. 2) and as portrayed in [14–16].
Here, $E_{\text{LUMO}}$ is considered to be 0, so it reduces to the form

$$g(E) = \frac{N_{\text{Deep}}}{\varphi_{\text{Deep}}} \cdot e^{-\frac{E}{k_B T_{\text{Deep}}}} + \frac{N_{\text{Tail}}}{\varphi_{\text{Tail}}} \cdot e^{-\frac{E}{k_B T_{\text{Tail}}}}$$

Therefore, the exact carrier density for the stated double-EDOS is

$$\delta = \frac{1}{N_i} \int_{-\infty}^{0} g(E) \cdot f_\xi(E) dE$$

Here, $N_i$ is a normalization parameter such that $\int_{-\infty}^{0} g(E) dE$ is 1. Hence, $N_i$ can be found as

$$N_i = N_{\text{Deep}} + N_{\text{Tail}}$$

Now, terms in both summations are similar in nature and differ only in coefficients $\varphi_{\text{Deep}}$ and $\varphi_{\text{Tail}}$, and coefficients outside the integral. Thus, we calculate only one of the terms of the summation and derive the other by simply substituting the parameters.

To solve the above integral, let us perform some substitutions:

$$x = \frac{E}{k_B T}, \quad \xi = \frac{E_F}{k_B T}, \quad \varphi_{\text{Deep}} = k_B T_{\text{Deep}}, \quad \varphi_{\text{Tail}} = k_B T_{\text{Tail}}$$

$$\delta = \frac{N_{\text{Deep}}}{\varphi_{\text{Deep}}} \int_{0}^{\infty} e^{-x} dx \cdot \varphi_{\text{Deep}} = \frac{N_{\text{Tail}}}{\varphi_{\text{Tail}}} \int_{0}^{\infty} e^{-x} dx \cdot \varphi_{\text{Tail}}$$

2.3 Solution of the integral using exact techniques

The equation is

$$\delta_1 = \frac{N_{\text{Deep}}}{\varphi_{\text{Deep}}} \cdot \frac{1}{N_i} \int_{0}^{\infty} e^{-\frac{E_F}{k_B T_{\text{Deep}}}} \cdot e^{\frac{-E}{k_B T_{\text{Deep}}}} \cdot f_\xi dE$$

Performing the substitutions mentioned above we get

$$\delta_1 = \frac{N_{\text{Deep}}}{\varphi_{\text{Deep}}} \cdot \frac{1}{N_i} \int_{0}^{\infty} e^{-\frac{E_F}{k_B T_{\text{Deep}}}} \cdot e^{\frac{-E}{k_B T_{\text{Deep}}}} \cdot f_\xi dE$$

$$\delta_1 = \frac{N_{\text{Deep}}}{\varphi_{\text{Deep}}} \cdot \frac{1}{N_i} \int_{0}^{\infty} e^{-\frac{E_F}{k_B T_{\text{Deep}}}} \cdot e^{\frac{-E}{k_B T_{\text{Deep}}}} \cdot f_\xi dE$$

Since $\xi < 0$ for all practical considerations, we substitute $\xi \rightarrow -|\xi|$ and get the equations as

$$\delta_1 = \frac{N_{\text{Deep}}}{\varphi_{\text{Deep}}} \cdot \frac{1}{N_i} \int_{0}^{\infty} e^{-\frac{E_F}{k_B T_{\text{Deep}}}} \cdot e^{\frac{-E}{k_B T_{\text{Deep}}}} \cdot f_{-|\xi|} \cdot e^{\frac{E}{k_B T_{\text{Deep}}}} dE$$

Now, consider $\frac{N_{\text{Deep}}}{N_{\text{Deep}} + N_{\text{Tail}}} = A_{\text{Deep}}$ so the equation reduces to

$$\delta_1 = A_{\text{Deep}} \cdot e^{-|\xi|} \int_{0}^{\infty} e^{-\frac{E}{k_B T_{\text{Deep}}}} \cdot f_{-|\xi|} \cdot e^{\frac{E}{k_B T_{\text{Deep}}}} dE$$

Now, using the techniques in Selvaggi [13] to evaluate an approximation for this integral for calculation purposes, let us consider integral $\int_{0}^{\infty} e^{-\frac{E}{k_B T_{\text{Deep}}}} \cdot f_{-|\xi|} \cdot e^{\frac{E}{k_B T_{\text{Deep}}}} dE$ as $I_1$ such that

$$\delta_1 = A_{\text{Deep}} \cdot e^{-|\xi|} I_1$$

$$I_1 = \int_{0}^{\infty} e^{\frac{E}{k_B T_{\text{Deep}}}} \cdot f_{-|\xi|} \cdot e^{-\frac{E}{k_B T_{\text{Deep}}}} dE$$

$$I_1 = \int_{0}^{\infty} e^{\frac{E}{k_B T_{\text{Deep}}}} \cdot f_{-|\xi|} \cdot e^{-\frac{E}{k_B T_{\text{Deep}}}} dE$$
As discussed in [17, 18], we have
\[
\frac{1}{1 + e^{-\eta}} = \lim_{{N \to \infty}} \sum_{{m=0}}^{{N}} f_m(-1) \times \left\{ e^{-(1+m)(\varepsilon-\eta)}, \text{ for } \varepsilon \geq \eta \right\}, \text{ for } \varepsilon \leq \eta
\]
It is also known that \( f_m(n) = \frac{1}{m!} \prod_{{i=0}}^{{n-1}} n-i \), so \( f_m(-1) = (-1)^m \).
Thus, writing \( I_1 \) as follows according to the expansion stated above
\[
= \int_{|\xi|} x \left( \frac{1}{1 + e^{x(1-|\xi|)}} \right) \, dx + \int_{|\xi|} x \left( \frac{1}{1 + e^{x(1-|\xi|)}} \right) \, dx
\]
\[
\frac{1}{1 + e^{-(\varepsilon-\eta)}} - 1 + \sum_{{p=1}}^{{\infty}} (-1)^p \times \left[ e^{\xi(1-\frac{\varepsilon}{\tau_{\text{Deep}}})} - e^{-\xi(1-\frac{\varepsilon}{\tau_{\text{Deep}}})} \right] + \frac{1}{1 + e^{-(\varepsilon-\eta)}} - 1 + \sum_{{p=1}}^{{\infty}} (-1)^p \times \left[ e^{\xi(1-\frac{\varepsilon}{\tau_{\text{Deep}}})} - e^{-\xi(1-\frac{\varepsilon}{\tau_{\text{Deep}}})} \right]
\]
Here, \( \phi(z, s, \alpha) \) gives the Hurwitz–Lerch transcendent \([19]\)

\[
\phi(z, s, \alpha) = \sum_{p=0}^{\infty} \frac{z^p}{\left(p + \alpha\right)^s}.
\]

The expression \([20]\)

\[
\phi(-1, 1, \frac{T}{T_{\text{Deep}}}) - \phi(-1, 1, 2 - \frac{T}{T_{\text{Deep}}})
\]

reduces to

\[
\frac{1}{1 - \frac{T}{T_{\text{Deep}}}} + \frac{\pi}{\sin\left(\frac{\pi T}{T_{\text{Deep}}}\right)} - \sum_{p=1}^{\infty} (-1)^p \frac{e^{-p |z|}}{p + \left(1 - \frac{T}{T_{\text{Deep}}}\right)}
\]

Therefore,

\[
I_1 = e^{\frac{|z|}{T_{\text{Deep}}}} \left(1 - \frac{T}{T_{\text{Deep}}}\right) - 1 + e^{\frac{|z|}{T_{\text{Deep}}}} \left(1 - \frac{T}{T_{\text{Deep}}}\right) - \frac{1}{1 - \frac{T}{T_{\text{Deep}}}} + \frac{\pi}{\sin\left(\frac{\pi T}{T_{\text{Deep}}}\right)} - \sum_{p=0}^{\infty} (-1)^p \frac{e^{-p |z|}}{p + \left(1 - \frac{T}{T_{\text{Deep}}}\right)} - 1 - \frac{T}{T_{\text{Deep}}}
\]

\[
I_1 = e^{\frac{|z|}{T_{\text{Deep}}}} \left(1 - \frac{T}{T_{\text{Deep}}}\right) - 1 - e^{\frac{|z|}{T_{\text{Deep}}}} \left(1 - \frac{T}{T_{\text{Deep}}}\right) + e^{\frac{|z|}{T_{\text{Deep}}}} \left(1 - \frac{T}{T_{\text{Deep}}}\right) - \frac{\pi}{\sin\left(\frac{\pi T}{T_{\text{Deep}}}\right)} - \sum_{p=0}^{\infty} (-1)^p \frac{e^{-p |z|}}{p + \left(1 - \frac{T}{T_{\text{Deep}}}\right)} + 1 + \frac{T}{T_{\text{Deep}}}
\]

\[
I_1 = e^{\frac{|z|}{T_{\text{Deep}}}} \left(1 - \frac{T}{T_{\text{Deep}}}\right) - \sum_{p=0}^{\infty} (-1)^p \frac{e^{-p |z|}}{p + \left(1 - \frac{T}{T_{\text{Deep}}}\right)}
\]

Now, since \( \delta_1 = A_{\text{Deep}} \cdot e^{-|z|}/I_1 \), computing \( \delta_1 \) using the simplified value of \( I_1 \), we get

\[
\delta_1 = A_{\text{Deep}} \cdot e^{-|z|} \left[ e^{\frac{|z|}{T_{\text{Deep}}}} \left(1 - \frac{T}{T_{\text{Deep}}}\right) - \sum_{p=0}^{\infty} (-1)^p \frac{e^{-p |z|}}{p + \left(1 - \frac{T}{T_{\text{Deep}}}\right)}\right]
\]

\[
= \frac{T}{T_{\text{Deep}}} \frac{N_{\text{Deep}}}{N_{\text{Deep}} + N_{\text{Tail}}} e^{\frac{|z|}{T_{\text{Deep}}}} \left[e^{\frac{|z|}{T_{\text{Deep}}}} \left(1 - \frac{T}{T_{\text{Deep}}}\right) - \sum_{p=0}^{\infty} (-1)^p \frac{e^{-p |z|}}{p + \left(1 - \frac{T}{T_{\text{Deep}}}\right)}\right]
\]

\[
\delta_1 = \frac{N_{\text{Deep}}}{N_{\text{Deep}} + N_{\text{Tail}}} e^{-\frac{r}{T_{\text{Deep}}}} \left[ e^{\frac{\pi T}{T_{\text{Deep}}}} e^{\frac{|z|}{T_{\text{Deep}}}} - \sum_{p=0}^{\infty} (-1)^p \frac{e^{-p |z|}}{p + \left(1 - \frac{T}{T_{\text{Deep}}}\right)}\right]
\]
### Table 1: Values of the physical parameters

| Parameters | Values |
|------------|--------|
| $N_{\text{Deep}}$ | $4.8 \times 10^{19}$ |
| $\phi_{\text{Deep}}$ | $1.28 \times 10^{-20}$ |
| $N_{\text{Tail}}$ | $4.2 \times 10^{21}$ |
| $\phi_{\text{Tail}}$ | $0.48 \times 10^{-20}$ |
| $E_{\text{LUMO}}$ | 0 |
| $E_F$ | $-1.6 \times 10^{-19}$ |
| $k_B$ | $1.38 \times 10^{-22}$ |
| $T$ | 300 |

### Table 2: Deviation from actual values as ($E_F$) is varied

| $E_F$ (eV) | Actual value | Percentage deviation in value of approximated expression as $p$ increases |
|------------|--------------|-----------------------------------------------------------------------|
| 0          | $3.033 \times 10^{21}$ | $p = 0$ | $p = 1$ | $p = 2$ | $p = 3$ | $p = 4$ | $p = 5$ | $p = 6$ |
| -0.1       | $4.346 \times 10^{20}$ | 71 | $-34$ | 22 | $-16$ | 12 | $-10$ | 9 |
| -0.5       | $1.122 \times 10^{17}$ | $10^{-11}$ | $10^{-11}$ | $10^{-11}$ | $10^{-11}$ | $10^{-11}$ | $10^{-11}$ | $10^{-11}$ |
| -1         | $2.138 \times 10^{14}$ | $10^{-7}$ | $10^{-7}$ | $10^{-7}$ | $10^{-7}$ | $10^{-7}$ | $10^{-7}$ | $10^{-7}$ |
| -1.5       | $4.127 \times 10^{11}$ | $10^{-13}$ | $10^{-13}$ | $10^{-13}$ | $10^{-13}$ | $10^{-13}$ | $10^{-13}$ | $10^{-13}$ |

### Table 3: Deviation from actual values as ($\phi_{\text{Deep,Tail}}$) varied

| $\phi_{\text{Deep}}$(eV) | $\phi_{\text{Tail}}$(eV) | Actual value | Percentage deviation in value of approximated expression as $p$ increases |
|--------------------------|--------------------------|--------------|-----------------------------------------------------------------------|
| 0.08                     | 0.03                     | $2.138 \times 10^{14}$ | $p = 0$ | $p = 1$ | $p = 2$ | $p = 6$ |
| 0.10                     | 0.05                     | $2.453 \times 10^{15}$ | $10^{-7}$ | $10^{-7}$ | $10^{-7}$ | $10^{-7}$ |
| 0.12                     | 0.07                     | $1.579 \times 10^{16}$ | $10^{-9}$ | $10^{-9}$ | $10^{-9}$ | $10^{-9}$ |
| 0.14                     | 0.09                     | $1.123 \times 10^{17}$ | $10^{-11}$ | $10^{-11}$ | $10^{-11}$ | $10^{-11}$ |
| 0.16                     | 0.11                     | $6.160 \times 10^{17}$ | $10^{-12}$ | $10^{-12}$ | $10^{-12}$ | $10^{-12}$ |

### Table 4: Deviation from actual values as $N_{\text{Deep,Tail}}$ are varied

| $N_{\text{Deep}} \times 10^{19}$ (cm$^{-3}$) | $N_{\text{Tail}} \times 10^{21}$ (cm$^{-3}$) | Actual value | Percentage deviation in value of approximated expression as $p$ increases |
|---------------------------------------------|---------------------------------------------|--------------|-----------------------------------------------------------------------|
| 0.0048                                      | 0.0042                                     | $2.138 \times 10^{11}$ | $p = 0$ | $p = 1$ | $p = 2$ | $p = 6$ |
| 0.48                                        | 0.42                                       | $2.138 \times 10^{13}$ | $10^{-7}$ | $10^{-7}$ | $10^{-7}$ | $10^{-7}$ |
| 4.8                                         | 4.2                                        | $2.138 \times 10^{14}$ | $10^{-7}$ | $10^{-7}$ | $10^{-7}$ | $10^{-7}$ |
| 0.48                                        | 42                                         | $2.138 \times 10^{13}$ | $10^{-5}$ | $10^{-5}$ | $10^{-5}$ | $10^{-5}$ |
| 0.0048                                      | 4200                                       | $3.045 \times 10^{11}$ | 0.142 | 0.142 | 0.142 | 0.142 |
Similarly, calculating $\delta_2$ by replacing $A_{\text{Deep}}$ by $A_{\text{Tail}}$ and $T_{\text{Deep}}$ by $T_{\text{Tail}}$ in $\delta_1$, we get
\[
\delta_2 = \frac{N_{\text{Tail}}}{N_{\text{Deep}} + N_{\text{Tail}}} e^{-[\xi] \frac{T}{T_{\text{Tail}}}} \cdot \left[ \frac{\pi T}{T_{\text{Tail}}} \right] - T_{\text{Tail}} e^{-\xi} \sum_{p=0}^{\infty} (-1)^p \frac{e^{-p[\xi]}}{p + 1 - \frac{T}{T_{\text{Tail}}}}
\]

Thus, $= \delta_1 + \delta_2$:
\[
\delta = \frac{N_{\text{Deep}}}{N_{\text{Deep}} + N_{\text{Tail}}} e^{-[\xi] \frac{T}{T_{\text{Deep}}}} \cdot \left[ \frac{\pi T}{T_{\text{Deep}}} \right] - T_{\text{Deep}} e^{-\xi} \sum_{p=0}^{\infty} (-1)^p \frac{e^{-p[\xi]}}{p + 1 - \frac{T}{T_{\text{Deep}}}} \\
+ \frac{N_{\text{Tail}}}{N_{\text{Deep}} + N_{\text{Tail}}} e^{-[\xi] \frac{T}{T_{\text{Tail}}}} \cdot \left[ \frac{\pi T}{T_{\text{Tail}}} \right] - T_{\text{Tail}} e^{-\xi} \sum_{p=0}^{\infty} (-1)^p \frac{e^{-p[\xi]}}{p + 1 - \frac{T}{T_{\text{Tail}}}}
\]

2.4 Modified charge carrier density

In order to develop a modified model, we approximate the above exact equation of $\delta$ by calculating it only for $p=0$ and neglecting higher order terms for $p=1,2,3 \ldots$

As can be seen in Table 2, deviation is quite negligible even for $p=0$, among values of $E_f$ greater than 10% of 1 eV, and the deviation remains fairly constant when we increase the value of $p$; hence, we can conclude that as far as $E_f$ is considered, the approximate expression for charge carrier density with $p=0$ is well suited to approximate the actual integral.

3 Analysis and results

The following values have been used from [9] for the delta equation to plot the charge carrier density function for various values of $E_f$ (Table 1).

Next, we compare the values of charge carrier density for varying values of $E_f$ for both the exact and approximate expressions for varying degrees of approximation.

Table 5 Deviation from actual values as temperature varies

| Temp (K) | Actual value | Percentage deviation in values of approximated expression as $p$ increases |
|----------|--------------|--------------------------------------------------------------------------|
|          |              | $p=0$ | $p=1$ | $p=2$ | $p=6$ |
| 50       | $1.797 \times 10^{14}$ | $10^{-12}$ | $10^{-12}$ | $10^{-12}$ | $10^{-12}$ |
| 100      | $1.823 \times 10^{14}$ | $10^{-13}$ | $10^{-13}$ | $10^{-13}$ | $10^{-13}$ |
| 200      | $1.933 \times 10^{14}$ | $10^{-13}$ | $10^{-13}$ | $10^{-13}$ | $10^{-13}$ |
| 250      | $2.021 \times 10^{14}$ | $10^{-11}$ | $10^{-11}$ | $10^{-11}$ | $10^{-11}$ |
| 300      | $2.138 \times 10^{14}$ | $10^{-7}$ | $10^{-7}$ | $10^{-7}$ | $10^{-7}$ |
| 350      | $2.288 \times 10^{14}$ | $10^{-9}$ | $10^{-9}$ | $10^{-9}$ | $10^{-9}$ |
| 500      | $3.063 \times 10^{14}$ | $10^{-10}$ | $10^{-10}$ | $10^{-10}$ | $10^{-10}$ |
Second, we see that increasing the $p$-values up to a reasonable level, such as $p = 6$, does not have any effect on deviation; i.e. as we change $N_{\text{deep}}$ and $N_{\text{tail}}$, the approximated expression converges very slowly to the real expression, and hence we can assume that the $p = 0$ term yields a reasonably accurate approximate solution.

Table 5 presents the variation in temperature from 50 to 500 K with a deviation in the approximate and exact models, keeping all other parameters fixed at the specified values.

As documented in Table 5, we can see that temperature does not affect the charge carrier density as much as the other factors do. Also, the error in the approximated expression is less than $10^{-7}$ for temperatures between 50 and 500 K. We also conclude that increasing the value up to the $p = 6$ term does not contribute much in increasing the accuracy as the order of the error remains the same. Hence, the $p = 0$ term is a good choice for approximation as far as temperature is concerned.

The variation of charge carrier density with temperature, and percentage error which corroborates our findings are shown in Figs. 3 and 4.

4 Conclusion

After using various approximation techniques and employing various mathematical methods, we have evaluated a fairly simple closed form of charge carrier density function with less
error for a wide range of parameter values. The literature for single exponential density of states are available, and techniques applied for this double exponential density of states are quite similar to those used for single exponential density of states. One of techniques used was expanding $\frac{1}{1+e^{x-y}}$ using binomial expansions. The second technique applied was writing a summation of form $\sum_{n=0}^{\infty} \frac{(-1)^n}{(n+q)}$ as a HurwitzLerchPhi transcendental notion. Finally, we put the higher order terms of a diminishing series to zero and took in account only the first term to get a closed form of the integral.

It is concluded that the approximations made are a very computationally efficient replacement to the exact expressions for a wide range of parameters involved in the charge carrier density evaluation and show a less relative error.

Also, the expression with the highest degree of approximation, i.e. the $p = 0$ term, can be selected as the primary expression to evaluate charge carrier density, as a further increase in the value of $p$ leads to increased computational complexity, whereas the increase in accuracy is marginal. Hence, the final approximated expression is obtained by keeping the $p = 0$ term and neglecting the higher order terms.

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Declarations

Competing interests The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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