An improved model for describing the net carrier recombination rate in semiconductor devices

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Abstract
Carrier recombination is a process that significantly influences the performance of semiconductor devices such as solar cells, photodiodes, and light-emitting diodes (LEDs). Therefore, a model that can accurately describe and quantify the net carrier recombination rate in semiconductor devices is important in order to further improve the performance of relevant semiconductor devices. The conventional model for describing the net carrier recombination rate is derived based on the condition that there is no electric current in the considered semiconductor, which is true only when the semiconductor is not part of a device, and hence, is not connected to an external circuit. The conventional model is adopted and used for describing the net carrier recombination rate in semiconductors that are part of devices (i.e., in semiconductor devices). In this paper, we derive and propose a new model for describing the net carrier recombination rate in semiconductor devices. The newly proposed model is an improvement to the currently used model by considering the fact that electric currents can flow in the semiconducting materials of semiconductor devices. We employ organic solar cells (OSCs) to validate the proposed recombination model and show that the proposed model can be crucial for modeling OSCs. Since the proposed recombination model is derived for general semiconductor devices, we expect that the use of the proposed model can also be crucial for modeling and analyzing the performance of other semiconductor devices, particularly optoelectronic devices such as LEDs and perovskite solar cells.

Keywords Bulk recombination · Charge recombination · Light-emitting diodes · Optoelectronic devices · Solar cells

1 Introduction
Recombination between electrons and holes is a fundamental process that occurs in a semiconductor whether the semiconductor is part of a semiconductor device or not. Carrier recombination is of special interest to several semiconductor devices. In solar cells and photodiodes, all carrier recombination processes should be minimized, whereas in light-emitting diodes (LEDs), radiative recombination should be maximized, and other possible recombination processes should be minimized. Therefore, an accurate description and quantification of the carrier recombination rate are important to accurately identify and evaluate the possible areas of improvement for those devices. An accurate description and quantification of the carrier recombination rate could also be important for studies on the fundamental properties of semiconductors.

For a given carrier recombination process, the net carrier recombination rate per unit volume \( R_{\text{net}} \) in a semiconductor is given by [1], pp. 313–324

\[
R_{\text{net}} = R_{\text{total}} - G_0,
\]

where \( R_{\text{total}} \) is the total carrier recombination rate per unit volume in the semiconductor, and \( G_0 \) is the carrier generation rate per unit volume that inherently or permanently occurs in the semiconductor. In a semiconductor that is not part of a device (called an isolated semiconductor here), it is well known that \( G_0 \) originates from thermal agitation, which causes electrons in the valence band to jump either directly or indirectly into the conduction band, thus producing electrons in the conduction band and electron vacancies (holes)
in the valence band [1, pp. 313–324]. In a semiconductor that is part of a device, there is an additional factor that contributes to $G_{n}$ as will be shown in this paper.

The conventional model for describing the detail expression of $R_{\text{net}}$ is derived under the condition that there is no electric current in the considered semiconductor, which is true only when the semiconductor is not part of a device and not connected to an external circuit. However, this conventional model is adopted and widely used to describe $R_{\text{net}}$ even in semiconductors that are part of devices (i.e., in semiconductor devices). In this paper, we derive a new model for describing $R_{\text{net}}$ in semiconductor devices and show that it should be different compared with the conventional $R_{\text{net}}$ model. The newly proposed $R_{\text{net}}$ model is an improvement to the currently used model by considering the fact that electric currents can flow in semiconductors that are part of devices. We validate the proposed model and show that the use of the proposed model is important to better analyze and enhance the performance of relevant semiconductor devices.

This paper is organized as follows. In Sect. 2, we describe the carrier continuity with a focus on the carrier recombination in semiconductors. In Sect. 3, first, we rederive the conventional model for quantifying $R_{\text{net}}$, and then, we derive a new improved model for quantifying $R_{\text{net}}$ in semiconductor devices. In Sect. 4, we employ organic solar cells (OSCs) as a case study to validate and demonstrate the significance of the newly proposed $R_{\text{net}}$ model. In Sect. 4, we also provide some physical insights on the newly proposed $R_{\text{net}}$ model and discuss the implication of the newly proposed $R_{\text{net}}$ model on the surface recombination model. The paper is then concluded in Sect. 5.

## 2 Carrier continuity and recombination in semiconductors

The continuity equations for electrons and holes in semiconductors are given by [1, pp. 58–63], [2, pp. 62–63]

$$\frac{1}{q} \nabla \cdot \mathbf{J}_n + G_n - R_n = \frac{dn}{dt}, \quad (2)$$

$$-\frac{1}{q} \nabla \cdot \mathbf{J}_p + G_p - R_p = \frac{dp}{dt}, \quad (3)$$

where $q$ is the elementary charge, $\mathbf{J}_n$ ($\mathbf{J}_p$) is the electron (hole) current density, $G_n$ ($G_p$) is the electron (hole) generation rate per unit volume due to external influences, usually external photon absorption, $R_n$ ($R_p$) is the net electron (hole) recombination rate per unit volume, $n$ ($p$) is the density or concentration of free electrons (holes), and $t$ is time. Carrier generation due to external influences (such as external photon absorption) is not part of carrier generation that inherently occurs in semiconductors, and therefore $G_n$ and $G_p$ have their own separate terms in the continuity equations and are not included as part of $R_n$ and $R_p$ [only inherent carrier generation rate should be considered in $R_n$ and $R_p$ as described by Eq. (1)]. For the one-dimensional case at steady state, the continuity equations become [2, p. 63]

$$\frac{1}{q} \frac{dJ_n}{dx} + G_n - R_n = 0, \quad (4)$$

$$-\frac{1}{q} \frac{dJ_p}{dx} + G_p - R_p = 0. \quad (5)$$

The electron current density $J_n$ and the hole current density $J_p$ for the one-dimensional case are given by

$$J_n = q\mu_n F n + qD_n \frac{dn}{dx}, \quad (6)$$

$$J_p = q\mu_p F p - qD_p \frac{dp}{dx}, \quad (7)$$

where $\mu_n$ ($\mu_p$) is the electron (hole) mobility, $F$ is the electric field, $D_n = \mu_n k_B T / q$ is the electron diffusion coefficient, and $D_p = \mu_p k_B T / q$ is the hole diffusion coefficient, where $k_B$ is the Boltzmann constant and $T$ is the absolute temperature. Here, we consider the case where there is no temperature gradient (i.e., $dT/dx = 0$) since the effect of the temperature gradient is negligible in general semiconductor devices (hence, the current densities consist of the drift and the diffusion components only), unlike in thermoelectric generators where the temperature gradient is purposely established.

In general, there are three main recombination mechanisms, which are the band-to-band (also called radiative) recombination, Shockley–Read–Hall (SRH) or trap-assisted recombination, and Auger recombination [1], pp. 39–44. The total band-to-band recombination rate is proportional to the product of the electron and the hole concentrations (i.e., $\propto np$) [1], pp. 313–315. The net band-to-band recombination rate per unit volume is therefore [1], pp. 313–315

$$R_{bb} = k_{bb} np - G_{0(\text{bb})}, \quad (8)$$

where $k_{bb}$ is the band-to-band recombination coefficient and $G_{0(\text{bb})}$ is the $G_0$ component [see Eq. (1)] for the band-to-band recombination process. It is worth noting that if $R_{bb}$ is zero, it does not necessarily mean that the band-to-band recombination process does not occur, but it simply means that the total band-to-band recombination rate per unit volume (i.e., $k_{bb} np$) is equal to $G_{0(\text{bb})}$. We may write Eq. (8) as [1], pp. 313–315

$$R_{bb} = k_{bb} (np - n_{0(\text{bb})} p_{0(\text{bb})}), \quad (9)$$

which means $G_{0(\text{bb})} = k_{bb} n_{0(\text{bb})} p_{0(\text{bb})}$.
The net SRH recombination rate per unit volume is given by [1], pp. 317–324]

\[ R_{SRH} = k_{SRH}np - G_{0(SRH)}, \]

(10)

where \( k_{SRH} \) is the SRH recombination coefficient (see Ref. [1], pp. 317–324) for the detail of \( k_{SRH} \) for example) and \( G_{0(SRH)} \) is the \( G_0 \) component [see Eq. (1)] for the SRH recombination process. We can write Eq. (10) as [1], pp. 317–324]

\[ R_{SRH} = k_{SRH}(np - n_{0(SRH)p_{0(SRH)}}), \]

(11)

which means \( G_{0(SRH)} = k_{SRH}n_{0(SRH)p_{0(SRH)}} \). Note that, since \( k_{SRH} \) depends on \( n \) and \( p \) [1], pp. 317–324], \( G_{0(SRH)} \) will definitely change if \( G_n \) and \( G_p \) change, as opposed to \( G_{0(bb)} \) which could remain constant even if \( G_n \) and \( G_p \) change.

The net Auger recombination rate per unit volume is [1], pp. 42–44]

\[ R_A = (k_{A1}^2p + k_{A2}p^2n) - G_{0(A)}, \]

(12)

where \( k_{A1} \) is the Auger recombination coefficient for the \( n^2p \) path, \( k_{A2} \) is the Auger recombination coefficient for the \( p^2n \) path, and \( G_{0(A)} \) is the \( G_0 \) component for the Auger recombination process. To be consistent with \( R_{bb} \) and \( R_{SRH} \), we can write Eq. (12) as [1], pp. 42–44]

\[ R_A = (k_{A1}n + k_{A2}p)(np - n_{0(A)p_{0(A)}}), \]

(13)

which means \( G_{0(A)} = (k_{A1}n + k_{A2}p)n_{0(A)p_{0(A)}} \). Note that, Eq. (13) indicates that \( G_{0(A)} \) also changes if \( G_n \) and \( G_p \) change.

The net electron and the net hole recombination rates per unit volume (i.e., \( R_n \) and \( R_p \)) are the sum of all possible processes and hence are

\[ R_n = R_p = R_{bb} + R_{SRH} + R_A. \]

(14)

From Eq. (14), it is also easy to see that the total carrier recombination rate is the sum of \( k_{bb}np \) (the total band-to-band recombination rate), \( k_{SRH}np \) (the total SRH recombination rate), and \( k_{A1}n^2p + k_{A2}p^2n \) (the total Auger recombination rate). Furthermore, the total \( G_0 \) is the sum of \( G_{0(bb)}, G_{0(SRH)}, \) and \( G_{0(A)} \). Since the total rate of a given recombination process cannot be less than the inherent carrier generation rate associated with that recombination process, this means \( R_{bb} \geq 0, R_{SRH} \geq 0 \) and \( R_A \geq 0 \). Therefore, when \( R_n = R_p = 0 \), this means \( R_{bb}, R_{SRH}, \) and \( R_A \) must all be zero since \( R_{bb}, R_{SRH}, \) or \( R_A \) cannot be negative.

3 Models for quantifying the net carrier recombination rate

In Sect. 3.1, we will rederive the conventional model for quantifying \( R_{net} \). The conventional model is derived based on semiconductors that are not part of semiconductor devices (called isolated semiconductors here). In Sect. 3.2, we will derive a new model for quantifying \( R_{net} \) based on semiconductors that are part of semiconductor devices. The purpose of rederiv ing the conventional \( R_{net} \) model is to assist us in deriving and understanding the newly proposed \( R_{net} \) model.

3.1 Model for quantifying the net carrier recombination rate in isolated semiconductors

Here, an isolated semiconductor is referred to a semiconductor, intrinsic or extrinsic (doped), that is not part of a semiconductor device, and hence it is not connected to an external circuit and no electric current can flow inside it. To determine \( G_{0(bb)}, G_{0(SRH)}, \) and \( G_{0(A)} \), we need to determine \( n_{0(bb)}, p_{0(bb)}, n_{0(SRH)}, p_{0(SRH)}, n_{0(A)}, p_{0(A)} \). Let us consider a special case where \( R_n = 0 \) and \( R_p = 0 \). Zero. Let us denote the electron concentration \( n \) and the hole concentration \( p \) in isolated semiconductors when \( R_n = R_p = 0 \) as \( n_{0(is)} \) and \( p_{0(is)} \), respectively. As mentioned in Sect. 2, when \( R_n \) and \( R_p \) are zero, \( R_{bb}, R_{SRH}, \) and \( R_A \) must all be zero, and hence according to Eqs. (9), (11), and (13), we have

\[ n_{0(is)} = n_{0(bb)} = n_{0(SRH)} = n_{0(A)}, \]

(15)

\[ p_{0(is)} = p_{0(bb)} = p_{0(SRH)} = p_{0(A)}. \]

(16)

The results given by Eqs. (15) and (16) are deduced provided that the recombination coefficients are not zero of course. If \( k_{bb} \) is zero for example, then there is no point to find \( n_{0(bb)} \) and \( p_{0(bb)} \). The results mean that according to Eq. (14), we can now write \( R_n \) and \( R_p \) in isolated semiconductors as

\[ R_n = R_p = k_{total}(np - n_{0(is)p_{0(is)}}, \]

(17)

where \( k_{total} = k_{bb} + k_{SRH} + (k_{A1}n + k_{A2}p) \).

If we can determine \( n_{0(is)} \) and \( p_{0(is)} \), then we can determine \( G_{0(bb)}, G_{0(SRH)}, \) and \( G_{0(A)} \). When \( R_n = R_p = 0 \), the carrier continuity equations at steady state become

\[ \frac{1}{q} \frac{\partial n}{\partial x} + G_n = 0, \]

(18)

\[ -\frac{1}{q} \frac{\partial p}{\partial x} + G_p = 0. \]

(19)
Since there is no current flow (i.e., $J_n$ and $J_p$ must be zero everywhere inside an isolated semiconductor), $\partial J_n/\partial x$ and
$\partial J_p/\partial x$ must also be zero, which means Eqs. (18) and (19) can be satisfied only if $G_n$ and $G_p$ are zero. This means that the situation $R_n = R_p = 0$ can only happen in an isolated semiconductor if there is no external carrier generation, which is well known.

To find out $n_{0(is)}$ and $p_{0(is)}$, we simply need to solve $J_n = 0$ and $J_p = 0$. An internal (or built-in) electric field can exist inside an isolated semiconductor, for example if the isolated semiconductor is attached to another isolated semiconductor with a different Fermi level, or if the isolated semiconductor is non-uniformly doped. An external electric field can cause free electrons and free holes in an isolated semiconductor to tend to accumulate on two opposite sides, thus inducing an internal electric field in the isolated semiconductor that opposes the external field. However, it is worth noting that the presence of an external electric field makes an isolated semiconductor to be out of thermodynamic equilibrium (the Fermi level in the semiconductor that is initially uniform becomes nonuniform due to the redistribution of carriers). Inside an isolated semiconductor, the electric field $F$ is determined by the gradient of the conduction band minimum $E_c$, given by $F = dE_c/\partial x$, or by the gradient of the valence band maximum $E_v$, given by $F = dE_v/\partial x$ [2], p. 46.

When $F$ is not zero, the conditions $J_n = 0$ [refer Eq. (6)] and $J_p = 0$ [refer Eq. (7)] lead to

\[
\frac{dn_{0(is)}}{dx} = -\frac{n_{0(is)} dE_c}{k_B T} \frac{dx}{x},
\]

(20)

\[
\frac{dp_{0(is)}}{dx} = \frac{p_{0(is)} dE_v}{k_B T} \frac{dx}{x}.
\]

(21)

When $F = 0$ (hence the gradients of $E_c$ and $E_v$ are zero), the conditions $J_n = 0$ and $J_p = 0$ lead to

\[
\frac{dn_{0(is)}}{dx} = 0,
\]

(22)

\[
\frac{dp_{0(is)}}{dx} = 0.
\]

(23)

Equations (20) and (21) are for isolated semiconductors (both intrinsic and extrinsic) when there are electric fields inside the semiconductors, whereas Eqs. (22) and (23) are also for isolated semiconductors (intrinsic and extrinsic) but when there are no electric fields inside the semiconductors.

First, we will try to determine $n_{0(is)}$ and $p_{0(is)}$ for the intrinsic semiconductor case. We know that $n_{0(is)}$ and $p_{0(is)}$ are the electron and the hole concentrations, respectively, when the net carrier recombination rate and the external carrier generation rate are zero. No net carrier recombination and no external carrier generation are two implications if an isolated semiconductor (whether intrinsic or extrinsic) is in thermodynamic equilibrium [1, 2]. For an isolated intrinsic semiconductor in thermodynamic equilibrium, the electron concentration and the hole concentration are called the intrinsic electron concentration $n_{int}$ and the intrinsic hole concentration $p_{int}$, respectively. Therefore, it seems that $n_{0(is)} = n_{int}$ and $p_{0(is)} = p_{int}$ for the intrinsic semiconductor case. $n_{int}$ and $p_{int}$ are given by [2], p. 20

\[
n_{int} = N_c \exp \left[ -\frac{(E_c - E_{Fi})}{k_B T} \right],
\]

(24)

\[
p_{int} = N_v \exp \left[ -\frac{(E_v - E_{Fi})}{k_B T} \right],
\]

(25)

where $N_c$ ($N_v$) is the effective density of states in the conduction (valence) band, $E_c$ ($E_v$) is the conduction (valence) band minimum (maximum), and $E_{Fi}$ is the Fermi level of the intrinsic semiconductor. Note that, the gradients of $E_c$ and $E_v$ in Eqs. (24) and (25) are zero if there is no electric field but are not zero if there is an electric field. However, the gradient of $E_{Fi}$ in Eqs. (24) and (25) must always be zero (whether there is an electric field or not) since Eqs. (24) and (25) are for intrinsic semiconductors in thermodynamic equilibrium, and the Fermi level of a material in thermodynamic equilibrium must be uniform [2]. It is also worth noting that the product of Eqs. (24) and (25) is actually independent of the Fermi level.

If there is no electric field ($dE_c/\partial x$ and $dE_v/\partial x$ are zero), it can be easily shown that $dn_{int}/dx = 0$ and $dp_{int}/dx = 0$, and therefore letting $n_{0(is)} = n_{int}$ and $p_{0(is)} = p_{int}$ can satisfy Eqs. (22) and (23), respectively. If there is an electric field ($dE_c/\partial x$ and $dE_v/\partial x$ are not zero), letting $n_{0(is)} = n_{int}$ and $p_{0(is)} = p_{int}$ can also satisfy Eqs. (20) and (21), respectively. Therefore, for both cases (when $F = 0$ and when $F$ is not zero), the parameters $n_{0(is)}$ and $p_{0(is)}$ for an isolated intrinsic semiconductor are indeed given by $n_{int}$ and $p_{int}$, respectively.

Next, to determine $n_{0(is)}$ and $p_{0(is)}$ for the extrinsic semiconductor case, we follow a similar procedure as for the intrinsic case above. First, we need to know the electron and the hole concentrations in isolated extrinsic semiconductors when there are no net carrier recombination and no external carrier generation (i.e., in thermodynamic equilibrium). When an isolated extrinsic semiconductor is in thermodynamic equilibrium, we know that the product of the electron and the hole concentrations is still equal to the product of the electron and the hole concentrations before the semiconductor is doped (i.e., equals to $n_{int}p_{int}$ [2], pp. 20–22). We already know that $n_{int}$ and $p_{int}$ can satisfy the conditions given by Eqs. (20), (21), (22), and (23). Therefore, for both cases (when $F = 0$ and $F$ is not zero), $n_{0(is)}p_{0(is)}$ for
an isolated extrinsic semiconductor is still given by \( n_{\text{int}}p_{\text{int}} \), where \( n_{\text{int}} \) and \( p_{\text{int}} \) are the intrinsic electron and the intrinsic hole concentrations, respectively, inside the extrinsic semiconductor before it is doped.

Since \( n_{\text{int}} = p_{\text{int}} \) [2], pp. 20–22], this means \( n_{\text{0(is)}}p_{\text{0(is)}} = n_{\text{int}}^2 \). Applying the obtained result to Eqs. (9), (11), and (13), the net band-to-band, the net SRH, and the net Auger recombination rates per unit volume in isolated semiconductors (whether intrinsic or extrinsic) are therefore given by

\[
R_{\text{bb}} = k_{\text{bb}} (np - n_{\text{int}}^2),
\]

\[
R_{\text{SRH}} = k_{\text{SRH}} (np - n_{\text{int}}^2),
\]

\[
R_A = (k_A n + k_{A2} p) (np - n_{\text{int}}^2).
\]

The results given by Eqs. (26), (27), and (28) are widely known [1], pp. 39–44. Therefore, the net carrier recombination rate per unit volume \( R_{\text{net}} \) in isolated semiconductors can generally be modeled as

\[
R_{\text{net}} = k_i (np - n_{\text{int}}^2),
\]

where \( k_i \) is the general coefficient of the considered recombination process. The recombination model given by Eq. (29) is the conventional model that is derived (and hence valid) for modeling \( R_{\text{net}} \) in isolated semiconductors, but the model is also adopted for modeling \( R_{\text{net}} \) in semiconductor devices. In the next subsection, we will derive a model to describe \( R_{\text{net}} \) in semiconductor devices and show that the model is not as described by Eq. (29).

### 3.2 Model for quantifying the net carrier recombination rate in semiconductor devices

To derive the parameters \( n_{\text{0(bb)}} \), \( p_{\text{0(bb)}} \), \( n_{\text{0(SRH)}} \), \( p_{\text{0(SRH)}} \), \( n_{\text{0(A)}} \), and \( p_{\text{0(A)}} \), for semiconductors that are part of semiconductor devices, we follow a similar procedure as for the isolated semiconductor case above. Again, let us consider the special case when \( R_n \) and \( R_p \) are zero. Let us denote the electron concentration \( n \) and the hole concentration \( p \) in the considered semiconducting material of a semiconductor device when \( R_n = R_p = 0 \) as \( n_{\text{0(d)}} \) and \( p_{\text{0(d)}} \), respectively. When \( R_n \) and \( R_p \) are zero, \( R_{\text{bb}}, R_{\text{SRH}}, \) and \( R_A \) must all be zero, and therefore according to Eqs. (9), (11), and (13), we have

\[
n_{\text{0(d)}} = n_{\text{0(bb)}} = n_{\text{0(SRH)}} = n_{\text{0(A)}},
\]

\[
p_{\text{0(d)}} = p_{\text{0(bb)}} = p_{\text{0(SRH)}} = p_{\text{0(A)}}.
\]

When \( R_n \) and \( R_p \) are zero, the continuity equations for the carriers inside the considered semiconducting material become

\[
\frac{1}{q} \frac{\partial J_n}{\partial x} + G_n = 0,
\]

\[
\frac{1}{q} \frac{\partial J_p}{\partial x} + G_p = 0.
\]

An external voltage bias (e.g., from a battery) can be applied to a semiconductor device which can result in nonzero \( J_n \) and \( J_p \), and this must be considered as an inherent feature of a semiconductor that is part of a device, otherwise the semiconductor is basically an isolated semiconductor. External carrier generation (e.g., due to external photon absorption) contributes to the excess free carriers. At any given bias condition, \( R_n \) and \( R_p \) are expected to reach their lowest possible value (i.e., zero) when the excess free carriers are at the lowest (i.e., when \( G_n = G_p = 0 \)). Therefore, at any given bias condition, \( R_n = R_p = 0 \) should happen when \( G_n = G_p = 0 \). Considering the case when \( G_n \) and \( G_p \) are zero, Eqs. (32) and (33) become

\[
\frac{\partial J_n}{\partial x} = \frac{\partial}{\partial x} \left[ q \mu_n F n_{\text{0(d)}} + q D_{\text{n}} \frac{\partial n_{\text{0(d)}}}{\partial x} \right] = 0,
\]

\[
\frac{\partial J_p}{\partial x} = \frac{\partial}{\partial x} \left[ q \mu_p F p_{\text{0(d)}} - q D_{\text{p}} \frac{\partial p_{\text{0(d)}}}{\partial x} \right] = 0.
\]

Up to this point, we show that both \( n_{\text{0(is)}} \) (for isolated semiconductors) and \( n_{\text{0(d)}} \) (for semiconductors that are part of devices) must satisfy the condition \( \frac{\partial J_n}{\partial x} = 0 \), and both \( p_{\text{0(is)}} \) and \( p_{\text{0(d)}} \) must satisfy the condition \( \frac{\partial J_p}{\partial x} = 0 \). However, for the isolated semiconductor case, those conditions are automatically satisfied due to the fact that \( J_n = J_p = 0 \) in isolated semiconductors. For the case of semiconductor devices, Eqs. (34) and (35) are satisfied without violating the fact that \( J_n = J_p = 0 \) can be nonzero. Therefore, it is clear that letting \( n_{\text{0(d)}} = n_{\text{int}} \) [Eq. (24)] and \( p_{\text{0(d)}} = p_{\text{int}} \) [Eq. (25)] would not give us the general solutions to Eqs. (34) and (35), respectively, since \( n_{\text{int}} \) and \( p_{\text{int}} \) lead to \( J_n \) and \( J_p \) that are always zero, which is not true in semiconductor devices. To obtain \( n_{\text{0(d)}} \) and \( p_{\text{0(d)}} \), Eqs. (34) and (35) need to be solved numerically together with the Poisson’s equation (the Poisson’s equation is used to determine the electric field \( F \)) and the boundary conditions at the edges of the considered semiconducting material.

To obtain analytical expressions for \( n_{\text{0(d)}} \) and \( p_{\text{0(d)}} \), we need to make simplifications by assuming \( F, \mu_n, \) and \( \mu_p \) to be uniform (i.e., independent of \( x \)). With these simplifications, Eqs. (34) and (35) become

\[
F \frac{d n_{\text{0(d)}}}{d x} + k_B T \frac{d^2 n_{\text{0(d)}}}{d x^2} = 0,
\]
\begin{align}
\frac{d^2p_{0(d)}}{dx^2} - \frac{k_B T}{q} \frac{d^2p_{0(d)}}{dx^2} &= 0. \tag{37}
\end{align}

The general solutions to Eqs. (36) and (37) are (note that \( F \) is uniform here)
\begin{align}
n_{0(d)} &= A_n \exp \left( -\frac{qF x}{k_B T} \right) + B_n, \tag{38}
p_{0(d)} &= A_p \exp \left( \frac{qF x}{k_B T} \right) + B_p, \tag{39}
\end{align}

where \( A_n, B_n, A_p, \) and \( B_p \) are constants that can be obtained by applying the boundary conditions at the edges of the considered semiconducting material. As opposed to \( n_{0\text{int}}^2 \) that appears in the conventional model as described in Sect. 3.1, \( n_{0(d)} \) and \( p_{0(d)} \) depend on \( F \), and hence, depend on the applied bias since the applied bias affects \( F \). Note that, \( n_{0(d)} \) and \( p_{0(d)} \) are not only influenced by the factors that clearly appear in Eqs. (38) and (39), respectively, but are also influenced by any factors that can influence the boundary conditions since the boundary conditions affect \( A_n, B_n, A_p, \) and \( B_p \). For example, the bandgap of the semiconductor material in a semiconductor device can influence the carrier concentrations at the boundaries of the semiconductor and hence can influence \( n_{0(d)} \) and \( p_{0(d)} \) (as can be seen later in Sect. 4.1).

It is worth noting that for the special case when \( F = 0 \), the first term on the left-hand side of each Eqs. (36) and (37) disappears, and the general solutions for this special case are
\begin{align}
n_{0(d)} &= A_n(F_0) x + B_n(F_0), \tag{40}
p_{0(d)} &= A_p(F_0) x + B_p(F_0), \tag{41}
\end{align}

where \( A_n(F_0), B_n(F_0), A_p(F_0), \) and \( B_p(F_0) \) are similar to the constants in Eqs. (38) and (39), which can be obtained by applying the boundary conditions.

Applying the obtained results to Eqs. (9), (11), and (13), the net band-to-band, the net SRH, and the net Auger recombination rates per unit volume in the semiconducting material of a semiconductor device are therefore given by
\begin{align}
R_{\text{bb}} &= k_{\text{bb}} \left( np - n_{0(d)} p_{0(d)} \right), \tag{42}
R_{\text{SRH}} &= k_{\text{SRH}} \left( np - n_{0(d)} p_{0(d)} \right), \tag{43}
R_A &= \left( k_A n + k_A p \right) \left( np - n_{0(d)} p_{0(d)} \right). \tag{44}
\end{align}

Based on our results here, we can propose that the net carrier recombination rate per unit volume \( R_{\text{net}} \) in the semiconducting material of a semiconductor device can be modeled as
\begin{align}
R_{\text{net}} &= k_n \left( np - n_{0(d)} p_{0(d)} \right), \tag{45}
\end{align}

where \( k_n \) is the general coefficient of the considered recombination process. \( n_{0(d)} \) is the electron concentration that results from the solution to \( \nabla \cdot J_n = 0 \) in the semiconducting material, and \( p_{0(d)} \) is the hole concentration that results from the solution to \( \nabla \cdot J_p = 0 \) in the semiconducting material. Concerning the physical meaning of \( n_{0(d)} \) and \( p_{0(d)} \), they are simply the electron and the hole concentrations, respectively, that inherently exist in the considered semiconducting material at any given voltage bias. Further insights regarding \( n_{0(d)} \) and \( p_{0(d)} \) will be given later in Sect. 4.2.

4 Model validation and discussion

4.1 Method

To support the newly proposed model for describing \( R_{\text{net}} \) in semiconductor devices (as derived in Sect. 3.2) and discuss its significance, we will compare between the use of the proposed \( R_{\text{net}} \) model and the use of the conventional \( R_{\text{net}} \) model (as derived in Sect. 3.1) in obtaining the current–voltage (J–V) characteristics of a specific semiconductor device. The semiconductor device considered here is an organic solar cell (OSC). A typical way to validate a proposed model is to use the model to fit the experimental J–V data. However, as can be clearly seen from the carrier continuity equations and the carrier (drift–diffusion) current equations, there are many factors that can affect the J–V characteristics such as the carrier mobility. Therefore, it is possible that we can satisfactorily fit the J–V data of an OSC by employing both the conventional and the proposed recombination models by adjusting the value of each input parameter accordingly without exceeding its valid range. Therefore, it can be difficult to make a conclusive validation using the typical approach. The approach that we will use here to validate whether the newly proposed \( R_{\text{net}} \) model or the conventional \( R_{\text{net}} \) model is better in describing \( R_{\text{net}} \) in semiconductor devices is by showing that under certain valid conditions, the better model produces a reasonable J–V characteristic whereas the other model produces an illogical J–V characteristic. The reason why an OSC is used here is because recently we developed an analytical model for describing the J–V characteristics of OSCs [3], and hence we have the source code for the J–V model that allows us to modify the recombination model in the code whether to follow the conventional model or the newly proposed model. The OSC considered here consists of an active layer (a blend of an electron accepting material and an electron donating material) sandwiched between two flat electrodes as shown in Fig. 1a and also as described in Ref. [3].
\[ p_{\text{conv}} = \gamma k_L (n^2 - n_{in}^2), \]  

where \( \gamma \) is the bimolecular recombination reduction coefficient, \( k_L = q(\mu_n + \mu_p) / \varepsilon \) is the Langevin recombination coefficient with \( \varepsilon \) being the effective permittivity of the active layer, and \( n_{in} \) is the intrinsic electron concentration. The net bimolecular recombination rate per unit volume in the active layer of the OSC according to the newly proposed model (see Sect. 3.2) is

\[ R_{b(new)} = \gamma k_{Lb} (n^2 - n_{in}^2), \]  

As mentioned earlier, the analytical model developed in Ref. [3] is used to calculate the J–V characteristics. The electric field in the model is taken to be uniform, given by

\[ F = \frac{V_a - V_{bi}}{L}, \]  

where \( V_a \) and \( V_{bi} \) are the applied voltage and the built-in voltage, respectively. The boundary conditions for the electron concentration \( n \) and the hole concentration \( p \) at the edges of the active layer (at \( x = 0 \) and \( x = L \)) of the OSC are given by [3]

\[ n|_{x=0} = N_e \exp \left[ -\frac{(E_g - \varphi_{p0})}{k_B T} \right] \]  

\[ n|_{x=L} = N_e \exp \left( -\varphi_{nc} \right), \]  

\[ p|_{x=0} = N_v \exp \left( -\varphi_{p0} \right), \]  

\[ p|_{x=L} = N_v \exp \left[ -\frac{(E_g - \varphi_{nc})}{k_B T} \right], \]  

where \( \varphi_{p0} \) is the hole injection barrier at anode given by the difference between \( \text{HOMO}_d \) and \( E_{Fb} \) (refer Fig. 1a), and \( \varphi_{nc} \) is the electron injection barrier at cathode given by the difference between \( \text{LUMO}_a \) and \( E_{Fc} \) (refer Fig. 1a).

The model in Ref. [3] considers the bimolecular recombination and the monomolecular recombination. The monomolecular recombination is basically a simplified (approximated) version of the SRH recombination and is neglected in our calculations. The bimolecular recombination (which is basically the band-to-band recombination) is considered in our calculations. The net bimolecular recombination rate per unit volume in the active layer of the considered OSC according to the conventional \( R_{b(new)} \) model (see Sect. 3.1) is

\[ R_{b(new)} = \gamma k_L (n^2 - n_{in}^2), \]  

where \( r_{0(d)} \) is given by Eq. (38) and \( p_{0(d)} \) is given by Eq. (39). For brevity, no calculations at exactly \( F = 0 \) (i.e., at \( V_a = V_{bi} \)) will be made here, and hence Eqs. (40) and (41) will not be used here [i.e., only Eqs. (38) and (39) will be used to describe \( n_{0(d)} \) and \( p_{0(d)} \), respectively]. The constants \( A_n, B_n, A_p, \) and \( B_p \) for \( n_{0(d)}, \) and \( p_{0(d)} \) can be obtained by applying the boundary conditions (i.e., \( n_{0(d)} |_{x=0} = n_{in}, n_{0(d)} |_{x=L} = n_{in}, p_{0(d)} |_{x=0} = p_{0(d)} |_{x=L} = p_{0(d)} |_{x=L} \)), which gives

\[ A_n = N_e \exp \left[ -\varphi_{nc} \right] - N_v \exp \left[ -\frac{(E_g - \varphi_{p0})}{k_B T} \right], \]  

\[ B_n = N_e \exp \left[ -\frac{(E_g - \varphi_{p0})}{k_B T} \right] - A_n, \]  

\[ A_p = N_v \exp \left[ -\frac{(E_g - \varphi_{nc})}{k_B T} \right] - N_v \exp \left[ -\frac{(E_g - \varphi_{p0})}{k_B T} \right], \]  

\[ B_p = N_v \exp \left[ -\frac{(E_g - \varphi_{p0})}{k_B T} \right] - A_p. \]  

The parameter values used in our calculations here are the same as used in Ref. [3] under the 1 sun condition (which
are based on the P3HT:PCBM solar cell in Ref. [4], except for the value of $\gamma$ [refer Eqs. (51) and (52)]. Here, $\gamma = 0.01$ is used compared with $\gamma = 0.001$ used in Ref. [3] and Ref. [4]. A reduction in the bimolecular recombination coefficient in comparison with the Langevin recombination coefficient was observed experimentally [5, 6]. The reduction is partly because free electrons and free holes are located in different materials of the active layer (which consists of donor and acceptor networks), and this reduces the probability for them to meet and recombine [7]. $\gamma$ can be affected by the fineness of the donor–acceptor morphology of the interpenetrating networks [8] and can have a value range of $0 \leq \gamma \leq 1$. A higher but valid value of $\gamma$ is used here compared with the value used in Ref. [3] and Ref. [4] because we want to obtain results that can clearly distinguish between the uses of the two models as explained at the beginning of this section and as will be shown later in Sect. 4.2.1.

4.2 Results and discussion

4.2.1 Validation and comparison

Figure 2 illustrates $n_n(0, d)$, $p_n(0, d)$, $n_{int}$, $n_n(0, d)p_n(0, d)$, and $n_n^2$ as functions of $x$. It can be seen that $n_n(0, d)p_n(0, d)$ is the same as $n_n^2$ at short-circuit point (at $V_a = 0$ V as shown in Fig. 2b) but not at a nonzero bias (e.g., at $V_a = 0.5$ V as also shown in Fig. 2b), which can be understood from the explanation in Sect. 4.2.2 later. As mentioned in Sect. 3, $n_{int}$ has no dependency on $F$, and therefore is invariant when $V_a$ is varied, unlike $n_n(0, d)$ and $p_n(0, d)$.

Figure 3 compares the J–V characteristic obtained using the proposed recombination model [using $R_{b(new)}$ given by Eq. (52)] with the J–V characteristic obtained using the conventional recombination model [using $R_{b(conv)}$ given by Eq. (51)]. The J–V characteristic obtained using $R_{b(new)}$ gives the expected J–V trend as $V_a$ is increased, but the J–V characteristic obtained using $R_{b(conv)}$ gives the wrong J–V trend as $V_a$ is increased starting from $V_a$ just below $V_{bi}$. The result in Fig. 3 suggests that the newly proposed recombination model is the better model for quantifying the net carrier recombination rate in the semiconducting material of a semiconductor device. Note that, if we use $\gamma = 0.001$ as in Ref. [3] instead of $\gamma = 0.01$, the J–V characteristics produced by both $R_{b(new)}$ and $R_{b(conv)}$ would give the correct J–V trend.

Figure 4 shows that the J–V characteristic obtained using $R_{b(new)}$ is noticeably different compared with the J–V characteristic obtained using $R_{b(conv)}$, where the difference is significant at $V_a$ just below the open-circuit voltage and all the way above that (the difference is due to the increase in the deviation of $n_n(0, d)p_n(0, d)$ from $n_n^2$ as $V_a$ is increased away from the short-circuit point, as can be seen in Fig. 2b). As shown in Fig. 4, the open-circuit voltage obtained using $R_{b(new)}$ is 0.5777 V, whereas the open-circuit voltage obtained using

![Figure 2](image1), ![Figure 3](image2)
process of from slightly below the short-circuit to slightly above the open-circuit

![Graph](image)

**Fig. 4** The same plot as Fig. 3 but focusing on the J–V characteristics from slightly below the short-circuit to slightly above the open-circuit.

$R_{b\text{(conv)}}$ is 5% lower, which is 0.5486 V. If higher values of $\gamma$ and $k_\text{i}$ are used (refer Eqs. (51) and (52)), then the difference between the uses of the proposed recombination model and the conventional recombination model in predicting the performance of the OSC would be even more significant. In addition to the band-to-band recombination, the SRH recombination can also be important in OSCs [9–11], while the Auger recombination can be important in perovskite solar cells [12], and hence the difference between the uses of the proposed model and the conventional model can even be more significant in practice than in the example shown here. Therefore, assuming that the newly proposed recombination model is the more accurate model for quantifying $R_\text{net}$ in semiconductor devices (as justified by the derivation in Sect. 3.2 and by the result shown in Fig. 3), we show here that the use of the proposed model is important in order to accurately evaluate the performance of OSCs. Since the proposed model is developed for any semiconductor devices made from any types of semiconducting materials (i.e., not specifically for OSCs), we also expect that the use of the proposed model is important to accurately evaluate the performance of other semiconductor devices (particularly optoelectronic devices) whose performance is influenced by carrier recombination such as hybrid perovskite solar cells and LEDs.

### 4.2.2 Understanding $G_0$ in semiconductor devices

Here, we will attempt to give some insights on the physical process of $G_0$ [refer Eq. (1)] in the semiconducting materials of semiconductor devices. As mentioned earlier in Sect. 1, $G_0$ is the generation rate of free carriers (i.e., free electrons or free holes) per unit volume that inherently or permanently occurs in a given semiconductor. In isolated semiconductors, it is well known that $G_0$ exists due to thermal agitation [1], pp. 313–324], which can be explained as follows. The product of the free electron concentration and the free hole concentration that inherently exists in an isolated semiconductor is $n_{\text{int}}p_{\text{int}}$. This means the total rate for any given recombination process that inherently occurs in an isolated semiconductor is $k_\text{r}n_{\text{int}}p_{\text{int}}$, where $k_\text{r}$ is the general coefficient of the considered recombination process [see Eq. (29)].

Since the free electron and the free hole concentrations must be maintained (i.e., the carrier concentrations must not keep increasing or decreasing), this means that $G_0$ in an isolated semiconductor must also be the same as the inherent carrier loss rate, which is $k_\text{r}n_{\text{int}}p_{\text{int}}$, and this explains why we get $n_{\text{0(0d)}}p_{\text{0(0d)}} = n_{\text{int}}p_{\text{int}}$. It is worth noting that $G_0$ depends on $k_\text{r}$, which may be influenced by external factors such as photon absorption as discussed immediately after Eq. (11). Since $n_{\text{int}}$ and $p_{\text{int}}$ exist due to thermal excitation process [refer Eqs. (24) and (25)], $G_0$ in an isolated semiconductor also simply exists due to carrier thermal excitation process (e.g., $T \to 0$, then $n_{\text{int}}$ and $p_{\text{int}}$ are basically zero, and this makes $G_0$ in an isolated semiconductor to be zero).

As shown in this paper, the significance of $n_{\text{0(0d)}}p_{\text{0(0d)}}$ for semiconductor devices is equivalent to the significance of $n_{\text{int}}p_{\text{int}}$ (or $n_{\text{0(d)}}^2$) for isolated semiconductors. $n_{\text{0(0d)}}p_{\text{0(0d)}}$ is the product of the free electron and the free hole concentrations that inherently exist in the semiconducting material of a semiconductor device at a given voltage bias, where the detail can be explained as follows. As can be seen in Eqs. (38), (39), (53), (54), (55), and (56), carrier injection (represented by the injection barriers and the electric field $F$ that appear in the mentioned equations, where $F$ depends on $V_\text{a}$) contributes to $n_{\text{0(0d)}}$ and $p_{\text{0(0d)}}$. When a semiconductor device is under a voltage bias, free carriers from outside the semiconducting material of the device can be forced into the semiconductor. Therefore, in the semiconducting material of a semiconductor device, electrons in the conduction band and holes in the valence band can also be created through carrier injection from outside the semiconductor, besides through carrier thermal excitation within the semiconductor (electrons jumping from the valence band to the conduction band in the semiconductor). A semiconductor that is part of a semiconductor device must be connected to an external circuit and its components (otherwise the semiconductor is an isolated semiconductor where no electric current can flow), and therefore, carrier generation due to carrier injection should be considered as part of the carrier generation that inherently occurs in a semiconductor that is part of a semiconductor device. This means that when a device is under a voltage bias, additional free carriers are injected into the semiconducting material of the device, and therefore, $n_{\text{0(0d)}}p_{\text{0(0d)}}$ must be larger than $n_{\text{int}}p_{\text{int}}$, and this explains why $n_{\text{0(0d)}}p_{\text{0(0d)}}$ is larger than $n_{\text{int}}p_{\text{int}}$ or $n_{\text{int}}^2$ when $V_\text{a} = 0.5$ V.
as shown in Fig. 2b. Furthermore, when a device is not under an applied bias \( V_g = 0 \), no carriers are injected into the semiconducting material of the device, and therefore, \( n_{0(d)}p_{0(d)} \) must be the same as \( n_{\text{int}}p_{\text{int}} \), and this explains why \( n_{0(d)}p_{0(d)} = n_0^2 \) when \( V_g = 0 \) V as shown in Fig. 2b. Since \( n_{0(d)} \) and \( p_{0(d)} \) exist due to carrier injection in addition to carrier thermal excitation, \( G_0 \) in the semiconducting material of a semiconductor device also exists due to carrier injection in addition to carrier thermal excitation.

4.2.3 The implication of the proposed recombination model on the surface recombination model

An enhanced carrier recombination rate and various transport possibilities at the interface can be modeled by using the surface recombination model [1], pp. 53–57, and therefore, the surface recombination model is usually used at the interface as a boundary condition [1]. To explain the implication of the newly proposed recombination model on the surface recombination model and vice versa, let us consider the OSC as described in Fig. 1. When the surface recombination is significant, it basically affects the minority carriers at the interface [13]. For the OSC of Fig. 1, electrons and holes are the minority carriers at the anode \((x = 0)\) and cathode \((x = L)\), respectively, and this leads to the boundary conditions [13, 14]

\[
J_n|_{x=0} = qS_n(n|_{x=0} - n_{\text{surf}}), \quad \text{Eq. (57)}
\]

\[
J_p|_{x=L} = qS_p(p|_{x=L} - p_{\text{surf}}), \quad \text{Eq. (58)}
\]

where \( S_n \) (\( S_p \)) is the electron (hole) recombination speed at the \( x = 0 \) (\( x = L \)) interface, and \( n_{\text{surf}} \) (\( p_{\text{surf}} \)) is the electron (hole) concentration at the \( x = 0 \) (\( x = L \)) interface if there is no surface recombination. Note that, \( n_{\text{surf}} \) and \( p_{\text{surf}} \) are given by the right-hand sides of Eqs. (47) and (50), respectively [13, 14]. Basically, according to the surface recombination model, the actual minority carrier concentration at a given interface is higher than the concentration if there is no surface recombination since the effect of the surface recombination makes the interface to attract the minority carriers in the active layer toward the interface, which leads to a leakage current that reduces the overall output current. Applying Eqs. (6) and (7) to Eqs. (57) and (58), respectively, the boundary conditions for \( n \) at \( x = 0 \) and \( p \) at \( x = L \) due to the surface recombination model are now given by

\[
n|_{x=0} = -\frac{D_n(\partial n/\partial x)|_{x=0} + S_n n_{\text{surf}}}{S_n - \mu_n F}, \quad \text{Eq. (59)}
\]

\[
P|_{x=L} = \frac{D_p(\partial p/\partial x)|_{x=L} + S_p p_{\text{surf}}}{p_{\text{surf}}}, \quad \text{Eq. (60)}
\]

Note that, Eqs. (59) and (60) replace Eqs. (47) and (50), respectively, only when we attempt to calculate the output \( J-V \) characteristics but not when we attempt to obtain \( n_{0(d)} \) and \( p_{0(d)} \). Since \( n_{0(d)} \) and \( p_{0(d)} \) are obtained when the net carrier recombination rate is zero, which means \( n|_{x=0} = n_{\text{surf}} \) according to Eq. (57) [leading to the boundary condition given by Eq. (47)] and \( p|_{x=L} = p_{\text{surf}} \) according to Eq. (58) [leading to the boundary condition given by Eq. (50)], the boundary conditions that should be used to obtain \( n_{0(d)} \) and \( p_{0(d)} \) for the OSC of Fig. 1 are still given by Eqs. (47), (48), (49), and (50). Therefore, in general, the newly proposed recombination model has no implication on the modeling of the surface recombination and vice versa.

5 Conclusion

We have investigated the modeling for the net carrier recombination rate in semiconductors. The net carrier recombination rate per unit volume \( R_{\text{net}} \) in a semiconductor is conventionally modeled as \( R_{\text{net}} = k_r (n p - n_{\text{int}}^2) \) where \( k_r \) is the general coefficient of the considered recombination process, \( n p \) is the product of the electron and the hole concentrations in the semiconductor, and \( n_{\text{int}} \) is the intrinsic electron concentration in the semiconductor. The conventional \( R_{\text{net}} \) model is derived based on the condition that the electric current in the considered semiconductor is always zero, which is valid only if the semiconductor is not part of a semiconductor device. To produce a better and more realistic model for describing \( R_{\text{net}} \) in semiconductor devices, we have derived and proposed a new model, where the model was derived by considering the fact that electric currents can exist in the semiconducting materials of semiconductor devices. We found that \( R_{\text{net}} \) in the semiconducting material of a semiconductor device can be modeled as \( R_{\text{net}} = k_r (n p - n_{0(d)} p_{0(d)}) \), where \( n_{0(d)} \) and \( p_{0(d)} \) are the carrier concentrations that arise from the solutions to \( \nabla \cdot J_n = 0 \) and \( \nabla \cdot J_p = 0 \), respectively, where \( J_n \) and \( J_p \) are the electron current density and the hole current density in the semiconducting material, respectively. By using an OSC as a case study, we analyzed the calculated \( J-V \) characteristics and showed that the newly proposed recombination model is the better model for describing \( R_{\text{net}} \) in OSCs. Hence, we expect the proposed recombination model to be the better model for describing \( R_{\text{net}} \) in other semiconductor devices too since the proposed model is derived for general semiconductor devices. We showed that the use of the proposed recombination model is important in order to accurately evaluate the performance of OSCs, and hence we also expect that the use of the proposed model is
important to better evaluate the performance of other optoelectronic devices whose performance is influenced by carrier recombination such as LEDs.

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