

Review Article

A Review of Organic Photovoltaic Energy Source and Its Technological Designs

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This study reviews and describes some of the existing research and mechanisms of operation of organic photovoltaic (OPV) cells. Introduced first are problems that exist with traditional fossil fuels that result in most of the world energy challenges such as environmental pollution. This is followed by the description of baseline organic solar cell (OSC) structures and materials. Then, some of the existing modelling approaches that have implemented either a one- or a two-dimensional drift-diffusion model to examine OSC structures are reviewed, and their reproducibility is examined. Both experimental and modelling approaches reviewed are particularly important for more and better designed research to probe practical procedural problems associated with OSCs that hinder the commercialization of OPV technology.

1. Introduction

The global share of photovoltaic (PV) technologies in electricity and energy production still remains marginal today and is likely to remain this way for a long period of time especially in poor developing countries. The evidence of the limited global impact of PV is marked by the increasing market share of fossil fuels in the generation of electricity [1]. Notably, about 65–70% of global electricity consumption is derived mainly from exhaustible fossil fuels such as petroleum, coal, and natural gas [1, 2]. The part of the remaining balance is largely derived from other energy resources, such as nuclear, biomass, rivers, geothermal, and wind [2]. Furthermore, due to the strong reliance on nonrenewable fossil fuels, the world energy supply has been experiencing many problems. These include energy market instabilities, technical or physical failures/threats of energy supply that comprise natural disasters, and different security sabotages that arise mostly due to strong global dependence on fossil fuel resources, which are also concentrated in few countries such as Russia, Iran, and Qatar [3]. This makes our world fossil fuel reserves unable to follow with the global energy demand,

which is rising continually as a result of human population growth and development. Additionally, some of these places that are concentrated with fossil fuel resources are affected by geopolitical and socioeconomical instabilities [3, 4].

Furthermore, the production of energy from fossil fuels is often toxic to the environment and health [5]. It is agreed generally that the increasing use of hydrocarbon-based fossil fuels, which represent the main part of the world energy consumptions [1, 2], is responsible for greenhouse gas emissions and the increasing ecosystem and climate instabilities [5–7] that result in the number of natural catastrophes occurring repeatedly in different areas of the world. These problems that are associated with the use of fossil fuels and the adverse social impacts such as those occurring in hydropower dams [8] along with the difficulties in the management of disposals from some of spent fuels such as radioactive wastes from nuclear energy plants [9] have increased the global interest and concerns about the security, sustainability, reliability, and consumption of energy that can be supplied from PV systems. They have also led policymakers, as well as scientists with PV expertise, to propose many strategies, based largely on research and development solutions that can improve

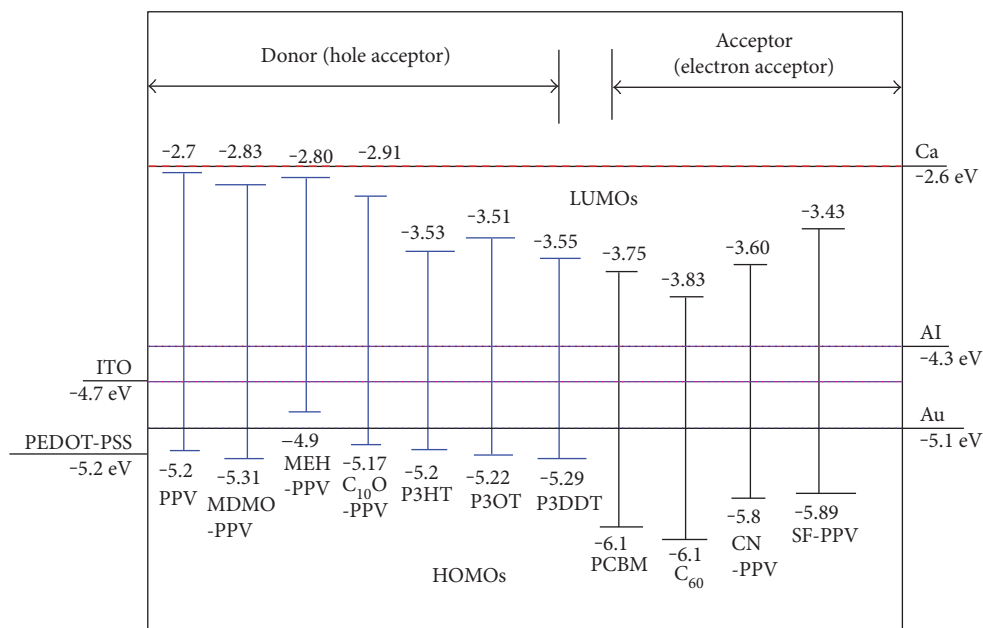


FIGURE 1: HOMO and LUMO energy (eV) levels of the commonly used OPV solar cell materials (source: Goswami et al., Adv. Sol. Ener., Vol. 17, Earthscan London).

the global PV production and market penetration [10]. One of the solutions that have been proposed is the increasing recourse to low-cost OPV systems that allow for the potential use of semiconducting polymers as low-cost material alternatives to crystalline silicon (c-Si) PVs that involve energy-intensive processes and expensive materials [1, 11, 12].

Although OPV technology is still at an early stage of its development, owing to its features of being eco-friendly, mechanical flexibility, vision for mass production, and/or large-area fabrication processes that include simple roll-to-roll or printing, spin coating, spraying, and vaporization, OPVs are considered to be one of the important future sources of energy [1, 13, 14]. This has prompted suggestions that OPV technology is an important energy source candidate for applications in most of the domestic energy needs (such as lighting) in remote rural places or off-grid poor urban communities [5, 10].

However, unlike fossil fuel technologies and some other renewable energy resources such as hydropower, biomass, wind, and inorganic PV technologies, which are technically mature and widely commercialized, only limited information is known on the fundamental material parameters, degradation mechanisms [1], and operation principles of OPV technology. This paper, therefore, attempts to review literature on OPV structures. The survey focuses on recently published knowledge that is relevant to materials, operational design, and fabrication of OSCs. The literature on the modelling of OSC structures is also presented for numerical predictions and optimization of OPV device configurations and their performances.

2. Organic PV Solar Cell Systems

OPV technology is still a relatively new type of thin film solar cells in the PV industry, in terms of performance, stability,

and maturity [1, 13]. It involves photoactive organic layers, comprised of chains and bucky-balls of p-type and n-type semiconducting polymers [14, 15] and oligomer [12] materials. In such polymeric OPV materials, the energy levels (Figure 1) of the highest occupied molecular orbitals (HOMOs) and lowest unoccupied molecular orbitals (LUMOs) are analogous to the respective valence and conduction bands of conventional inorganic semiconductors [16, 17]. Organic semiconductors are thus selected, characterized, and tailored (through different chemical syntheses) based on the energy gaps between LUMO and HOMO levels [16]. The representative examples of the commonly used organic donors (p-type polymers) include poly(p-phenylenevinylene) (PPV), poly(2-methoxy-5-(2-ethylhexyloxy)-1-4-phenylenevinylene) (MEH-PPV), and poly[2-methoxy-5-(3',7'-dimethyloctyloxy)]-p-1-4-phenylenevinylene (MDMO-PPV) [17]. Others are poly(p-phenylene benzobisthiazole) (PBZT) and poly(3-hexylthiophene) (P3HT) [14, 15].

Additionally, prior to depositions of the photoactive organic films, layers of poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT:PSS) are usually coated on top of substrates that are smeared with indium tin oxide (ITO). PEDOT:PSS is a hole-transporting layer (HTL) that blocks electrons while transporting holes to the transparent anode of the OSCs, thus enhancing the charge collection and PV effects of the solar cell system [18]. The other types of polymers that are needed in the fabrication of OSCs are acceptors (n-type organic semiconductors). Examples of the commonly used organic acceptors include [19] poly(2,5,2',5'-tetraalkoxy-7,8'-dicyanodi-p-phenylenevinylene) (CN-PPV), [6,6]-phenyl-C₆₁-butyric acid methyl ester (PCBM), poly(benzamidazobenzophenanthroline) (BBL), and poly[2-alkoxy-5-alkanesulfonyl-1-4-phenylene vinylene] (SF-PPV). More examples of semiconducting polymeric donors, acceptors, and other baseline materials that are needed

generally for the fabrication of OSC systems are summarized in Figure 1.

3. Advances in OPV Technology and Designs

Historically, the first OSC was based on anthracene and was reported by Pochettino in 1906 [20]. Subsequently, after Pochettino's discovery, a number of research efforts have been made to develop high-performance semiconducting polymers together with the enhancement of organic electronic device performances. Such devices include OSCs [20], organic light-emitting diodes (OLEDs) [21], and layered memory structures [22]. Recently, the OPV technology has shown tremendous development [14], evolving from its primitive stage to a relatively reliable source of clean energy in terms of power conversion efficiencies (PCEs) [14]. As shown in Figure 2, literature [23–25] has continually shown increases in organic PV solar cell PCEs, with laboratory solar cell efficiency reaching 10% in 2012 [10] and recently increased to ~11.2% [26] in OSCs with inverted device structures [27] and ~12% in well-optimized OPV systems with nonfullerene acceptor materials [14, 28], while more efforts are being explored to improve semiconducting polymeric materials [29–34], OPV devices [35], and inorganic-organic hybrid structures [36]. This has led to OSCs and other organic device systems that are integrated with portable devices already being tested [37, 38]. The commonly investigated types of OSC structures include those based on the following:

- (i) Dye-sensitized solar cell systems (DSSCs) [39]
- (ii) Metal/polymer junction solar cell systems, which however show very low PCEs that are less than 0.1% [40]
- (iii) Planar organic semiconductor solar cell systems [41–43], which consist of donor/acceptor bilayers and show a relatively low performance with PCEs as low as ~1% [44]
- (iv) Bulk heterojunction (BHJ) OSC systems, which are characterized by a high degree of interactions between donor and acceptor constituents due mainly to the high interfacial surface area between donor and acceptor materials [45–48].

Classically, BHJ OSCs are produced from a solid-state mixed layer of conjugated donor polymers such as P3HT and acceptor molecules such as PCBM [14]. BHJ OSC structures are fabricated generally by codepositions of the two molecules (donor and acceptor) within a thoroughly mixed blend [18, 47, 49].

Note that OPV systems with BHJ structures have been shown to result in the most promising solar cell properties in terms of device PCEs [48, 49]. This enhanced device performance has been attributed to the proper rationing of the polymeric donor and acceptor molecules within the photoactive blends [46]. The donor and acceptor materials are chosen and mixed in a well-controlled way that optimizes

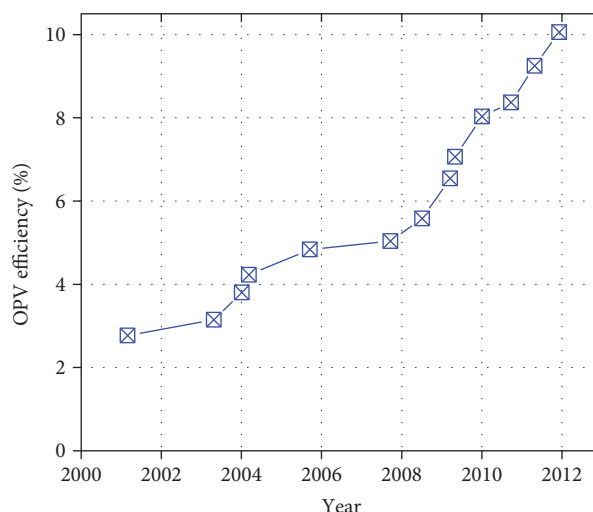


FIGURE 2: Yearly developments of laboratory organic solar cell PCEs [23–25].

the configuration and the local contact area of the final mixtures [35]. This type of blending improves ultimately the light absorption, the exciton/polaron pair dissociation, and the charge transport, thus enhancing the PV effect of BHJ OSC systems [50].

In BHJ OSC structures, the donor and acceptor molecules are also very close to each other, typically less than 10 nm apart. Such distances are within the order of exciton pair mean free-path lengths (the minimum diffusion distance before the exciton can be annihilated via recombination). This suggests that appropriate rationing of the donor and acceptor blends of BHJ OPV cells enables most of the excitons to reach the donor/acceptor interfaces [17], whereupon they dissociate to form loosely bound polarons. Furthermore, BHJ OSC structures are characterized by continuous percolated pathways through which charge carriers migrate to their respective anode and cathode electrodes for collection [5, 51, 52], before they are extracted to the external OSC circuitry.

OSC systems that are based on BHJ structures have been widely studied [1, 20]. Such research efforts have enhanced the OSC PCEs to high values [14, 23–26, 53, 54] that were not thought of before (Figure 2). This advancement has fueled further interest in OPV systems and has also pushed several established companies to turn their focuses on OSC systems and other organic electronic devices and components such as OLEDs [1, 20]. As mentioned earlier, due partly to the high interfacial contact area between the blended donor and acceptor molecules, which enhance the ionization of the strongly bound excitons, OSCs with BHJ structures have been shown to exhibit relatively good PCEs [27].

This performance is also associated with the increase in charge-transporting percolation networks of BHJ OSC structures through which the ionized free charge carriers travel, by hopping and drift-diffusion motions, to the electrodes at the terminal of solar cells. Additionally, studies have shown that blending of an absorber donor polymer, P3HT [17, 45, 55], with an electron-transporting material, PCBM (acceptor

bucky-ball molecules), results in optimum classical BHJ structures so far with better PCEs [1]. This has been attributed to structural factors that the blends of P3HT and PCBM have in improving performances of BHJ OSC systems. These potentials include [44, 45, 56–59] the following:

- (i) Fast free charge carrier transport of high-molecular weight P3HT. This is due mainly to the P3HT morphological crystalline chain-packing abilities, which enhance the mobility of holes [45, 60].
- (ii) The side groups of P3HT that result in good cosolubility with PCBM when they are mixed together inside a well-rationed blend. This not only enhances the interpenetrability of the donor/acceptor blends but also increases the interfacial area of BHJ solar cell systems, thus increasing exciton diffusion length and enhancing their dissociations [61].
- (iii) Proper rationing of the donor polymer, P3HT, and the acceptor molecule, PCBM, in the mixture results in good overlap between the absorption property of the blend and the electromagnetic solar emission spectrum. As shown in Figure 3, for a well-prepared blend, the absorption property has been shown to be compared favourably with the absorption characteristics of c-Si materials and those of the other inorganic thin film solar cell semiconductors, such as cadmium telluride (CdTe) and copper indium gallium selenide (CIGS). Classically, this makes P3HT the best OPV donor material so far when blended with PCBM [19, 50].

As a result, OPV devices with optimized BHJ structures that are based mostly on TCO/PEDOT:PSS/P3HT/PCBM/Al materials have generally been adopted and studied as baseline OSC structures [1, 5, 17, 19, 62, 63]. These can be prepared on top of rigid or flexible substrates [64]. However, PSS (poly(styrenesulfonate)) is acidic and hence a strongly hydrophilic material [65]. This results in serious OPV solar cell problems. The hydrophilicity of PSS is known to accelerate the solar cell degradation mechanisms as a result of increased water moisture absorption [1]. It does so by permeating the OSC ITO layer, the transparent conducting oxide (TCO) film that is commonly used in most of the optoelectronic devices and components [66–68]. These permeation processes increase the degradation rates of the OPV systems [1] and introduce contaminations into the OSC structures [55, 65].

In an effort to overcome the obstacles above while maintaining practical requirements of the HTL materials, some researchers [55] have demonstrated the use of transition metal oxides as alternatives to PEDOT:PSS. These oxides include molybdenum oxide (MoO_3) and vanadium oxide (V_2O_5) [55]. Such metal oxides have been shown to prevent most of unwanted chemical reactions and corrosion processes between the ITO-anode electrode and photoactive layers of OSCs [55]. Furthermore, as explained elsewhere [50], the optoelectronic properties such as energy levels and work functions of MoO_3 and V_2O_5 were compared favorably

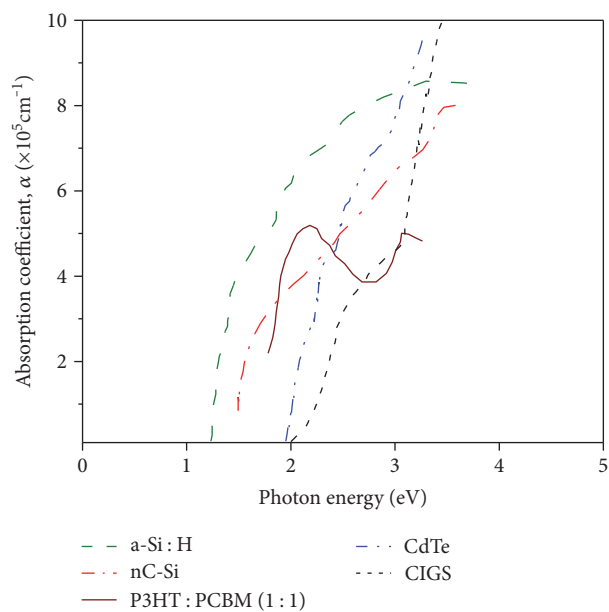


FIGURE 3: Comparison of absorption coefficients for the commonly used solar cell photoactive absorber materials [50].

to those of the baseline materials that are used currently in the operation of BHJ OSC structures (Figure 4). Also, the use of ITO/ MoO_3 -coated substrates has been shown [55] to result in BHJ OSC devices with good performances that are relatively better than those of OPV solar cell systems that are fabricated with traditional PEDOT:PSS buffer layers.

4. Organic BHJ Solar Cell Operation Principles

Preparation of BHJ OSCs requires sandwiching of a blended photoactive solid-state layer of organic donor and acceptor materials between a transparent anode (commonly ITO) with large work function and a cathode (commonly aluminum) with small work function (Figure 1). Charge generation comprises the following steps [69]: first, photons are absorbed by the donor polymer within OSC structures. This creates excitons with charges bound together by strong electrostatic bonds. In order to guarantee a PV effect, the photogenerated excitons have to diffuse inside the OSCs to reach the donor/acceptor interfaces whereupon they dissociate [70] to form weakly bound pairs of charge transfer complexes known as polarons.

Notably, BHJ OSCs are activated by illumination from the anode side of the devices. This is in opposite to the injection conditions of OLEDs, the first broad area of application of organic electronics and optoelectronics [71, 72], such as flat panel displays [73] and other energy devices [74]. Material selection for optimization of photogeneration, transportation, and collection of charges at electrodes requires the cathode Fermi energy to be less than the acceptor LUMO level and the anode Fermi energy to be larger than the donor HOMO level [69]. This leads to the attractive combinations of optical and electrical properties that are relevant for improved OPV system performances. This has further led to the proposition of an optimized empirical relation for

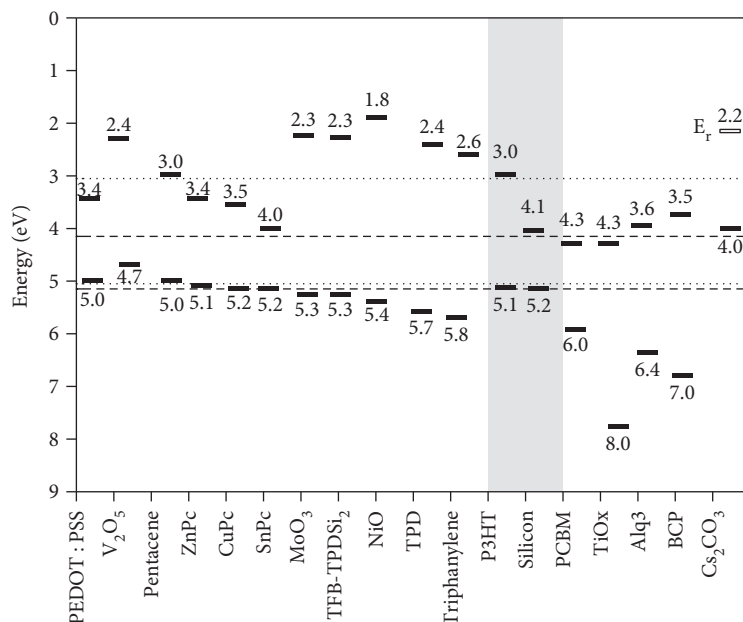


FIGURE 4: Bandgap energies (LUMO-HOMO levels) for several HT/EB layer materials to the left of the absorbers (P3HT, silicon in gray stripe) and ET/HB layer materials to the right [50].

the prediction of open-circuit voltage of OSCs with BHJ structures [75].

However, unlike inorganic semiconductors in which the photogenerated excitons are easily dissociated and separated into free charge carriers [1], organic excitons are strongly bound with energies of ~ 0.4 eV [76]. Such energy values are between 0.5 and 2 eV stronger than those of the thermal energy at room temperature [77–80]. As a result, at the donor/acceptor interfaces, excitons dissociate into short-lived, weakly bound polarons [70]. This is why the photoactive layers of BHJ OSCs are made of interpenetrating blends with phase-segregated donor and acceptor materials. This helps to reduce the separated domain sizes of the photoactive layers, thus increasing the exciton mean free-path lengths and their dissociation probability [81–83].

The weak coulombic force-bounded polarons require further mechanisms to separate them into free charge carriers. Their separation, transportation, and extraction are determined largely by the local internal and external electric fields along with the ambient conditions, such as temperature [70]. This explains the role of the work functions of the two electrodes at the terminals of OSC systems. It also suggests the importance of local morphological configuration of donor and acceptor materials [35], after phase segregation through controlled thermal treatments [5, 84].

In a case where the electric field from external electrodes and local photoactive domain-assisted internal fields are sufficiently large, the polarons separate into free charge carriers, before they are transported for collection [85] at the terminal electrodes. The charge carriers can still, however, annihilate each other by recombining during migration to their respective electrodes. It has been shown that, provided that there are no traps such as impurities/defects, reorganization of chains, and significant variations in the degree of

crystallinity, which hinder charge carrier mobility [86], the transportation of charge carriers depends largely on the morphology of blended photoactive solid-state layers [35, 63, 86].

In BHJ OSC systems, the transportation phenomena of free charge carriers occur primarily by hopping and drift-diffusion movements through bicontinuous percolation paths within the photoactive layers [69, 87, 88]. These movements depend also on the quality of the internal and external electric field of OSC systems. The magnitude of the electric field is determined largely by the work functions of anode and cathode electrodes that are attached on the terminals of the cell [70]. At the electrodes, the electrons at the cathode and holes at the anode can either recombine or become extracted through drift-diffusion processes [70], resulting in the open-circuit voltage of the OSC system.

Therefore, overall performances of BHJ OSCs depend significantly on the exciton/polaron dissociation, separation, recombination, and collection of charge carriers at the respective electrodes [17]. This suggests the importance of a well-engineered interfacial adhesion [64] and contacts for the design of organic PV systems [65, 84, 89]. These issues are investigated largely by experiments using BHJ OSC structures with photoactive organic baseline materials that use polymer-fullerene [83], polymer-polymer [46, 90], and polymer-nanoparticle blends [91] or polymer-inorganic hybrids [36]. Furthermore, typical BHJ OPV systems with low-bandgap blended donor/acceptor copolymers [14, 92–94] and those that are based on fullerene-free polymer structures [95, 96] with reasonably high PCEs have been recognized and widely investigated [14, 92, 95].

Consequently, numerical modelling and theoretical analyses of OSC PCE are also performed based on collective contributions of efficiencies from separate individual mechanistic steps of OPV solar cell operation processes, starting

from cell illumination to charge collection and extraction at the electrodes [17]. A comprehensive physics of OSCs can be cited from the work by Wolfgang [23] while the contemporary historical development of organic PV solar cell systems can be found in literature [1, 13, 20]. Recently, there have also been remarkable research efforts to develop insights of the combined science of organic semiconductors and the associated OPV technology with emphasis on enhancements of PCEs [14, 95, 97–99] and stability of OSC devices [1]. For example, different OPV material tailoring approaches [14, 29–34] along with wide ranges of technological OSC designs and configurations have been established [100–103]. Undeniably, these efforts have led to extensive improvements of the characteristic performances of OPV material structures and PCEs of BHJ OSC devices and components [14, 28, 92–103].

5. Modelling of BHJ OSC Structures

Besides experimentally engineered polymeric functional materials and corresponding investigations of OPV devices [28–34, 92–104], electrical models are also increasingly being developed to ascertain the dependency of OSC performances on their structural and material properties [17, 99]. These models are developed generally based on one spatial dimensional solar cell electrical systems and concepts [17, 104–109]. Recently, however, a number of research groups [110–115] have also applied a two-dimensional space geometry modeling approach to study the properties of BHJ OSC structures. These models are being used to probe sensitive performance issues in the operation of OPV systems such as impacts of active layer morphological factors on the electrical performances and associated limiting issues on the efficiency of OPV devices [116].

So far, finite difference computational methods that are based on drift-diffusion models [17, 104–115] have widely been developed and implemented to study the electronics and kinetic processes of OSC systems with different configurations [17]. In principle, these drift-diffusion electrical models [17, 104–115] are also applicable to inorganic solar cell systems as well as to organic and inorganic light-emitting diodes and other semiconductor devices and components [116]. This is due mainly to the driving forces for charge carrier transport in electronic semiconductor structures that have been shown to be closely similar for organic and inorganic electronic semiconducting materials [117, 118].

The finite difference continuum method is essentially a combination of Poisson's and current continuity drift-diffusion models [17]. The model is usually solved iteratively with appropriate self-consistent boundary conditions [116]. The basic equations that are used in writing drift-diffusion continuum models for simulations of OSCs and other semiconductor devices were discussed by Koster et al. [17] and XinYan et al. [116]. These include Poisson's equation, which relates the position-dependent electrostatic potential to charge carrier densities that are also function of position within the solar cell device [17, 116]. For simplicity, the models and the respective current continuity equations for

electron and hole densities of a given PV system are often written and solved under steady-state condition [17, 116].

It is well known that in semiconductor structures such as solar cells, both electrons and holes contribute to the photocurrent of the device [119]. This has led to the definition of series of postulates for the evaluation of the performance of PV devices, based on Poisson's equation and the current densities, for electrons and holes [17]. These postulates are written in a way relating electron and hole current densities to the electrostatic potential, which is also related to the electric field strength of the solar cell system. The current density equations, therefore, combine both drift and diffusion characteristic transport of charge carriers to arrive at current density continuum models for the prediction of solar cell behaviors [104–115].

To obtain the solution of the drift-diffusion models, the entire device is discretized into a finite number of discrete grid units [17]. This is done using either the forward or the backward difference approximation method [120]. For example, through assuming ohmic contacts, the drift-diffusion equations were discretized and solved iteratively in a one spatial dimension with appropriate anode and cathode boundary conditions [17]. Furthermore, in recent numerical studies of OSCs [17, 104, 105, 108], comprehensive numerical guidelines for modeling of boundary conditions for the respective electron and hole densities were also discussed.

The production of OSC excitons is induced by the absorption of photons inside the photoactive semiconducting polymeric materials, before diffusing to the interfaces for dissociation. The contemporary description of the exciton diffusion phenomenology for inclusion in BHJ OSC models can be found in literature [86]. Note that the photogenerated organic excitons are only capable of diffusing across a certain distance called organic exciton diffusion length/mean free path [115]. This implies that simulations and modeling of OSCs need to account for the effects of exciton diffusion on the operation of OPV devices.

However, studies [115] have shown that the distances between the donor/acceptor interfaces and the excitons in BHJ OSCs are generally very short, in the order of exciton diffusion length. This makes the typical exciton diffusion efficiency in BHJ OPV devices to be considerably effective, very close to 100% [1]. This consideration enabled disregarding of the excitonic diffusion processes in the modeling of BHJ OSCs, using electrical drift-diffusion models [17, 116]. Hence, for OSC systems at steady-state condition, the dissociation and recombination of excitons at the donor/acceptor interface are usually combined to describe the net photogeneration of electron-hole pair density [17, 121].

There are also several theories that have been developed to describe the generation, recombination, and separation of electrostatically bound electron-hole pairs into free charge carriers in organic-like amorphous semiconductors [17, 116]. These include the Langevin recombination [120], Onsager's geminate generation-recombination model [122, 123], and its successful refinement by Braun [124]. Onsager's geminate recombination model [123] applies generally to cases like OSC electronic systems in which there are weak electrolytes [116]. This was further

refined by Braun [124] to derive the field-dependent separation rate constant theory. In the case of a disordered polymer, fullerene solar cell systems, the distance between electron and hole within the exciton or polaron pair is known not to be constant throughout the device [124]. Hence, it has been ascertained that the probability of electron-hole pair separation can be obtained generally as an integral over the spherical averaged Gaussian distribution of electron-hole pair separation distances [17].

After separation of charge carriers, during transportation to their respective electrodes at the terminal of the solar cell, they may still suffer losses due to different factors [116]. These factors may include the Shockley-Read-Hall [125–128], the trap-assisted [128, 129], the surface [130, 131], and the bimolecular [132, 133] recombination phenomenologies of free charge carriers. However, while the trap-assisted recombination has been shown to occur dominantly in OSCs with polymer-polymer structures [128], they do not play significant effects on OPV devices with polymer-fullerene structures [116]. The trap-assisted recombination has, therefore, been neglected in the modeling and operation of OSCs with polymer-fullerene structures [17]. This implies that, during transportation of carriers, the dominant loss mechanisms of charge carriers occur generally by bimolecular recombination [17, 124, 134].

The bimolecular recombination model [17, 124, 134] was used, in a modified form initially by Koster et al. [17]. The authors [17] refined the bimolecular recombination model in order to account for the charge carrier density gradients that occur generally in BHJ amorphous organic semiconductor devices. It was revealed by these authors [17] that the dominant bimolecular recombination rate in OSCs is determined mainly by the type of charge carriers with minimum mobility, generally the holes. The bimolecular recombination rate model was extended further by Deibel et al. [135, 136] to describe the generally observed experimental recombination rates in OSCs that are often lower than the Langevin recombination rate. Their modification led, ultimately, to the description of the bimolecular recombination rate constant for the OPV solar cell devices [135, 136]. Combining the generation and bimolecular recombination rate models, the net expression for the generation/recombination rate of charge carriers is readily obtained as reported by Koster et al. [17].

To obtain the solution of the drift-diffusion model, the basic Poisson and continuity equations are solved based on either Gummel or Newton iteration scheme [116, 137]. However, in most computational simulations and numerical predictions, Gummel iteration scheme [137] is chosen due mainly to its simplicity as compared to the Newton scheme [116]. Note also that the values of the original parameters such as electron/hole densities and the potential difference that are used in the drift-diffusion equations might be relatively large. The equations can, therefore, be normalized, and the model was operated with reduced variables (with arbitrary units) using suitable carrier density and differential equation operator scaling factors [116].

6. Reproducibility of 1D Numerical Method in 2D Space Geometry

In order to ascertain the reproducibility of a one-dimensional spatial drift-diffusion model in 2-dimensional space geometry, numerical simulation was performed on organic BHJ solar cell structure with perfect planar interlayer contacts. The numerical procedure was purposely tested based largely on the model reported earlier by Koster et al. [17]. However, this part of the review compares the reproducibility of the 1D drift-diffusion model developed by the group [17] with a two-dimensional version (Figure 5) of the same model and then with experiments that were also reported by the authors [17]. In the first part, a finite difference method was employed in writing a computer source code that is capable of simulating the relevant characteristics of semiconductor devices with particular accent on BHJ organic solar cells.

The model was purposely implemented in MATLAB computer software package. This enabled numerous random and reasonably easy modifications of the code to allow suitable implementation of the different OPV solar cell electronics and kinetic phenomenologies reported elsewhere in literature [17, 104–118]. The modeling results were then compared with a 1D numerical finding that was obtained earlier by Koster et al. [17] for similar organic BHJ solar cell structures. In comparison, the numerical results obtained from 1D and 2D models are largely in agreement. As it was with a 1D OSC model, studied by Koster and coauthors [17], the fits of the 2D model to the experimental profiles (Figure 6) are in agreement with the data that were obtained for both dark and illuminated OSC devices. This suggests that the conditions that were described in Koster's group 1D model [17] that were also assumed in the 2-dimensional numerical simulations of a similar OSC with perfect planar contacts are closely mimicking the electronics, kinetics, and charge carrier transfer interfaces in actual structures of BHJ OSC systems.

6.1. Implications. The 1D models are significantly important and form the widely studied numerical methods for the investigation of organic, inorganic, and other semiconductor devices [17, 104–109]. However, higher spatial dimensional models such as 2D and 3D models can enable probing of some of solar cell interfacial and contact phenomena such as analyses of the broad dimensional features found inherently in organic PV and other organic semiconductor devices. These may include numerical analysis of the recently reported experimental polymer morphological [35, 63] and nonuniformity nature of the entire BHJ OPV structures and components [125].

Hence, the reproducibility of the 1D model to 2D space geometry suggests further that the OPV drift-diffusion models can be extended into high-spatial dimensions such as 3D models in a way making them broader to address the most complex interfacial/interlayer optoelectronic processes [64, 65] and experimental morphological issues [35, 64] that influence the PCEs of BHJ organic solar cells. Such efforts should attempt to explore effects of other forms of charge carrier transport, such as thermionic emission and the

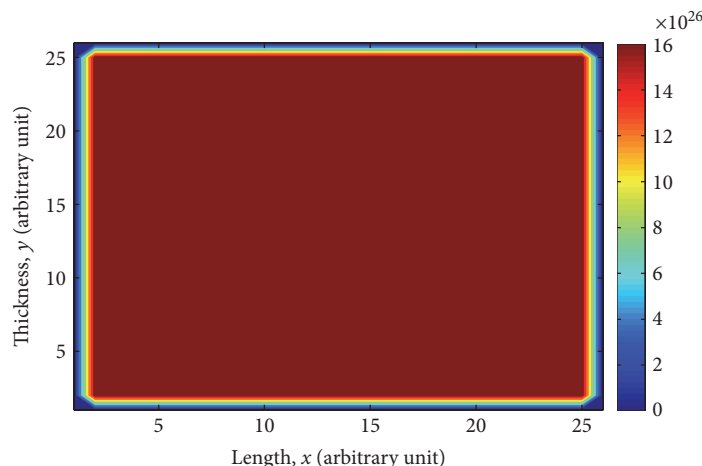


FIGURE 5: (Colored online) simulation illustrating the generation rate of charge carriers from a drift-diffusion model of a BHJ OSC structure with planar contacts in two spatial dimensions.

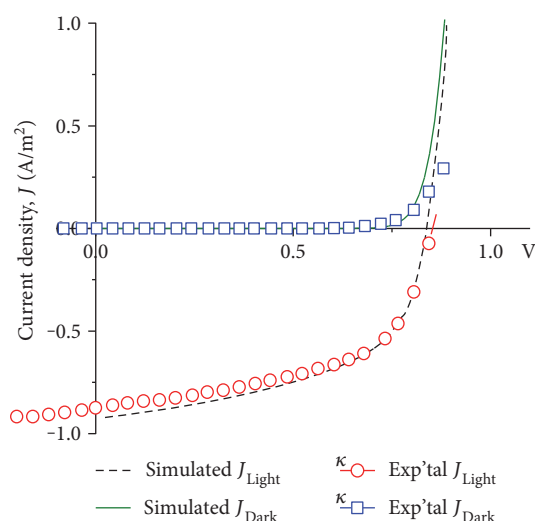


FIGURE 6: Comparison of 2D simulated J-V characteristics of an OPV solar cell system with perfect planar interface with experimental profiles (κ) adapted from Koster et al. [17].

different quantum charge tunneling on the operation of OPV structures. These are clearly some of the challenges and opportunities for future work. Such work is particularly important due to the fact that the potential of PV is not exploited to the level it deserves [138], resulting in marginal share of its technologies in energy and electricity production.

7. Concluding Remarks

In summary, the work and research efforts on organic-based solar cells to date have not provided the answer to the question: can OPV technology improve the global share of PV technology in energy and electricity production? This is an important question that still requires research-based answers commenting on the reliability, adoption, and commercialization of OSCs and modules. As of today, there are sufficient research efforts that have been made to improve the

polymeric semiconductor materials, structure, PCE, stability, and designs of OSCs at the laboratory level. There is, however, insufficient research evidence to support the recommendation that organic photovoltaic technology can contribute significantly to our current global energy consumption or replace the traditional c-Si-based solar cell technology in the near future. This entails that the research on OSC materials, processes, and technological design is very far from being exhausted. The review in this paper showed further that it has been increasingly clear that there remains lots of scope for further research and improvements to be achieved in terms of the necessary OSC technological requirements that include performance, material reliability, stability, solar cell processing, and commercialization of the OPV solar cells and modules.

Conflicts of Interest

The author reports no conflict of interests in this review paper.

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