

Working principle of photovoltaic device

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The working concept of all PV cells is virtually based on ‘ photovoltaic effect’. In common, photovoltaic effect implies generation of voltage difference at the junction of 2 dissimilar materials in reply to ultraviolet/visible/near infrared or other type of radiation. Hence, a cell is a 2 terminal semiconductor device which conducts exactly like a junction diode in the dark region and produces a potential difference when illuminated by sunlight [29]. A p-n junction semiconductor device in the dark region, gives the characteristics similar to rectifier diode.

Solar cell device characterization parameters

The important parameters that are utilized to characterize performance of photovoltaic device are: peak power (P_{max}), fill factor (FF), short circuit current density (J_{sc}) and open circuit output voltage (V_{oc}). The power conversion efficiency (PCE i. e. η) is determined by using these photovoltaic parameters. Brief descriptions and formulae for photovoltaic parameters are illustrated below for a p-n junction semiconductor device.

Short-Circuit Current Density (J_{sc}):

The short-circuit current density is the maximum photo-generated current delivered by a solar cell when the terminals of the solar cell are in contact with each other (i. e. short-circuited). The solution for can be gotten from the net current density in the solar cell given as [27]

$$J(V) = J_{sc} - J_{dark}(V)$$

Where $J_{dark}(V)$ is the dark current density.

Under illumination, the solar cell behaviour is described using the ideal diode equation (2. 2) and an additional current source due to illumination. Thus, with the electronic charge ($q = 1.603 \times 10^{-19} \text{ C}$) and Boltzmann's constant ($k_B = 1.38 \times 10^{-23} \text{ JK}^{-1}$) the illuminated solar cell equation. The open-circuit voltage (V_{oc}): V_{oc} is the voltage at which no current flows through the external circuit when the terminals of the solar cell are not connected to each other. It is the maximum voltage that a solar cell can deliver. The V_{oc} depends on the photo generated current density, J_{ph} . For the simple p-n junction, It is given by [27]: This is obtained from equation (2. 3b) by setting the net current, $J(V)$ to zero. This leads to compensation effect between the dark and the photocurrent, such that $J(V) = 0$, $J_{sc} = J_{ph}$ and $V = V_{oc}$.

Fill factor, FF

The fill factor is the ratio between the maximum power generated by a solar cell and the product of V_{oc} and J_{sc} and FF describes the 'squareness' of the J-V curve and V_m and J_m are the maximum point voltage and current density generated by a solar cell.

Power Conversion Efficiency

The power conversion efficiency is calculated as the ratio between the generated maximum power and the incident power. This is given by: (2. 6)

The irradiance value, of 1000 W/m^2 of AM1.5 spectrum has become a standard for measuring the conversion efficiency of solar cells. Where the irradiance power, P_{in} , is the standard incident power as function of solar cell area. It has a value of 1000 W/m^2 of spectrum[27].

Junctions in solar cell device

P-N Junctions in PV devices are the interfaces amidst the semiconductor materials that make up the cells or semiconductor and different materials. For instance, the regions between the P and N semiconductor, result in electric fields being produced. These fields are important in the separation of carriers which drift in inverse directions to contacts. As stated, these junctions are called p-n junctions [27]. Other junctions that are important in cell designs, combine the P-I-N and metal-semiconductor junctions [29].

PSCs

To develop inexpensive photovoltaic systems substitutes to Si solar cells, PSCs have drawn great interest [22]. These have enhanced the efficiencies of PSCs to high levels, exceeding the PCEs of many photovoltaics, such as DSSCs Ref.[30], OPV Ref.[30] and a-Si solar cells [31]. Further, the efficiency of PSCs compares favourably with many PV systems that are utilized currently in the photovoltaic industry (Figure 2. 2). A perovskite refers to any material with structure ABX_3 same as $CaTiO_3$ (calcium titanium oxide). Here X is an anion, A and B are cations of organic/inorganic substance of abstract sizes. [22]. The structure of the perovskites presently used in photovoltaics consists of a mechanism of corner-sharing BX_6 octahedral with the B cation and X is a halogen. The cation A is picked to balance the charge and it can be organic (i. e. Methylammonium, Formamidinium) or inorganic such as Cs^+ ion [32], [33]. Perovskites are known for phase complexity, with admissible cubic, tetragonal, monoclinic polymorphs, orthorhombic, trigonal etc. depending on rotation and tilting of the BX_6 polyhedral. [34]. Transition in phase is generally observed in Pb perovskites under the effect of

temperature, pressure or electric field. [35]. MASnI₃ perovskite consists a tetragonal structure same as the MAPbI₃ but under different temperature [36] with the lattice parameters $a = 8.7912 \text{ \AA}$ and $c = 4.4770 \text{ \AA}$.

MASnI₃ consists the following properties which makes it suitable for solar cell applications. Low optical band gap of 1.23 eV, broad absorption edge of $\sim 1000 \text{ nm}$ and an good hole transporter. [37].

2. 4. 1 Properties of organic-inorganic hybrid perovskite materials

Perovskite materials are used as light absorbers in PSCs. The interest has been due to interesting characteristics of the inorganic materials, which include thermal stability, structural ordering because of the properties of the organic component like the functional versatility, mechanical flexibility and low production cost. [39][40].

Therefore, the possibility of merging the properties of inorganic crystals with molecular organic solids has motivated research into the properties of organic inorganic hybrid perovskites.

Furthermore, organic-inorganic hybrid perovskites have some tempting potential for applications in solar cells. Which include:

1. Excellent photoabsorber characteristics as well as excellent hole transporting properties [41].
2. Low processing cost.
3. Low temperature photovoltaic processing via the printing techniques which makes it possible to be deposited on a flexible substrate [38], [42].
4. It increases light absorption, thus increasing the photogeneration of free charge carriers. This enables low energy-loss by the charges generated and increase their collection at the electrodes.[43], [44].

5. Low energy payback time due to low processing cost and high efficiency. Energy payback time is the time or duration it takes for solar cells to give back the equivalent energy used or expended on its production. A low payback time can be achieved in a material with low cost of production and high performance. Despite these advantages of organic-inorganic hybrid perovskites, there are generally four major challenges facing PSCs, which hinder their commercialization. Researchers have worked on addressing some of these challenges in various capacities. These efforts have proffered solutions in overcoming them. These problems include.

Perovskite materials are extremely sensitive to oxygen and water vapor, which degrade the solar cells by dissolving the salt-like perovskite crystal structure. This has been addressed by preparing the perovskite thin films in an inert atmosphere such as Nitrogen [25],[28] or Argon [35] filled glove boxes. This is followed with immediate encapsulation of the whole device within an air tight sealant with the same inert condition. Although it is not cost effective for large scale production, this method has been used to reduce the degradation of tin perovskite and oxidation of Sn^{2+} to Sn^{4+} . Thus increasing the solar cell lifetime for a period of 4-months for tin perovskite.

It is challenging to prepare large continuous films in glove boxes, which limits it for large scale production of PSCs. However, sequential deposition of the constituents components perovskite materials can be used to get a continuous film over a larger area without degradation of the cell efficiency [24].

Lead, which is the most-used PSCs, is toxic. This could leach out of the solar panel into the environment causing health and ecological challenge. Hence, environmentally-benign element such as tin has recently been proposed as solar cell materials alternatives to lead perovskites.

Low lifetime due to phase transition: the longer-term stability of PSCs has not been verified. There are a few studies on storage lifetime. However, they are only limited on an operating cell (under illumination at the maximum power) sealed at $\sim 45^{\circ}\text{C}$ ambient temperature [24]. In that, study, the authors observed a decrease in initial solar cell power conversion efficiency of less than 20% after 500 h. While much work has been done on lead halide PSCs, there are relatively few reports on tin halide PSCs.

Much experimental efforts have been made in addressing the problems listed above; the optimization of tin halide PSCs with accent on their efficiencies has not been fully examined. There is also a need to develop models and numerical simulations complements to experiments, which are relatively difficult to understand. Therefore, this work will use numerical modeling to obtain insight into the details of the physical operation of thin-film organic-inorganic hybrid tin PSCs with planar-interface heterojunction structure.

Prior work on the organic-inorganic hybrid PSCs Single and mixed halides perovskite such as $\text{CH}_3\text{NH}_3\text{PbI}_3$ and $\text{CH}_3\text{NH}_3\text{PbI}_{3-x}\text{Cl}_x$ have recently been used as light harvesters. Due to their high light absorption coefficients, these materials have been shown to have resulted in solar cells with efficiencies of over 15%. Furthermore, an efficiency of 17.9% has been recently recorded

by Soek et al. who produced a PSC with mixed-halide $\text{CH}_3\text{NH}_3\text{PbI}_{3-x}\text{Br}_x$ using poly-triarylamine as hole transport material (HTM).

However, lead being a toxic element has really been a concern. In an effort to address this concern, tin has been proposed for effective replacement of lead. Kanatzidis et al. have reported on lead-free PSC that was based on methylammonium tin iodide ($\text{CH}_3\text{NH}_3\text{SnI}_3$). They observed a decrease in V_{oc} as compared to lead-containing PSC devices with the same configuration. Also, these authors have investigated the possibility of using a mixed halide of $\text{CH}_3\text{NH}_3\text{SnI}_{3-x}\text{Br}_x$ as the light-absorbing material in solution-processed solid-state photovoltaic devices. The mixed halide was tried in realization of its tunable band gap, which should allow increases in V_{oc} of the devices. For comparison, Table 1 summarizes some important results obtained in Ref. In a different work, with a similar $\text{CH}_3\text{NH}_3\text{SnI}_3$ perovskite material having a slightly lower bandgap energy of 1.23 eV, Snaith et al. reported a solar cell with efficiency of 6.4%.

Optical band gaps and refined lattice parameters of the ABX_3 ($x = 0, 1, 2, 3$) perovskites and their corresponding solar cell performance parameters 2.5. 1 PSCs device architecture PSCs have been produced using different device structures, shown in Figure 2.4. These show the possible ways that have been recently used in the design and fabrication of PSC devices with different performance. For numerical modeling and simulation, it is straightforward to use the solar cell configuration in fig. 2.4(c). The later has the structure of a thin-film p-i-n solar cell with planar heterojunction structure. This allows the use of numerical software packages such as Solar

Cells Capacitance Simulation (SCAPS) for modeling and numerical characterization of PSC devices, in a way similar to the structure of thin-film compound semiconductor solar cells, such as CIGS.

The above configurations are popularly used in PSC devices. Fig. 2. 4a, b contain a mesoporous and nanowire material which serve as scaffold (support) to the perovskite compound. In the three structures, they have in common the transparent conducting oxide (TCO) which is deposited on a glass substrate and a cathode (Au) layer which serve as the electrodes. The electron transport material, ETM (compact TiO_2) and hole transport material, HTM (spiroOMeTAD) just like the name, extract the electrons and holes generated in the absorber layer (perovskite) and transport them to the electrodes which are in contact with the load.

Charge carriers in perovskite material ($\text{CH}_3\text{NH}_3\text{PbX}_3$) The determination of charge carriers in organic-inorganic hybrid PSCs has been a challenge. This is due largely to the presence of both organic and inorganic components. This uncertainty on the nature of charge carriers transported in perovskite material has been experimentally investigated by Edri et al. It was found that the lead halide PSCs (thin film and/or inert mesoporous configuration) operate generally as p-i-n junction. A p-i-n junction has an intrinsic semiconductor material sandwiched between a p and n type extrinsic semiconductor. Their study was carried out on a solar cell with mixed halide lead based perovskite, $\text{CH}_3\text{NH}_3\text{PbI}_3 - x\text{Cl}_x$ absorber. Figure 2. 5 (c) shows the band diagram of perovskite structure. Note that, the PSC band diagram resembles a typical p-i-n band diagram shown in fig. 2. 5 (b).

In agreement with a previous report[50], Minemoto et al. and Tanaka et al. have observed that the dominant charge carrier in lead halide perovskite is a typical Wannier- type exciton. This is similar to the type of charge carriers observed in inorganic materials. Wannier type excitons occur when the electric field screening tends to reduce the Coulomb interaction between electrons and holes. The screening reduces the binding energy of the electron-hole pair and makes them move independently, unlike Frenkel excitons which occur in organic materials.

E_v and E_f represent the vacuum and Fermi energy level while CB and VB are the conduction and valence band edge (conduction and valence band energy level).

Operational principle of PSCs As discussed earlier, lead PSCs operate like p-i-n junction devices. The perovskite material serves as an intrinsic semiconductor layer, -i- while the n-type material serves as the electron transporting material (ETM) and a p-type material as the hole transporting material (HTM). A p-i-n solar cell structure is basically a p-n junction device with an undoped - i- layer sandwiched between n-type and p-type materials. The intrinsic layer, i, extends the electric field generated in the space charge (depletion) region of the p-n junction over a wider range. The photo-generated carriers at the -i- layer are then transported towards the contacts (attached at the ends of n-type and p-type materials) by the same built-in electric field generated at depletion layer of the cell. The extension of the electric field over a wider range of the device increases the survival of the photogenerated carriers over a greater distance than those in the

conventional doped semiconductor materials. The planar configuration without mesoporous structure corresponds to a p-i-n solar cell structure. Such PSCs (without mesoporous scaffold) has been shown to have highest recorded efficiency of 19.3%. This suggests shows that the mesoporous PSC structure is not a prerequisite for obtaining a better performing solar cell device.

Excitons

Excitons are elemental quantum of electronic excitation combining of a -vely charged electron and a +vely charged hole stained to each other through coulombic attraction. They are made when a solid absorbs light photons. There are two types of excitons, the Wannier and Frenkel excitons, on the basis of size relative to the interatomic/intermolecular distances in the material.

In Wannier type excitons, generally observed in covalent bond semiconductors/insulators, the charge carriers are separated by a distance greater than the atomic spacing, so the effect of the lattice on the exciton is almost zero. In Frenkel type excitons, which are typically found in organic substances, charge carriers are separated by a distance that is almost same to the atomic spacing, so the exciton is localized to a single site at any given time. Wannier excitons move like free particles, whereas motion of Frenkel excitons is considered as hopping from one site to another.