Optimal design of organic–inorganic hybrid tandem solar cell based on a-Si:H and organic photovoltaics for high efficiency

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Thin-film solar cells based on hydrogenated amorphous silicon (a-Si:H) and conjugated polymers have been studied extensively. However, organic–inorganic hybrid tandem solar cells incorporating the two materials as subcells are yet to be extensively studied. Here, a computational study on the optimal design of organic–inorganic hybrid tandem solar cells to achieve the maximum possible efficiency is presented. The optical simulations predict the optimal design of an organic–inorganic hybrid tandem solar cell, desirable for a wide range of spectral response and high efficiency. The optimum combination of thicknesses of a-Si:H and organic photovoltaic (OPV) subcells to achieve the highest possible efficiency in terms of short circuit current (J_{sc}) is determined. Thicknesses of 400 and 140 nm for a-Si:H and OPV subcells, respectively, are suggested for the optimised tandem solar cell to achieve current matching and a maximum power conversion efficiency of 11.57%.

1. Introduction: The last few decades have seen rapid development of hydrogenated amorphous silicon (a-Si:H) solar cells. In recent years, solution-processed bulk-heterojunction organic photovoltaics (OPVs) have developed remarkably. To overcome the theoretical limit of the power conversion efficiency (PCE) of single solar cells calculated by Shockley and Queisser [1], tandem solar cells have been suggested. These are multi-junction photovoltaic devices, in which two subcells are stacked to achieve a higher overall solar absorption [2–4].

One of the advantages of tandem solar cells is the higher open circuit voltage (V_{OC}) obtained by the addition of the two V_{OC} because of the serial connection of two subcells. Moreover, in tandem solar cells, the stacking of subcells with different band gaps enables complementary light absorption over the entire solar spectrum. Different absorbers such as inorganic–inorganic solar cells with a-Si/μc-Si [5, 6], organic–organic solar cells [7, 8], hybrid dye sensitised solar cells, and copper–indium–gallium–diselenide solar cells [9, 10] have been reported in earlier works on the design of tandem solar cells. Recently, an organic–inorganic hybrid tandem cell using an a-Si solar cell and an organic solar cell has been reported [11], and subsequent to the report by Kim *et al.* in 2011 [12–14], few more reports have followed. However, the efficiency of the tandem solar cells is lower than that of each single subcell. This is mainly because the top and bottom cell lack the optimal thicknesses to ensure that the subcell absorbs light equally. The study of such problems is a new and developing field of research, with numerous challenging issues, such as current matching and device design, yet to be resolved.

In this Letter, we propose an optimal structure design of a highly efficient organic–inorganic hybrid tandem solar cell through optical simulations. Using rational combination of single cells of OPV and amorphous silicon (a-Si), we develop a structured organic–inorganic hybrid tandem solar cell with a maximum efficiency of 11.57% and a short-circuit current (J_{SC}) of 8.91 mA/cm^2 for each subcell exhibiting high performance. Until now, hybrid tandem solar cells have had a maximum reported PCE of 5.72% and J_{SC} below 7 mA/cm^2 [14]. Our optical simulations and calculations suggest that organic–inorganic hybrid tandem solar cells with OPV and a-Si have the potential for drastic improvement in performance.

2. Experimental details: The structure of the hybrid organic–inorganic tandem solar cell is illustrated in Fig. 1. It is used in the simulations to vary the thicknesses of a-Si:H photovoltaic and OPV subcells to obtain the corresponding J_{SC} values. The finite dimension time domain (FDTD) method enables an optical calculation of absorption for each solar cell using the measured refractive index (n) and extinction coefficient (k). The simulations were performed with the Lumerical package [15]. The chosen optical parameters were obtained from a highly efficient single solar cell of a-Si:H and OPV subcells with appropriate band gap. To detect the incident light of AM 1.5 G equally, and to obtain a balanced spectral response from the top and bottom cell, a low band gap of OPV subcelll is set at 1.3 eV since a wide band gap of the top cell of a-Si:H remains at 1.83 eV because of known acceptable efficiency in hybrid organic–inorganic tandem solar

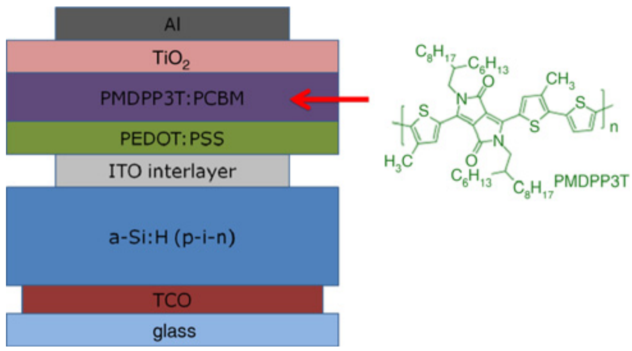

Figure 1 *Schematic of a-Si:H photovotaic and OPV subcells in hybrid tandem solar cell*

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cells. For this purpose, a newly synthesised donor polymer was used to blend with a [6, 6]-phenyl-C61-butyric acid methyl ester. This novel polymer, poly[[2,5-bis(2-hexyldecyl-2,3,5,6-tetrahydro-3,6-dioxopyrrolo[3,4-c]pyrrole-1,4-diyl]-alt-[3′,3″-dimethyl-2,2′:5′,2″-terthiophene]- 5,5″-diyl] (PMDPP3T), and its chemical structure are shown in Fig. 1. It has a low band gap of 1.3 eV, and the absorption edge is ∼950 nm. Single junction OPV cells fabricated with the novel polymer exhibit increased efficiency of up to 7%, thus making it a suitable building block to achieve low band gap and high performance criteria [16]. Vapour-deposited a-Si:H, produced by plasma-enhanced chemical vapour deposition, was used as a wide band gap absorber as the top cell. Optical constants of a-Si:H were fabricated by adhering to methods used in earlier reports [11–13], and were obtained by ellipsometry measurement.

3. Results and discussion: Fig. 2 shows the calculated capacity of J_{SC}, corresponding to the maximal value when it approaches the limit. The contour plot of maximal J_{SC} against the thicknesses of the front cell with a-Si:H and the back cell with OPV is obtained by applying basic Kirchoff's law to determine the total current in serial circuitry; that is, the total current is limited by the lower current of the component in a serial circuit. The optical simulations were performed for the tandem structure shown in Fig. 1, and the absorption of each cell is calculated by simultaneously varying the thicknesses of both the front and back cells. The lower value of absorption in those two cells is the determining factor to calculate the maximal J_{SC} from the total number of absorbed photons in each cell.

In the case of total conversion of absorbed photons to electrons, the absorption of each cell is calculated by optical simulation, which gives the potential value that J_{SC} can obtain for the tandem solar cell. The contour map shown in Fig. 2 can be plotted from the thicknesses required to obtain the potential maximum value of J_{SC}. The optimal condition occurs when the front cell of a-Si:H has 550 nm and the back cell of OPV has 140 nm. This ideal condition indicates that the internal quantum efficiency (IQE) of each cell is 100%. Although IQE cannot be 100%, if the IQE of each cell is equal, the optimal thickness in Fig. 2 should be realisable. However, the IQE of OPV and a-Si PVs inhibits intrinsic variance because of their different photon to electron conversion and electron conduction mechanisms. Careful precautions were taken to resolve this issue in order to account for the variations in IQE and to obtain realistic values of J_{SC}. Moreover, other parameters such as open circuit voltage (V_{OC}) and fill factor (FF) were also taken into account.

To calculate the parameters of the tandem solar cell, IQE is obtained from a single cell while varying the thicknesses [17] and is fitted as a function of thickness. IQE of a-Si is independent of thickness for a scale of several hundred nm, and IQE of OPV with PMDPP3T remains stable at about 80% regardless of thickness [16]. In general, a maximum of 95% for IQE is feasible on a-Si PVs, such that 80 and 90% of IQE are obtained for OPVs and a-Si PVs, respectively.

Open circuit voltage is also a complicated issue to predict. Here, we determine the V_{OC} using the following equation:

$$V_{OC,a\text{-}Si} = E_g - 0.8\ \text{eV} \tag{1}$$

where $V_{OC,a\text{-}Si}$ is the open circuit voltage of a-Si PV and E_g is the band gap. For V_{OC} of a-Si PV, the subtraction of 0.8 eV was empirically determined from the band gap.

For the calculation of V_{OC} of OPV, we should also consider exciton dissociation. The following equation gives the open circuit voltage for OPV:

$$V_{OC,OPV} = E_g - 0.3\,\text{eV} - \Delta_{LL} \tag{2}$$

where $V_{OC,OPV}$ is the open circuit voltage of OPV and Δ_{LL} is LUMO-LUMO offset. Δ_{LL} ranges between 0.3 and 0.4 eV. Here, we take 0.3 eV [18].

As a result, we obtain 1.03 V for $V_{OC,a\text{-}Si}$ and 0.7 V for $V_{OC,OPV}$. According to Kirchhoff's law, the open circuit voltage of tandem solar cell ($V_{OC,tandem}$) is simply the sum of the two V_{OC} ($V_{OC,a\text{-}Si}$ + $V_{OC,OPV}$). This gives 1.73 eV for $V_{OC,tandem}$.

Finally, the FF is calculated from the average FF of a-Si PV and OPV. The FF is obtained from the FF of a single cell with various thicknesses. FF shows an inverse relationship with thickness for OPV while a-Si shows a weakly similar relationship.

Throughout this process, power conversion efficiency (η) is given by the following equation:

$$\eta = (J_{SC}) \times (V_{OC}) \times (\text{FF}) \tag{3}$$

Fig. 3 shows the contour plot of calculated efficiency against thickness. The plot is shown as a function of thicknesses of an organic–inorganic hybrid tandem solar cell with respect to the thickness of the front cell (a-Si:H) and back cell (OPV). The optimal thicknesses are illustrated with the deep red colour in Fig. 3, where an a-Si:H

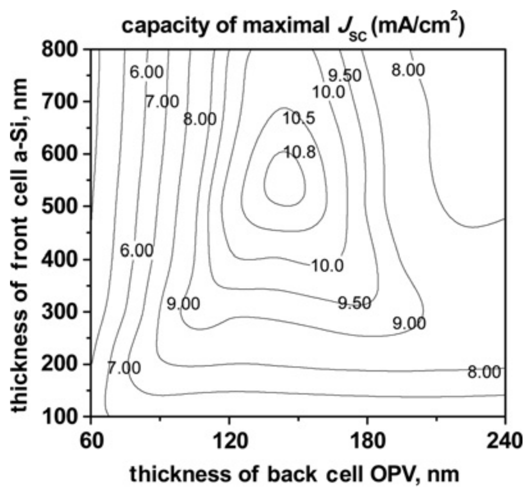

Figure 2 *Contour plot of J_{SC} against thicknesses of organic–inorganic hybrid tandem solar cell with a-Si:H as the front cell and OPV as the back cell*

J_{SC} is obtained from the total number of absorbed photons of tandem solar cell depending on thicknesses of each subcell

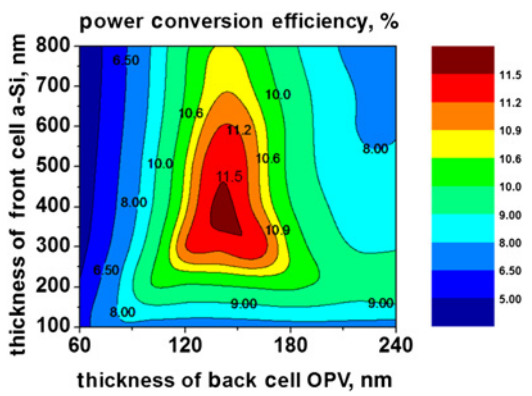

Figure 3 *Contour plot of efficiency against thicknesses of organic–inorganic hybrid tandem solar cell with a-Si:H as the front cell and OPV as the back cell*

From this, the efficiency of the tandem solar cell with respect to thicknesses of each subcell can be determined

Table 1 Photovoltaic parameters of organic–inorganic hybrid tandem solar cell with the highest efficiency

a-Si thickness, nm	Intrinsic a-Si, nm	Absorber of OPV, nm	J_{SC}, mA/cm^2	Efficiency, %
412	400	140	8.91	11.57

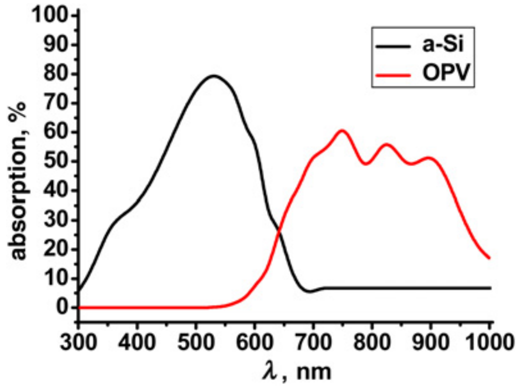

Figure 4 *Absorption spectra of the tandem solar cell with contributions from two subcells, a-Si:H and OPV*

front cell with a 400-nm observer and 145-nm OPV is the best performing hybrid tandem solar cell in terms of efficiency. This tandem solar cell obtained a J_{SC} value of 8.91 mA/cm^2 and a PCE value of 11.57%. Our results predict a greater than 10% increase in the efficiency of an organic–inorganic hybrid tandem solar cell with a-Si:H and OPV, making them promising candidates as photocells.

The thickness value and other solar cell parameters for maximum efficiency are given in Table 1. The total thickness of a-Si is 412 nm, with 7 and 5 nm being the thickness of p-type and n-type a-Si, respectively, in PIN structure.

Absorption spectra are given in Fig. 4. The maximum efficiency is obtained because of current matching between a-Si PV and OPV in the tandem structure. Spectral response is divided equally by a-Si and OPV, leading to current matching and maximum efficiency with thicknesses of 400 nm of a-Si and 140 nm of OPV.

4. Conclusion: The optical simulations reported in this Letter predict the optimal design of an organic–inorganic hybrid tandem solar cell with a wider range of spectral response and high efficiency. Our computational simulations using FDTD shows the dependence of J_{SC} on thickness combination of a-Si:H and OPV and also determines the most optimal combination of thicknesses to achieve the highest possible efficiency. Here, we suggest 400 and 145 nm of absorber for a-Si:H and OPV subcells, respectively, as this combination provides the ideal condition for the hybrid tandem solar cell in terms of current matching. Our optimised hybrid tandem solar cells obtained maximum PCE and J_{SC} values of 11.57% and 8.91 mA/cm^2, respectively. This study provides a new direction for achieving a rational layout for an optimal device and shows the potential to improve the performance of hybrid tandem solar cells. Further attempts will soon be made to develop and test the proposed design experimentally.

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