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Design and Development of Energy Efficient Hybrid Solar Cell Based on Polymer

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ABSTRACT
Hybrid Solar Cell (HSC) consisting of poly (3-hexyl thiophene) (P3HT) as donor conducting polymer and core shell cadmium selenide/zinc sulphide (ZnS/CdSe) quantum dots (QDs) as an acceptor have been developed using thermal inter-diffusion process. This unique technique was needed to deposit the QD layer because P3HT has a good solubility in toluene (in which QDs are already dispersed) and there is a possibility that it would dissolve the already existing P3HT layer. Thermal inter-diffusion process forming BHJ of P3HT and QDs is confirmed by scanning electron microscope (SEM) in which QDs are observed to be diffused in to the polymer layer in the film annealed at 1200C at an optimized duration of 7 min. Photoluminescence (PL) studies of P3HT: QDs films confirm that the presence of QDs quenches the PL of pristine P3HT by an order of magnitude. It is a clear indication of charge transfer from donor to acceptor when desired BHJ is formed. With this approach we have been able to achieve power conversion efficiency (PCE) of 5.1% using P3HT: QDs inter-diffusion process. Further improved the device by incorporating single walled carbon nano tube (SWCNT) to P3HT: QDs cell. It is found that SWCNT acts as an absorber in the near infrared (NIR) region and makes the absorption spectrum much wider as compared to that of P3HT: QDs film. From AFM studies we found that there is a clear phase segregation of the QDs and SWCNT in the polymer matrix. The performance of SWCNT in P3HT: SWCNT: QDs solar cell has been examined in detail and a PCE of 5.4% is achieved.

***Keywords*-**Polymer Solar Cell, Thermal Inter Diffusion, Polymer Matrix, Absorption Spectrum, Quantum Dots.

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I. INTRODUCTION

The high electro negativity of ZnS/CdSe core shell Quantum Dot (QD) allows for the ultrafast charge transfer to each electrode and the dissociation of polymeric excitons. The presence of this nanomaterial enhances the efficiency of Organic Photovoltaic (OPV) due to highly conductive polymer-QDs film in comparison to the low conductivity of the photocatalyst pristine polymer film. Multiple excitons generation improves the device's charge collection efficiency and open circuit voltage (Voc), but the device's low efficiency—8 to 10% [2]—and instability remain significant obstacles for researchers studying OPV devices, which have a lower efficiency than silicon solar cells—25% [3]. The presence of a donor polymer that is conductive and an acceptor with a higher adsorption coefficient and a broad solar radiation absorption spectrum is one of the fundamental requirements for an OPV.

When compared to PCBM, which is an electron acceptor nanomaterial, ZnS/CdSe QDs have very little visible absorption (at about 575nm for QDs of size 5nm). We have already demonstrated that adding QDs increases absorption by roughly 70% while maintaining the same spectrum range. QDs and fullerene derivatives like PC60BM, which have a high electron affinity, aid in the dissociation of polymeric excitons, which improves the electrical output parameters of OPV devices. However, these nanomaterials have a high percolation threshold and low aspect ratio in the polymer matrix. Because of these disadvantages, high levels of doping (immediately >75%) occur, which can impair the polymer composites mechanical properties [4-6]. SWCNTs with a high electronic conductivity and low percolation threshold on the other hand, can be used to significantly improve the level of doping [7].

As a result, materials with high electron mobilities, conductivities, and affinities can be used as additives to boost the device's performance. With

this addition, polymer: QDs: SWCNT complex could be used to increase the effectiveness of OPV devices. The process of excitons dissociating will, in theory, be dependent on a sufficient potential difference in energy between the energy of polymers and nanomaterials and the energy of excitons binding. [9]. SWCNT aids in exciton dissociation and attracts the electrons produced in the poly(3-hexylthiophene) (P3HT) and QDs complex due to its low lowest unoccupied molecular orbital (LUMO) and appropriate potential energy level. As is well known, the hopping process is the mechanism of charge conduction in QDs. Additionally, QDs have more traps centers, which limits mobility and increases transportation costs [10]. SWCNT, an alternative is a ballistic conductor, which transports charged particles with less coulombic interaction and thus a lower rate of recombination.

Due to their high electron affinity and conductivity, SWCNT improves the efficiency of electron conduction to the electrode. With the aid of Fig. 1, in which the electrons are transported without scattering, it is possible to comprehend the ballistic electron conduction in SWCNT, which is well known. SWCNT is also an effective light absorber in the near infrared (NIR), which absorbs photon flux with lower energy. Due to the fact that trio materials absorb light in various spectral ranges, we will assume that P3HT: SWCNT: QDs composite is comparable to traditional triple junction solar cell [11]. Using the inter-diffusion process, the BHJ was created from a bilayer of QDs and P3HT: SWCNT composite. According to the photoluminescence (PL) measurements, QDs, the hybrid P3HT, and SWCNT film's PL is significantly more effectively quenched than that of P3HT film of pristine. This demonstrates that there was a sizable electron transfer from the SWCNT to the electrode [12]. Using an atomic force microscope, the topography of the QDs inter-diffused film was examined (AFM).

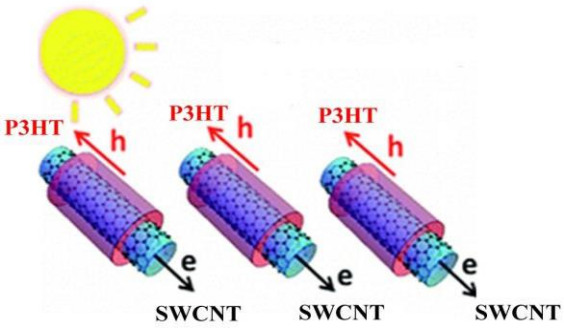

Fig. 1: Electron transport in composite of P3HT and SWCNT.

II. RELATED WORKS

Li et al. [13] show that incorporating functionalized SWCNTs embellished with ZnS/CdSe core-shell colloidal QDs (CQDs) into natural polymers improves the performance HSC. This improvement is due to SWCNTs' high electron-transporting capacity and ZnS/CdSe CQD's increased absorption in the visible region. Tenario et al. [14] proposed the incorporation of pure SWCNT into P3HT to produce Composite Films (CF) with varying SWCNT wt.%. The contact of the conjugated polymer and CNT could explain this phenomenon. The electrical conductivities of the CF improved as the SWCNT weight percentage increased, which was critical. Li et al. [15] introduced mild solution-process method to achieve carrier transfer into accumulating electrode. According to PL measurements, conjugating ZnO QDs with MWCNTs increased charge transfer effectiveness by more than 90%. The PCE of the UV photovoltaic cells was found to be greater than 1% in heterojunctions. Jindal et al. [16] used the solvothermal method to create the eco-friendly bulk heterojunction device with CuInS2/ZnS QDs. Using ultra violet photoelectron spectroscopy, bulk heterojunction hybrid devices were created using solar simulator. Characteristics of bulk heterojunction show that increasing the amount of CuInS2/ZnS QDs improves PCE.

Polymer/inorganic HSCs based on nanorods were created by Luo et al. [17]. By modifying composition, the PCE of hybrid solar cells can be significantly increased, reaching 2.58% and 2.79%, respectively. They performed better than the substrates of CdSe. As a result, formation and separation was increased, which improved the device's performance. Kumari et al. [18] introduced

graphene concentrations in polymer film range from 0 to 0.01% w/w for this intent. It is discovered that graphene has no negative effects on the composite film's absorption. About 95% of PL is quenched at a graphene concentration of 0.01% weight per weight. The electrical properties demonstrate that adding graphene improves the device's effectiveness by creating interconnected conducting pathways within the polymer matrix. At a graphene content of 0.005% w/w, the maximum efficiency is measured to be 1.5%.

Li et al. [19] demonstrated that introducing lead selenide (PbSe) CQDs to active material improves polymer solar cell efficiency by extending absorption into the infrared spectrum. Inorganic ligands and post-annealing conditions have been thoroughly investigated for their effects on system performance. Following optimization of these parameters, a solar cell made of Poly(3HT: PCBM:PbSe/Al) has a maximum PCE of 3.31% and 14.5% increase over the control device. Meherbian et al. [20] used spin coating to create ZnSQDs (spin-SILAR). Under single solar illumination, an improved ZnS QDs sensitized solar cell demonstrated a maximum short-circuit current of 10.53 mA/cm2. ZnS QD layer acts as a recombination-blocking and light-absorbing layer. Yu et al. [21] investigated antireflection polymer layer. According to data analysis, these layers have the ability to decrease cell surface transmittance and thus raise the amount of solar radiation that silicon can absorb without negatively impacting the photovoltaic junction. Jeong et al. [22] created a Si NT array that provided 13.4% improvement over the cell that uses the most well-known Si structure. Within the nanotubes, light is effectively trapped.

III. MATERIALS AND METHODS

ZnS/CdSe, P3HT and PEDOT: PSS along with QDs were used with SWCNT. To obtain fine electrodes, it was patterned by etching with concentrated HCl. The substrate was then cleaned using an ultrasonicator and isopropyl alcohol and acetone. This substrate was spin coated for 50 seconds at 4000 rpm with a thin film of PEDOT:PSS. To remove any remaining water in the PEDOT: PSS, the substrate underwent a 30-minute annealing process at 120°C. The solubility parameters of the chosen solvent and the solute are compatible. To create a homogeneous solution, the solution was ultrasonically treated for two to three hours.

The polymer was annealed at 10000C for about 20 minutes to remove any remaining solvent before ZnS/CdSe QDs were deposited on it. After that, the floating method [24] was used to deposit the QDs layer on top of and placed in oven for 7 minutes at an optimum temperature of 12000C to obtain QDs in polymer. A thermal evaporator was used to grow an Al electrode. To prevent Al atoms from migrating into the device, a layer is added between QDs and aluminum. The structures of the HSC produced by the above procedure are depicted in Fig. 2.

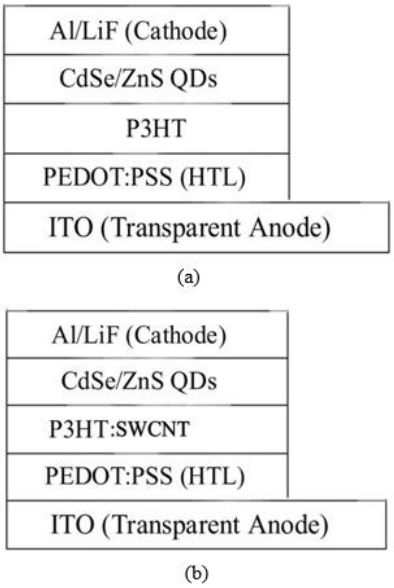

Fig. 2: Hybrid Solar Cell Structures (a) without SWCNT, (b) with SWCNT composite.

To serve as a baseline for comparison, we simultaneously created a C1 without SWCNT in the active layer. Spectro-Fluro-Photometer and double beam UV-VIS Spectrophotometer were used, respectively, to measure the samples' PL and absorption spectra. All measurements were performed without any device encapsulation in air at room temperature. Measurements were made using a TEM to determine the average size of aggregates.

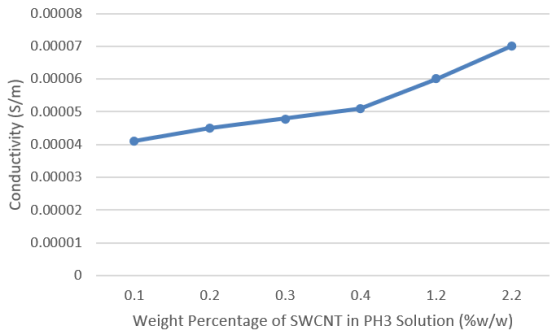

Fig. 3: Conductivity of the P3HT: SWCNT CF for various SWCNT concentration.

Prior to the creation of device, to optimize the SWCNT concentration in the polymer, conductivity measurements were used as shown in Fig. 3. The limit of percolation was discovered as 0.8% w/w. In our case, concentration of SWCNT in the polymer matrix is maintained at 0.5% w/w. Due to its large surface area, SWCNT can establish the greatest possible contact network with the polymer at very low percolation rates without disturbing the host polymer. For J-V measurements using a Keithley Source Meter, the conductivity of the films was found for various concentrations of SWCNT.

IV. RESULTS AND DISCUSSION

A. Optical Characteristics

As depicted in Fig. 4, It has been discovered that absorption is also increasing in the visible region. According to Geng et al. [24], polymer SWCNTs can be attributed to lower wavelength absorption. Clusters of SWCNT: ZnS/CdSe QDs may have created, which could explain the higher absorption observed in SWCNT-containing samples.

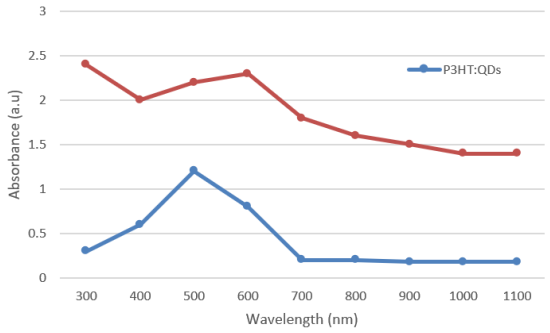

Fig. 4:Absorbance Analysis

Composite structure's PL measurements can be used to follow electron movement. PL of P3HT is quenched by QDs and then further quenched by SWCNT, it is rapidly transferred to SWCNT. SWCNT concentration has been optimized to achieve the greatest P3HT quenching of 0.5% w/w. Fig. 5 displays Photo Luminance (PL) spectrum of various polymer combinations. SWCNT structure is quenched by a factor of 15 at the optimized concentration of SWCNT (0.5% w/w). The charge transfer efficiency is indicated by the combination P3HT: ZnS/CdSe: SWCNT.

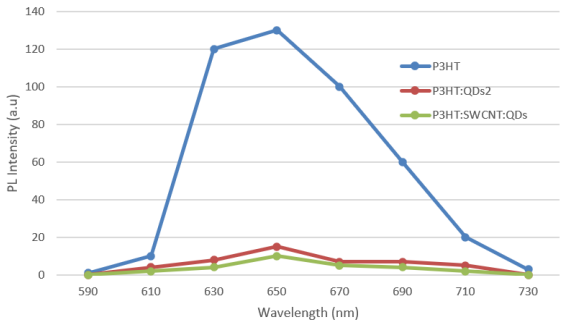

Fig. 5: Photoluminescence spectra for HSC.

B. Morphological Characteristics

The typical Atom Force Microscope (AFM) images for HSC are shown in Fig. 6. SWCNTs appear as thread-like structures, whereas QDs appear as white spots. Large QD aggregates have also been observed in some locations.

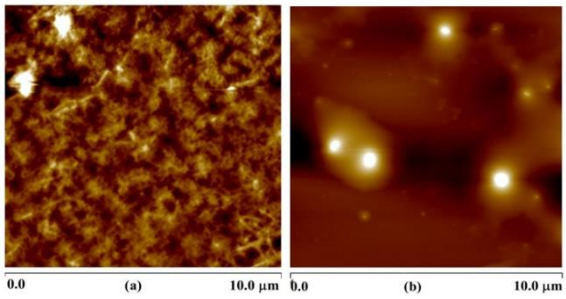

Fig. 6: AFM images (a) P3HT: SWCNT (b) P3HT: SWCNT: QDs

The bundles of SWCNT with P3HT polymer are seen in Fig. 7(b). The aggregate formation of P3HT: QDs of size 25nm to 40nm are also observed as shown in Fig. 7(c). The aggregate formation of controlled size also helps for transportation of electrons.

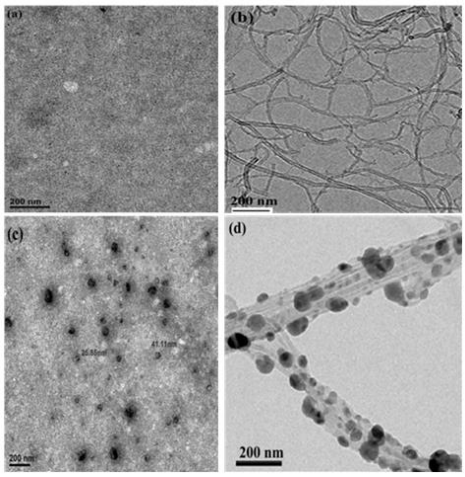

Fig. 7:(a)PristineP3HT,(b)P3HT: SWCNT composite, (c)P3HT: QDsaggregates, (d)P3HT: SWCNT: QDsstructure-TEMimages

It should be noted that SWCNTs shown in Fig. 7(d) are coated with the QDs and it is beneficial for transportation of charge to Al through SWCNT. The variation in HSC parameters with annealing duration is provided in Table 1. It is clear that the value of these parameters is directly proportional to the annealing time.

Table 1: Variation of HSC parameters with Annealing Time

Time (min)	V_{OC} (V)	P_{MAX} (mW)	J_{SC} (mA)	FF	PCE (%)
0	0.58	0.071	0.71	0.30	0.9
6	0.60	0.178	1.05	0.39	2.3
7	0.61	0.285	1.33	0.48	3.9
8	0.62	0.411	1.48	0.55	5.4
10	0.64	0.467	1.52	0.62	6.9

C. Electrical Characteristics

Energy level diagram of P3HT: SWCNT: QDs is depicted in Fig. 8. Photogenerated electrons from P3HT is shown in this figure. Through SWCNT, these electrons are gathered at Al. Similar to how P3HT's is easily accessible to the holes created in CdSe QDs' valence band. Through PEDOT: PSS, ITO collects these holes.

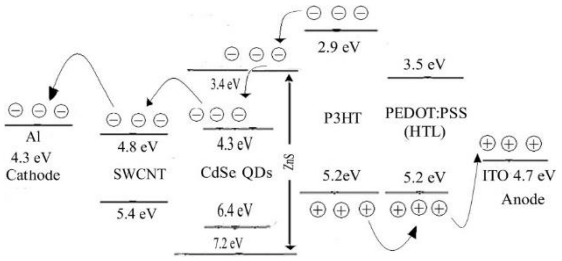

Fig. 8: Energy levels of HSC

When the temperature of the annealing process is increased, there is a variation in the electrical parameters of HSC. The value of these parameters gradually increases and then decreases after a threshold temperature. The electrical parameter variation with respect to annealing temperature is provided in Table 2. This calculation is made by increasing the temperature for 10 minutes duration.

Table 2: Variation of HSC parameters with Annealing Temperature.

Temp:	V_{OC} (V)	P_{MAX} (mW)	J_{SC} (mA)	FF	PCE (%)
27ºC	0.57	1.03	4	0.47	1.9
100ºC	0.73	4.14	10.9	0.52	4.4
150ºC	0.78	5.44	12.24	0.57	5.7
200ºC	0.58	2.49	8.42	0.50	2.3
250ºC	0.61	2.96	10.31	0.46	2.1

Fig. 9 displays J-V curves and maximum output power (P_{MAX}), of solar cells are observed to be better for cell C2. It is discovered that the VOC for the two devices, C2 and C1, is 0.75 and 0.7V, respectively. It is discovered that the JSC for cells C2 and C1 is~11mA/cm2 and 9.6mA/cm2, respectively. In contrast, it is discovered that the PMAX for cells C1 and C2 is 4.09mW/cm2 and 5.3mW/cm2, respectively. So, the cell's overall efficiency is improved by the increase in current. The efficiency of cell C2, which uses SWCNT as an electron transporter in the active layer, is found to be 5.4%, as opposed to C1's 4.1%. Additionally, it has been discovered that cells containing SWCNT have better fill factors (0.65 for cells C2 and 0.59 for cells C1). These values are very encouraging. In this instance, the P3HT: SWCNT solar cell's PCE is only 0.9%. But it increases very significantly with the addition of QDs and SWCNT.

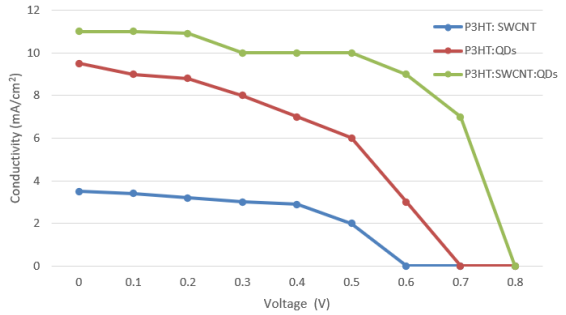

Fig. 9: J-V Characteristics of HSC

V. RESULTS AND DISCUSSION

The optical absorption, PCE and charge transfer of the P3HT: ZnS/CdSe QDs-based cell are improved by 4.1% to 5.4% by the addition of SWCNT. But in order to prevent short circuits (above the percolation limit) or poor charge transport (very low than the threshold limit), the concentration of SWCNT in the polymer matrix must be optimized. The proposed polymer-based HSC exhibit better electrical properties. The bandgap of the material affects a device's efficiency as well as Low bandgap materials (LBGPs). In comparison to P3HT and poly (3-octyl thiophene), proposed HSC demonstrate better light harvesting capability.

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