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Experimental and Theoretical Comparable Study of Pure and Zinc Porphyrin Surface Modified ZnO Nanorod Arrays for Hybrid Solar Cell Applications

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Abstract- Experimental and theoretical study Porphyrin-grafted ZnO nanowire arrays were investigated for organic/inorganic hybrid solar cell applications. Two types of porphyrin – Tetra (4-carboxyphenyle) TCPP and *meso*-Tetraphenylporphine (Zinc-TPP)were used to modify the nanowire surfaces. The vertically aligned nanowires with porphyrin modifications were embedded in graphene-enriched poly (3-hexylthiophene) [G-P3HT] for p-n junction nanowire solar cells. Surface grafting of ZnO nanowires was found to improve the solar cell efficiency. There are different effect for the two types of porphyrin as results of Zn existing. Annealing effects on the solar cell performance were investigated by heating the devices up to 225 °C in air. It was found that the cell performance was significantly degraded after annealing. The degradation was attributed to the polymer structural change at high temperature as evidenced by electrochemical impedance spectroscopy measurements.

Keywords- graphene, P3HT, ZnO Nanowire, Porphyrin,DFT, Solar Cells

I. **Introduction**

Organic and inorganic hybrid structures own advantages natural from both types of materials, such as the high charge transport with high mobility in inorganic materials and high absorption in visible region with low-cost processing of organic materials in addition to intrinsic flexibility.

They have fascinated attention for optoelectronic applications such as light emitting diodes (LEDs) and photovoltaics due to their exceptional properties(Abdulalmohsin *et al.*,2012). ZnO as thin films or nanostructures have been extensively investigated for applications in solar cells because it has wide band gap semiconductor, and use as window materials at the same time active n-type layers (Yin*et al.*,2017). The advantages behind using ZnO its low-cost, easy of deposition, lack of toxicity, and transparency in the visible region. Among various morphologies such as nanocrystals, nanowires, and nanoplates, ZnO nanonwires have shown their possible in the next generation solar cells. These nanowires can be used to enhance charge separation at the junction interface, improve charge collection as well as used as the nanoelectrode, so increase light absorption due to trapping effects. To increase the junction area, randomly distributed ZnO nanowires embedded in polymer and self-assembled ZnO nanorods/polymer core-shell structures have been investigated recently (Abdulalmohsin and Cui,2012; Lee *et al.*,2011).Although the junction interfaces can be significantly improved in these bulk junction configurations,It was inefficient charge transport in these structures because the embedded nanoparticles or nanorods so they isolated from the back electrode. Vertically aligned ZnO nanowire arrays embedded in polymers have been used to facilitate efficient charge collection due to their direct contact with the electrode (Abdulalmohsin*et al.*,2012; Lin *et al.*,2017; Ajee *et al.*,2017). ZnO nanowire arrays have also been widely studied for uses in dye-sensitized solar cells(Abdulalmohsin and Cui, 2012).

Poly (3-hexylthiophene) (P3HT) is a p-type polymer and an important organic material for solar cells. The drawback of P3HT is its low conductivity, which restricts charge collection efficiency. To improve the electrical properties, graphene has been added into P3HT as a hole collector . In general, the efficiency of polymer-inorganic cells based on ZnO nanorods and P3HT are still far from satisfactory (Zafar*et al.*,2017).

This deficiency is usually attributed to poor charge separation at the junction interface, which may be improved via a surface modification of ZnO NWs by organic molecules (Ajeel*et al.*,2017; Prima and Narula,2018; Abdulalmohsin *et al.*,2012). In our recent study, it is found that a combination of surface modification of ZnO NW arrays with porphyrin and graphene-enriched P3HT (G-P3HT) could help to improve solar cell performance, which resulted from the improved energy level alignment between ZnO and P3HT, enhanced charge inject at the junction interfaces, and efficient electron collection through ZnO NW arrays and hole collection via G-P3HT polymer (Abdulalmohsin and Cui, 2012)

In this work, it has been investigated the surface modification of ZnO nanowire arrays with two types of porphyrin (Tetra (4-carboxyphenyle) porphyrin (TCPP) or *meso*-Tetraphenylporphine(**(**zinc-TPP**)**) for solar cell applications and Theoretical calculation with and without Zinc atom in porphyrin have been studied for improving light harvesting efficiency ,and electron injection from the porphyrin in to the TiO2 conduction bands .In addition the study focus on molecular design of the Zinc porphyrin by density functional theory .The main point of improving the photovoltaic performance has focused on a relationship between electron injection into the ZnO .Our purpose in the present paper is to characterize the porphyrin modified ZnONW solar cells and study the effects of annealing on the solar cell performance. It was found that the surface modifications help to improve both open circuit voltage and short circuit current. Annealing at temperatures above the process temperature of 110 °C causes the cell performance to deteriorate continuously.

Possible mechanisms are studied by electrochemical impedance spectroscopy (EIS) and discussed in terms of polymer property change at elevated temperatures.

Ii. Experimental Details

The vertically aligned ZnO NW arrays were fabricated on FTO glass substrates (SPI Supplies) by a low temperature electrochemical method(E et al.,2017). The detailed fabrication procedures can be found elsewhere (Prima and Narula,2017).They were typically prepared in a two-step process. First, a layer of ZnO thin films was grown on the FTO substrates in zinc nitrate (Alpha Aessar) solution at 70 °C. Second, ZnO NW arrays were grown on top of the ZnO thin film 95 °C using an electrolyte containing zinc nitrate and hexamethylenetetramine in de-ionized water.

P3HT was synthesized by chemical polymerization of 3-hexylthiophene (3HT) monomer in the presence of anhydrous FeCl3 at room temperature (Liuet al.,2018). After the P3HT was obtained, graphene was added into P3HT by mixing 0.1 g P3HT and 5 mg graphene (from Cheap tubes) in 1 ml tetrahydrofuran (THF) to be sonicated at 60 °C for 2 h.TCPP or zinc-TPP was purchased from Sigma Aldrich and used as received without further purification. The TCPP or zinc-TTP dye of 0.0002 M was dissolved in THF at room temperature. After FTO/ZnO NWs were immersed in the porphyrin solution overnight, the TCPP or zinc-TTP grafted ZnO nanowires were rinsed by DI water, and dried by nitrogen gas.

The structure of hybrid solar cells containing ZnO NW arrays and polymer is shown in Figure 1(a). They were fabricated by depositing G-P3HT composites onto the TCPP or zinc TPP grafted ZnO NW arrays by a spin coating process with a speed of 1000 rpm for 1 min. Then the samples were annealed at 110 °C for 120 min to improve the infiltration of polymer. A contact electrode of 50 nm Au was deposited on top of the polymer surface by thermal evaporation at room temperature.

The structure and morphology of the as-prepared ZnO nanowire arrays and the nanowire/P3HT structures were characterized by scanning electron microscopy (SEM, JSM 7000F). Optical absorption spectra were measured by an Angstrom Sun Technologies TFProbe reflectometer. The photovoltaic properties were measured by monitoring current density–voltage (J-V) characteristics of solar cell devices under dark and illumination of AM1.5. A Keithley 2400 Source-Measure unit collected the data. Electrochemical impedance spectroscopy was measured by using a Gamry potentiostat

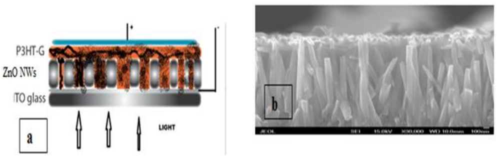


Fig. 1. Schematic diagram of organic-inorganic hybrid solar cells using surface modified ZnO NWs and G-P3HT (a) and the corresponding SEM cross section image of the nanowire arrays embedded in P3HT (b).

III. Computational Details

The optimized ground state geometries and electronic structures of natural dyes are performed by employing density functional theory (DFT) method using Gaussian 09 package(Ajeel et al.,2016). The unrestricted Becke's three parameter gradient-corrected exchange potential and the Lee- Yang-Parr gradient-corrected correlation potential (UB3LYP), and 6-31+G(d,p) have been used for all the calculations(E et al.,2017; Yang et al.,2019).

III. Results and Discussion

1) Experimental Part

Figure 1(b) displays a cross section image of the ZnO nanowire array embedded in P3HT polymer. Some of the nanowires are still visible in the image. However, most of them covered and infiltrate .As it can be seen that the nanowires were wrapped by P3HT .The SEM measurements indicate that the P3HT infiltrated deeply inside the gaps among the ZnO NWs by using this solution process with spin Coater Technic, which guarantees the construction of good heterojunctions between the two semiconductors.

To see the effects of porphyrin on the optical properties of ZnO Nw, optical absorption spectra of ZnO NW films modified with Porphyrin and zinc-Porphyrin were measured and compared as shown in figure. 2.

As shown in figure. 2, The zinc-Porphyrin/ZnONW showed strong absorptionpeaksat 432,519,559,600and 620 nm which cover the strong visible absorption peaks specially at 556nm and UV strong peak at 432 nm and there are number of small peaks in the visible range see figure. 2 which is similar to that reported in the literature (Paredes-Gil*et al.*,2017). The modification of ZnO NW with porphyrin exhibits a strong increase in absorption around 432 nm - 620 nm which is attributed to the additional absorption of the coated porphyrin. Similar effect was observed on porphyrin coated ZnO NW although has strong and main peak at 420 nm and number of small peaks at513 nm,546 nm,590 nm and 646 nm in visible region .One can be seen that the Zinc atoms make big differences in the amount of light which absorbed .

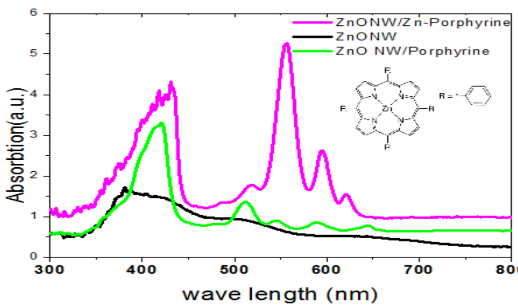


Figure. 3. Current density vs. voltage measured on G-P3HT/ZnO nanowire arrays with and without porphyrin grafting.

Figure 3 shows the typical J-V characteristics of the hybrid structures based on G-P3HT and ZnO NW arrays modified with TCPP and Zinc TTP porphyrins. Both devices show similar photovoltaic effect. The ZnO NWs grafted with zinc- porphyrin show better PV performance than that modified with pure porphyrin.

The open circuit voltage V_{oc} was increased from 0.479 V for solar cells with porphyrin to 0.505 V for that with zinc-porphyrin. The corresponding current density J_{sc} was also increased slightly from 1.67 to 1.87 mA/cm^2. Note that the solar cells based on ZnO NWs without porphyrin modification has very poor performance where the current density J_{sc} was 0.214 mA/cm^2 and the open circuit voltage V_{oc} was 0.149 Volt(Fu*et al.*,2018). Improvement in PV performance was observed in the modified ZnO nanowire arrays by both porphyrins.

A few factors associated with the surface modification may result in the increase of solar cell efficiency by porphyrin modification (Fu*et al.*,2018).

As shown in the absorption spectroscopy, the porphyrin grafting results in additional absorption in the near UV and visible regions, and therefore improves the energy harvesting. In addition, it is generally accepted that the V_{oc} for organic bulk heterojunction solar cells depends on the energy difference between the LUMO level of the electron acceptor and the HOMO level of the electron donor. The addition of porphyrin on the ZnO surface may form an intermediate band between P3HT and ZnO, which enables easier charge transfer through the junction interfaces.

The dense nanowires with length up to micrometers pentrate into P3HT, which not only helps to transport the electron charge efficiently to the electrode but also remarkably reduces the distance needed for the excitons in P3HT to reach the junction interface. This structural configuration would help to reduce the charge recombination rate.

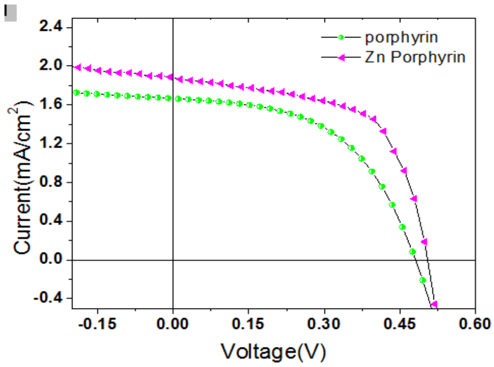


Figure. 3. Current density vs. voltage measured on G-P3HT/ZnO nanowire arrays with and without porphyrin grafting.

Table1. Short circuit current, open circuit voltage, fill factor and Efficiency of P3HT+G/ZnO NWs modified with TCPP and TPP.

System	I_{sc}(mA/cm^2)	V_{oc}(Volt)	FF	Efficiency
Porphyrin	1.67	0.479	0.57	0.456%
Zinc porphyrin	1.868	0.505	0.59	0.558%

From the J-V curves, series (R_s) and shunt resistance (R_{sh}) can be calculated using (Keawin*et al.*,2017),

From the ideal I-V relationship for organic solar cells

$$I=\frac{I_L-\frac{V}{R_{sh}}}{1+\frac{R_s}{R_{sh}}}-\frac{I_0}{1+\frac{R_s}{R_{sh}}}\cdot\left(e^{\frac{V-IR_s}{\frac{nKT}{q}}}-1\right) \text{----- (1)}$$

The series resistance calculated from equation (1) where V greater than V_{oc},

The Shunt resistance calculated from equation (1) where V approach to zero

$$R_s \approx \left(\frac{I}{V}\right)^{-1} \quad \text{for } V>V_{oc} \text{ -------- (2)}$$

$$R_s \approx \left(\frac{I}{V}\right)^{-1} \quad \text{for } V \longrightarrow \text{Zero -------- (3)}$$

From ideal solar cells when the Series Resistance approach to Zero ,the Shunt Resistance should be close to infinity from the Table 2 decreases in Series resistance with increase annealing temperature indicate worse electron transport in active layer

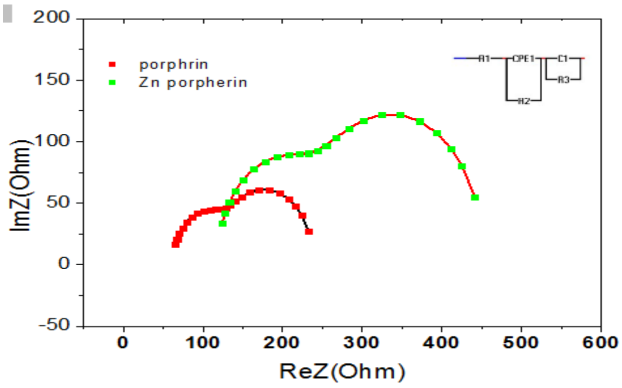
$$R \approx (1/V)^{-1} \qquad (4)$$

As V is larger than V_{oc} and approaches to zero, respectively. An ideal solar cell has a R_s close to zero and a R_{sh} approaches to infinity.

the calculated R_s and R_{sh} from porphyrin devices. As expected, the series resistance of porphyrin greater than Zn porphyrin while the shunt resistance decreases for Zn-Porphyrin where Shunt Resistance increase from 3100 Ohm to 5600 Ohm and the Series Resistance reduced from 186 Ohm for porphyrin to 78 Ohm for Zn porphyrin . This change is ascribed to the existing of Zinc in porphyrin which help to increase the absorption density to be in more strong than pure porphyrin as well as reduced the series resistivity due to increase the number of electrons in the porphyrin which resulting in good solar cell performance.

Electrochemical impedance spectroscopy was measured in order to further understand the impact of the annealing on the solar cell performance. Figure 4 shows the EIS spectra obtained on the solar cell structures after annealing at different temperatures. The measurements were carried out at 0.3 V and a frequency range of 0.005 to 1 MHz under illuminated 1.5 AM. The data can be used to directly quantify the charge-transfer process associated with the annealing. The EIS spectra from the cells annealed at 200 °C and 225 °C show semi-circle curves while the as prepared and annealed at 150 °C and 175 °C exhibit double semi-circle characteristics. The double semi-circle feature may imply the role of the porphyrin played in the solar cells.

The EIS showed a single semi-circle feature. These EIS spectra show that the series resistance decrease as the Zinc in the structure of porphyrin , which agrees with the data obtained from the J-V curve measurements of the solar cells.



. Fig. 4. Electrochemical impedance spectroscopy of G-3HT/Porphyrin/ZnO NW solar cells for Zn-porphyrin ,and pure porphyrin.

The solid squares are experimental data and the solid curves are simulations using an equivalent circuit shown in the inset of the figure.

2) Computational part

In our system, the porphyrin consisted of 73 atoms (44carbon, 4 Nitrogen,1 Zinc and 29 hydrogen atoms at the edge of the porphyrin) with bond lengths 1.429 , 1.5007 and 1.07 ˚A for C –C ,C –N, and C –H respectively. Porphyrin were considered without Zn and withZn atom in the center of porphyrin molecule. The electronic properties, DOS analysis, and the calculations of the energies were performed using the Gaussian 09 program package, with the DFT at the B3LYP level and the 3–21 G basis set(Mohammed et al.,2017). The relaxation and optimization structures of all of our systems consider the first step of our investigations and calculations before and after adding Zn atom. Theoretically, it was investigated how the Zn atom in the center affect the electronic properties of the porphyrin,calculate the electronic band gaps (E_g), dipole moments (α) total energy (E_T), HOMO energies (E_{HOMO}), Fermi level energies (E_{FL}), LUMO energies (E_{LUMO}), and the change of band gaps (E_g).

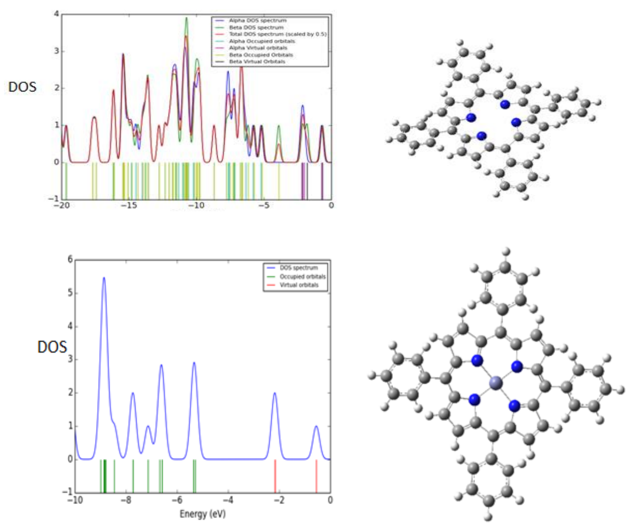


Fig.7 Optimization of pristine Zn-porphyrin and its DOS .

The optimization structure with geometers and DOS of pristine porphyrin and Zn-Porpheren are explained in fig.5 and fig.6. there are three types of bond lengths-C and C-N,and C-H bonds that can be recognized ; ordered 1.4,1.5,and 1.07 respectively .It was studied the electronic properties of pristine and ZincC porpherene ,such as the DOS ,electronic band gap,and Fermi level energy ,as shown in fig.5 and table 3 it has beenfound out that the electronic band gap (3 eV) and (1.9 eV) respectively for pristine and porphyrin Zn are in agreement with (Paredes-Gil*et al.*, 2017).After that it is figured out how the porphyrine and porphyrine Zn are appropriate to use them as a dye in adye sensitive solar cells application

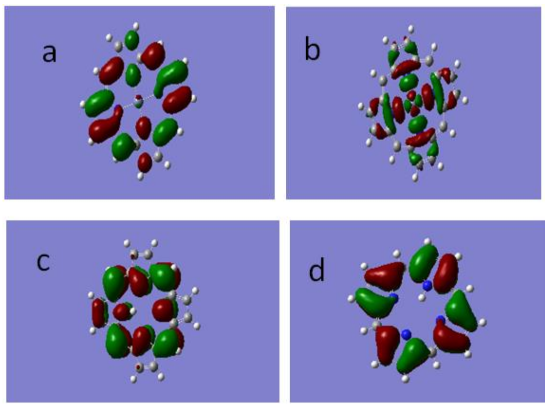


Fig.7.influence of chemical substitution of (a) ,(b)porphyrin ZinC ,(c),(d) pure porphyrin on chemical

structures , on electronic structure .the molecular orbital were varied with energy level states atHOMO and LUMO

.

Our extracted parameters indicate the value of the electronic band gaps (E_g), dipole moments (α), total energy (E_T), HOMO energies (E_{HOMO}), Fermi level energies (E_{FT}), LUMO energies (E_{LUMO}), and change of band gaps (ΔE_g) in the pristine of porphyrin and Porphyrin-Zn

Table2. shows E_{HOMO} and E_{LUMO} energies.

System	?? (eV)	α(Debye)	E_T (eV)	E_{HOMO}	E_{LUMO}	? E_g	Wavelength (nm)
Porphyrin	2.88	0.1	36	-5.25	-2.37		425
Porphyrin - Zn	2.19	5	101	-5.56	-3.366	0.69	558

We compared the electronic properties of pristine porpherene with theZn- porphyrin case ,it has found out that the $E_g$is affected by adding Zn atom in the center of the pristine porphyrin.In addition the results indicate that the E_g for pristine is wider than Zn-Porphyrin ,then ,we found out that the Zn- porphyrin improved the electronic properties of the porphyrin .The energy gap is changed from 2.88 eV in the pristine porphyrin to 2.19 eV for Zn-porphyrin therefore the absorption spectrum shifted from 425 nm to 558 nm which represent the peak of most absorption wavelength so the power conversion efficiency increase from 0.456 to 0.558 These results indicate that the Zn- porphyrin has more effect on the electronic band gap of the porphyrin if we compared with the pristine case. Another important result concerns the dipole moments (μ) of the porphyrin .Our results show that the dipole moment value is highly changed where it is changed from 0.1 to 5, so the properties can be developed through the electrostatic interaction due to the dipole – dipole interaction between or polar species there can be increase physisorption energy then increase the stability of the device.We also calculated the total energies of the porphyrin with and without Zinc atom. The total energy (E_T) plays an important role in the assessment in the stability of the structure. The total energy (E_T) is increase with adding Zinc atom which are used in this study in the above comparing with the pristine case, as shown in Table 3 . The porphyrin structure becomes more stable due to $E_T$being increase from 36 eV to 101 eV with Zinc atom structure. That means the Zincporphyrin have more amount of light absorption and cover wide spectrum of wavelength in the presence Zinc atom. Then the total energy for the porphyrin withthis atom is increased due to the interaction force being dependent on bonding between the Zinc atom and four atom of Nitrogen make the system molecules more stable and wider spectrum absorption. Similarly, our results show that a changing of electronic band gap can play an importantrole in absorption spectrum of light to be very good candidate for using the Zinc porphyrin as dye in solar cells in both hetrostructure solar cells and dye sensitive solar cells .

3) DFT-based solar cells modeling :

Our solar cells analysis has been analyzed from DFT data of porphyrin .the charge transfer rate from porphyrin to the ZnO NW surface can be determined using the general Marcus theory (Roy et al.,2017)
The light harvesting efficiency (LHE)

$$LHE = 1 - 10^{-f} \quad \text{-----------(1),}$$

where f is the oscillating strength
The theoretical open circuit voltage can be expressed as given in eq (2)

$$eV_{0c} = E_{F,n} - E_{LUMO} \quad \text{---------------(2)}$$

where EF,n is a quasi fermi level of ZnO
Short circuit current of the solar cells theoretically in eq (3)

$$J_{sc} = \int LHE(\lambda).\phi_{injection}.\eta_{injection} d\lambda \quad \text{-----------(3)}$$

where $\phi_{injection}$ which is free energy of change of electron injection

And $\eta_{injection}$ which is ratio of electron injection
Improve the interface structure between the ZnONW and the porphyrin will support the inhibition recombination between the electrons and holes .Its yield increase the short circuit current and the power conversion efficiency .
The photovoltaic performance affected by distribution of electron density on the electronic structure at HOMO ,LUMO and the HOMO-LUMO gap which is important factor to make performance under control our pure porphyrin and Zinc porphyrin have been investigated by quantum calculation using DFT.Fig.8 shows the molecular orbital with energy levels at HOMOand LUMO .Addition role of chemical substitution such as Zinc atom in the porphyrin ring as electron donating affinity was shown in figure 8 there was a lack of uniformity in electronic structure density ,which caused to separate considerable splitting of degenerated energy levels at the HOMO and next HOMO with a decrease of energy levels at HOMO,increase of energy levels at LUMO and a wide band gap between HOMO and LUMO .In conclusion that a strong accepting Zinc atom would increase of charge transfer .The exciting of Zinc atom provides to control the electronic donating and accepting affinity. The Zinc porphyrin structure has a great influence on the photovoltaic propertiessuch as open circuit voltage , short circuit current ,and power conversion efficiency .The charge transfer behavior would be increase from improvement of effective separation with injection of electron exaction at interface between the porphyrin and ZnO NW .In addition to increase the diffusion of porphyrin adsorbed on to ZnONW would guide to increase diffusion of exciton .The separated electron would inject from ZinC porphyrin in increase rate of injection than pure porphyrin. The new molecular design of Zinc porphyrin is important factor to increase the light

charge separation .Electronic transportation for improving conversion efficiency in the solar cells.

IV. Conclusions

Graphene enriched P3HT (G-P3HT) and porphyrin grafting of the ZnO nanowire surface have been studied for applications in hybrid solar cells. Two types of porphyrin (Pure and Zinc porphrin) have shown positive impact on the solar cell performance. Influence of adding Zinc to porphyrin as donating efficiency in the hetrojunction solar cells on the photovoltaic properties were investigated by light –induced current density by using density functional theory. Electrochemical impedance spectroscopy was also measured in order to understand the effect of annealing on the solar cell devices.

VI. Acknowledgment

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