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(Prof. Satyabrata Jit) Supervisor Department of Electronics Engineering IIT (BHU), Varanasi (Dr. Bratindranath Mukherjee) Co-Supervisor Department of Metallurgical Engineering IIT (BHU), Varanasi

DECLARATION BY THE CANDIDATE

I, Amit Kumar, certify that the work embodied in this thesis is my own bonafide work and carried out by me under the supervision of Prof. Satyabrata Jit and Dr. Bratindranath Mukherjee from "21/07/2015" to "12/04/2021", at the Department of Electronics Engineering, Indian Institute of Technology (BHU), Varanasi. The matter embodied in this thesis has not been submitted for the award of any other degree/diploma. I declare that I have faithfully acknowledged and given credits to the research workers wherever their works have been cited in my work in this thesis. I further declare that I have not willfully copied any other's work, paragraphs, text, data, results, *etc.*, reported in journals, books, magazines, reports, dissertations, theses, *etc.*, or available at websites and have not included them in this thesis and have not cited as my own work.

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(Prof. Satyabrata Jit) Supervisor Department of Electronics Engineering IIT (BHU), Varanasi (Dr. Bratindranath Mukherjee) Co-Supervisor Department of Metallurgical Engineering IIT (BHU), Varanasi

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Date:

(Amit Kumar)

Dedicated To My Family

CONTENTS

List of Figure	25	xvii-xix
List of Tables	5	xxi
List of Abbre	viations	xxiii-xxiv
List of Symbo	bls	xxv-xxvi
Preface		xxvii-xxix
CHAPTER Introduction	1 and Scope of the Thesis	1-36
1.1	Introduction	3
1.2	Photovoltaic Devices	4
1.3	Organic photovoltaic (OPV) Devices	5
1.3.1	Materials for Organic Photovoltaic Cells	6
1.3.2	Type of Organic Photovoltaic Devices	10
1.3.2.1	Single Layer OPV Device	10
1.3.2.2	Bilayer Heterojunction OPV Device	11
1.3.2.3	Bulk Heterojunction (BHJ) OPV Device	13
1.3.3	Working Principles of BHJ OPV Device	15
1.3.3.1	Light Absorption	16
1.3.3.2	Exciton Diffusion	18
1.3.3.3	Exciton Dissociation	18
1.3.3.4	Charge Collection	19
1.3.4	Equivalent Circuit of BHJ OPV Devices	20
1.3.5	Parameters of BHJ OPV Devices	22
1.3.5.1	Short Circuit Current (Isc)	23
1.3.5.2	Open Circuit Voltage (Voc)	24
1.3.5.3	Fill Factor (FF)	25

1.3.5.4	Power Conversion Efficiency (PCE)(η)	26
1.4	Literature Review	27
1.4.1	Review of BHJ OSCs	27
1.4.2	Review of PCDTBT:PCBM based BHJ OSCs	30
1.4.3	Major Observation from the Literature Review	32
1.5	Challenges in the BHJ OSC	33
1.6	Motivation and Problem Definition	34
1.7	Scope of the Thesis	34

CHAPTER 2

37-53

Effect of PQT-12 Interface Layer on the Performance of PCDTBT:PC₆₁BM Bulk Heterojunction Organic Solar Cells

2.1	Introduction	39
2.2	Experimental Details	41
2.2.1	Materials and Synthesis	41
2.2.2	Device Fabrication	42
2.3	Results and Discussion	44
2.3.1	Thin Film Characterization	44
2.3.2	Solar Cell Characterization	47
2.4	Conclusion	52

CHAPTER 3 55-68 Effects of HTL and ETL Thicknesses on the Performance of PQT-12/PCDTBT:PC₆₁BM/ZnO QDs Organic Solar Cells

3.1	Introduction	57
3.2	Experimental Details	58
3.2.1	Materials and Synthesis	58

3.2.2	Solar Cell Fabrication	58
3.3	Results and Discussion	61
3.3.1	Optical Characterization	61
3.3.2	Electrical Characterization	63
3.4	Conclusion	68

CHAPTER 469-83Synergistic Effect of CdSe Quantum Dots (QDs) and PC61BM inPCDTBT:PC61BM:CdSe QDs Bulk Heterojunction Based Organic Solar Cells

4.1 Introduction 71 4.2 **Experimental Details** 72 4.2.1 Materials and Synthesis 72 4.2.2 Solar Cell Fabrication 73 4.2.3 Film and Device Characterization 75 4.3 **Results and Discussion** 75 4.3.1 **Optical Characterization** 76 4.3.2 **Electrical Characterization** 79 4.4 Conclusion 82 **CHAPTER 5** 85-92 **Conclusion and Future Scope**

5.1	Introduction	87
5.2	Chapter-Wise Major Observations	87
5.3	Future Scope of Work	90
Referenc	es service and the service of the se	93-110
Author's	Relevant Publications	111-112

Contents

LIST OF FIGURES

Figure 1.1:	Renewable energy resources.	4
Figure 1.2:	The comparative energy band diagram for conjugated polymer and conventional inorganic semiconductor.	8
Figure 1.3:	(a) Device structure and (b) Energy band diagram of single- layer OPV cell.	11
Figure 1.4:	(a) Device structure and (b) Energy band diagram of bilayer heterojunction OPV device.	12
Figure 1.5:	(a) Device structure and (b) Energy band diagram of bulk heterojunction (BHJ) OPV device.	14
Figure 1.6:	Bulk heterojunction organic (BHJ) OPV device with buffer layer.	15
Figure 1.7:	Working of BHJ OPV device: Step 1 to 4.	16
Figure 1.8:	Extraterrestrial solar spectrum (AM0, gray) and terrestrial solar spectrum (AM1.5, blue).	17
Figure 1.9:	Equivalent circuit of OPV device under (a) Dark and (b) Solar light.	22
Figure 1.10:	Current-voltage (I-V) characteristics of BHJ OPV.	23
Figure 1.11:	Maximum limit for open circuit voltage in OPV.	25
Figure 1.12:	Factors influencing the open circuit voltage in OPV.	25
Figure 1.13:	Comparison of power conversion efficiency of cell 1 and cell 2.	27
Figure 2.1:	Synthesis process of ZnO QDs.	42
Figure 2.2:	The schematic diagram of floating film transfer method (a) Dropping of PQT-12 on hydrophilic solution (ethylene glycol and glycerol in 1:1 ratio), (b) Thin film of PQT-12 over liquid surface, (c) Transferring of film on substrate, (d) PQT-12 coated substrate and (e) Empty space in PQT-12 film over liquid surface.	44
Figure 2.3:	Device structure of fabricated OSCs (a) Device 1 and (b) Device 2.	45
Figure 2.4:	Energy band diagram of (a) Device 1 and (b) Device 2.	46

Figure 2.5: Absorption spectra of ZnO/Active layer and ZnO/Active 47 layer/PQT-12 films. 47 Figure 2.6: Photoluminescence (PL) of ZnO/Active. spectra ZnO/Active/PEDOT:PSS, and ZnO/Active/POT-12/PEDOT:PSS films taken from glass side at an excitation of 540 nm. Current density versus voltage (J-V) characteristic of the 49 Figure 2.7: fabricated OSCs. Figure 2.8: External quantum efficiency of the fabricated OSCs. 50 Figure 2.9: (a) Nyquist plot of the fabricated OSCs under dark condition, 52 (b) Equivalent circuit of the OSCs under dark, (c) Nyquist plot of Device 2 under dark and light illumination, and (d) Equivalent circuit of the Device 2 under dark and light illumination. Figure 3.1: (a) FTM deposition steps for PQT-12 film and (b) Energy band 60 diagram for the OSCs structure. Figure 3.2: HRSEM cross-sectional image of the optimized OSC structure 60 without Ag and complete OSC device structure in the inset. Figure 3.3: Absorbance of PQT-12 and PCDTBT:PC₆₁BM film. 61 Figure 3.4: Transmittance of ZnO QDs thin film with different thicknesses. 62 Figure 3.5: EOE characteristics for different HTL thicknesses with fixed 62 ZnO of 20 nm. Figure 3.6: EQE characteristics for different ETL thicknesses with fixed 63 POT-12 of 20 nm. J-V characteristics of solar cells for fixed ETL thickness of 20 Figure 3.7: 65 nm and different PQT-12 thicknesses of 20 nm, 40 nm, and 60 nm. Figure 3.8: J-V characteristics of solar cells for a fixed PQT-12 based HTL 65 thickness of 20 nm with four different ZnO QDs based ETL thicknesses of 20 nm, 25 nm, 30 nm, and 35 nm. Figure 3.9: J-V characteristics of device with 20 nm and 35 nm of PQT-12 66 and ZnO QDs, respectively to realize seven days stability. **Figure 3.10:** Nyquist plot with variation in PQT-12 thickness with fixed 67 ZnO QDs of 20 nm. **Figure 3.11:** Nyquist plot with variation in ZnO QDs thickness with fixed **68** PQT-12 of 20 nm.

Figure 4.1:	Synthesis process of CdSe QDs	73
Figure 4.2:	Device structure (a) Binary OSC without CdSe QDs (b) Ternary OSC with CdSe QDs.	75
Figure 4.3:	The absorbance in ZnO QDs thin film, CdSe QDs thin film, ZnO QDs/PCDTBT:PC ₆₁ BM and, ZnO QDs/PCDTBT:PC ₆₁ BM:CdSe QDs.	77
Figure 4.4:	Photoluminescence (PL) spectra of PCDTBT:PC $_{61}$ BM and PCDTBT:PC $_{61}$ BM:CdSe QDs.	77
Figure 4.5:	Energy band diagram (a) Binary OSC without CdSe QDs, and (b) Ternary OSC with CdSe QDs.	78
Figure 4.6:	Ternary thin film made of PCDTBT, PC61BM, and CdSe QDs. The charge carrier transport through CdSe QDs due to better band alignment.	78
Figure 4.7:	The external quantum efficiency of the fabricated binary and ternary OSC devices.	79
Figure 4.8:	J-V characteristics of the fabricated binary and ternary OSCs.	79
Figure 4.9:	Nyquist plot of binary and ternary OSC devices under 1 sun illumination at zero applied voltage.	81
Figure 4.10:	Frequency vs. imaginary part of impedance (Z_2) of the binary and ternary OSC devices.	82
Figure 4.11:	Frequency vs. real part of impedance (Z_1) of the binary and ternary OSC devices.	82

LIST OF TABLES

Table 2.1:	Performance parameters of the OSC devices.	49
Table 2.2:	Reverse saturation current of the OSC devices.	49
Table 3.1:	Photovoltaic Parameters with Varying PQT-12 Thickness	64
Table 3.2:	Photovoltaic Parameters with Varying ZnO QDs thickness.	64
Table 3.3:	Seven days analysis of the device with 20 nm and 35 nm of PQT-12 and ZnO QDs, respectively.	66
Table 4.1:	Photovoltaic parameters of the binary and ternary OSCs	80

LIST OF ABBREVIATIONS

Abbreviation	Details
OPV	Organic photovoltaic
OSC	Organic solar cell
ВНЈ	Bulk heterojunction
EPBT	Energy payback time
EQE	External quantum efficiency
MEH-PPV	Poly[2-methoxy-5-(2'-ethylhexyloxy)-1,4-phenylene vinylene]
PCDTBT	poly[N-9'-hep- tadecanyl-2,7-carbazole-alt-5,5-(4',7'-di-2-thienyl-2',1',3'-ben- zothiadiazole)]
РСВМ	[6,6]-phenyl- C_{61} -butyric acid methyl ester
ETL	Electron transport layer
HTL	Hole transport layer
РЗНТ	Poly(3-hexylthiophene)
PQT-12	Poly(3, 3 ^{'''} -dialkylquaterthiophene) or
	Poly(3,3 ^{'''} -didodecylquaterthiophene)
FTM	Floating-film transfer method
IL	Interface layer
НОМО	Highest occupied molecular orbital
LUMO	Lowest unoccupied molecular orbital
AM	Air mass
PBTTT	Poly[2,5-bis(3-tetradecylthiophen-2-yl)thieno[3,2- b]thiophene]
PEDOT	Poly(3,4-ethylenedioxythiophene)
PSS	Polystyrene sulfonate
eV	Electron volt
V ₂ O ₅	Vanadium oxide
PPV	Poly(p-phenylene vinylene)

TiO ₂	Titanium dioxide
PCE	Power conversion efficiency
MDMO-PPV	([2-methoxy-5-(3',7'-dimethyloctyloxy)]-1,4- phenylenevinylene)
HRSEM	High resolution scanning electron microscopy
UV-Vis	Ultraviolet-visible
PL	Photoluminescence
ZnO	Zinc oxide
PET	Polyethylene terephthalate
CdSe	Cadmium selenide
QDs	Quantum Dots
SnO ₂	Tin oxide
Au	Gold
Ag	Silver
Al	Aluminum
MoO ₃	Molybdenum trioxide
ITO	Indium-doped tin oxide
FTO	Fluorine-doped tin oxide
Si	Silicon
In_2O_3	Indium oxide
MEA	Monoethanolamine
PVDF	Polyvinylidene fluoride
DI	Deionized
IPA	Isopropanol alcohol

Symbol	Details
λ	Wavelength
П	Power conversion efficiency
n	Ideality factor
R	Responsivity
α	Absorbance coefficient
IV	Current-voltage
JV	Current density-voltage
Eg	Energy band gap
IP_D	Ionization potential of the donor
EA_A	Electron affinity of the acceptor
E_B	Binding energy of the excitons
μ	Mobility
E _{HOMO}	Energy level of HOMO
ELUMO	Energy level of LUMO
е	Charge of electron
I _{dark}	Dark current
I _d	Diode current
I _{so}	Reverse saturation current
I_{ph}	Photo generated current
Jo	Reverse saturation current density
V_T	Thermal equivalent voltage
Rs	Series resistance
Rsh	Shunt resistance

LIST OF SYMBOLS

Isc	Short circuit current
Jsc	Short circuit current density
Voc	Open circuit voltage
FF	Fill factor
Vm	Maximum voltage
Im	Maximum current
Pmax	Maximum output power
Pin	Input incident power

PREFACE

Bulk heterojunction (BHJ) based organic solar cells (OSCs) are gaining greater attention for clean energy production due to various features, namely low-cost, easy fabrication process, the feasibility of solution process, mechanical flexibility, nontoxicity, and biodegradability. Recently, the low bandgap polymer, poly[N-9'-heptadecanyl-2,7-carbazole-alt-5,5-(4',7'-di-2-thienyl-2',1',3'-benzothiadiazole)] (PCDTBT) has been considered to be more suitable p-type donor polymer for the OSC. The PCDTBT is blended with the commonly used acceptor polymer $PC_{61}BM$ for the fabrication of OSC and provides better stability as well as improved photovoltaic parameters. Considering the above aspects, the present thesis is focused to fabricate and characterize the PCDTBT:PC₆₁BM active layer based BHJ OSC by modifying the interface layer, transport layers, and the photoactive layer. The works of the thesis are intended to enhance the photovoltaic parameters through thin film engineering. The thesis consists of five chapters which are briefly outlined in the following sentences.

Chapter-1 introduces the inorganic and organic semiconductors and charge conduction mechanism through them. A brief discussion on solar cells is included. Further, various types of organic solar cells, including the BHJ OSC, are discussed along with working principles and important photovoltaic parameters. A detailed literature survey followed by the scope of the present thesis has been finally outlined in this chapter.

Chapter-2 reports the PQT-12 polymer-based interface layer (IL) effect for the improvement in the photovoltaic parameters of the BHJ OSC. The floating film transfer method (FTM) is adopted for the deposition of PQT-12 thin film. Two distinct BHJ

OSCs have been fabricated in the device structure of ITO/ZnO QDs/PCDTBT:PC61BM/PEDOT:PSS/Ag and ITO/ZnO QDs/PCDTBT:PC61BM/PQT-12/PEDOT:PSS/Ag for the comparative study. The effect of PQT-12 IL has been investigated by several characterizations, namely current-voltage characteristics, absorbance, photoluminescence (PL), impedance spectroscopy, and external quantum efficiency. The OSC with the PQT-12 based IL has shown improved photovoltaic parameters.

Chapter-3 investigates the effect of thickness variations of the electron transport layer (ETL) as well as hole transport layer (HTL) on the performance of PCDTBT:PC₆₁BM based BHJ OSCs. The BHJ OSCs are fabricated in ITO/ZnO QDs/PCDTBT:PC₆₁BM/PQT-12/Ag structure, where ZnO QDs and PQT-12 are used as ETL and HTL, respectively. ZnO QDs ETL has been deposited by a solution-processed spin coating method, whereas PQT-12 HTL has been deposited using the FTM technique. The best OSC device performance has been obtained with the 35 nm ZnO QDs and 20 nm PQT-12 thicknesses.

Chapter-4 deals with the fabrication and characterization of two distinct BHJ OSCs in the device structures, ITO/ZnO QDs/PCDTBT:PC₆₁BM/MoO₃/Ag and ITO/ZnO QDs/PCDTBT:PC₆₁BM:CdSe QDs/MoO₃/Ag. The synergistic effect of CdSe QDs and PC₆₁BM is investigated in the ternary OSC device, where ZnO QDs and MoO₃ are used as ETL and HTL, respectively. The device structure, ITO/ZnO QDs/PCDTBT:PC₆₁BM:CdSe QDs/MoO₃/Ag has shown the improved photovoltaic parameters compared to other OSCs described in Chapter-2 and Chapter-3. The maximum efficiency of 5.02% is achieved due to the synergistic effect of CdSe QDs and PC₆₁BM.

Chapter-5 includes the major findings of the thesis along with a brief outline for the future scope of research related to the present thesis.

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Preface

Introduction and Scope of the Thesis

Contents

1.1	Introduction	3
1.2	Photovoltaic Devices	4
1.3	Organic Photovoltaic (OPV) Devices	5
1.3.1 Ma	aterials for Organic Photovoltaic Cells	6
1.3.2 Ty	ppe of Organic Photovoltaic Devices	10
1.3.2.1	Single-Layer OPV Device	10
1.3.2.2	Bilayer Heterojunction OPV Device	11
1.3.2.3	Bulk Heterojunction (BHJ) OPV Device	13
1.3.3 Wo	orking Principles of BHJ OPV Device	15
1.3.3.1	Light Absorption	16
1.3.3.2	Exciton Diffusion	18
1.3.3.3	Exciton Dissociation	
1.3.3.4	Charge Collection	19
1.3.4 Eq	quivalent Circuit of BHJ OPV Devices	20
1.3.5 Pa	arameters of BHJ OPV Devices	
1.3.5.1	Short Circuit Current (Isc)	
1.3.5.2	Open Circuit Voltage (Voc)	24
1.3.5.3	Fill Factor (FF)	25
1.3.5.4	Power Conversion Efficiency (PCE)(η)	

1.4	Literature Review	27
1.4.1	Review of BHJ OSCs	27
1.4.2	Review of PCDTBT: PCBM based BHJ OSCs	30
1.4.3	Major Observation from the Literature Review	32
1.5	Challenges in the BHJ OSC	33
1.6	Motivation and Problem Definition	34
1.7	Scope of the Thesis	34