

**COLLOIDAL QUANTUM DOTS AND HYBRID  
NANOSTRUCTURES FOR SOLUTION PROCESSED  
OPTOELECTRONIC DEVICES**

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by

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Submitted

in fulfillment of the requirements of the degree of Doctor of Philosophy

to the



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*Dedicated to  
My Parents*

# CERTIFICATE

This is to certify that the dissertation entitled, “**COLLOIDAL QUANTUM DOTS AND HYBRID NANOSTRUCTURES FOR SOLUTION PROCESSED OPTOELECTRONIC DEVICES**” being submitted by **Mr. RAZI AHMAD** to the **Indian Institute of Technology, Delhi** for the award of the degree of “**Doctor of Philosophy**” in Chemistry, is a record of the bonafide research work carried out by him. **Mr. RAZI AHMAD** has worked under our supervision and guidance. In our opinion, the dissertation has reached the standard of fulfilling the requirements of all the regulations relating to the degree. The results contained in it have not been submitted in part or full, to any other University or Institute for the award of any degree or diploma.

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# ABSTRACT

Colloidal semiconductor nanocrystals (NCs) or quantum dots (QDs) have been widely investigated nanomaterials for possible application in solution processed optoelectronic devices. The unique size and shape dependent optical properties of quantum dots and high carrier mobility make it an ideal candidate for light harvesting component in photovoltaic devices. Despite the above mentioned advantages, the use of QDs in optoelectronic applications has been limited by poor transport properties arising due to insulating ligands, interparticle hops and absence of interconnected percolation network for charge transport. In order to improve the charge separation and electron transport, semiconductor QDs can be conjugated with high mobility network of 1D nanostructure such as single-walled carbon nanotube (SWCNT) or with 2D nanostructure of graphene and transition metal dichalcogenide (TMDs). Thus, a hybrid combination (0D–1D) of the type QDs/SWCNT and (0D-2D) can provide the advantage of increased photon absorption/exciton generation obtained by the QDs and high charge mobility by the 1D SWCNT and 2D TMD, two properties which are very useful in the development of QDs based optoelectronic devices.

The present thesis is mainly focused on the synthesis of photoactive QDs and its hybrid nanostructures (0D QDs, 0D-1D hybrid of QDs decorated SWCNT and 0D-2D hybrids of QDs decorated MoS<sub>2</sub> nanosheet) to promote charge separation and enhanced charge transport for efficient optoelectronic devices. The detailed plan of work is as follows:

**Chapter I** of the thesis is devoted towards the extensive literature survey on past and present research work of quantum dots and its hybrid nanostructures based

optoelectronic devices. It summarizes the general review on various methods for the enhancement in the performance of optoelectronic devices by improved charge separation and transport. This chapter introduces the reader about the rationale and objectives of the present research work.

Methods used for the syntheses of quantum dots and their hybrid nanostructures are described in **Chapter II**. The detailed process for the fabrication of solution processed optoelectronic devices such as solar cells and photoconductive devices are discussed. Brief accounts of the techniques used to characterize the newly synthesized materials are provided.

In **Chapter III**, we present the effective enhancement of exciton dissociation and electron transport in the active layer of organic solar cells, by incorporation of tetrapod CdSe nanocrystals. We observed that the open circuit voltage ( $V_{OC}$ ) of ternary blends based hybrid devices depend upon concentration of CdSe TPs. The  $V_{OC}$  gradually increases with the increasing concentration of CdSe TPs in ternary blends. The increase in  $V_{OC}$  with CdSe TPs may be due to enhanced carrier life time due to creation of new interfacial energy level induced by CdSe TPs

In **Chapter IV**, we have synthesized a series of different size and nearly monodisperse  $Ag_2S$  quantum dots by using thioacetamide as a sulfur source at a relatively lower temperature ( $< 100$  °C). A hybrid solar cell based on blends of poly (3-hexylthiophene) and  $Ag_2S$  QDs were fabricated and tested for photovoltaic application.

In **Chapter V**, a photoactive hybrid nanostructure based on zero dimension (0D) light harvesting components of  $CuInS_2$  quantum dots (QDs) and one-dimensional (1-D) transporting channel of single-walled carbon nanotube (SWCNT) was synthesized by

hydrophobic interaction. The photophysical studies and electrical characteristics of hybrid with hole transporting polymer demonstrated enhanced charge separation and transfer will occur from QDs to CNT.

In **Chapter VI**, we present ligand assisted exfoliation of MoS<sub>2</sub> nanosheet in non-polar organic solvent 1,2 dichlorobenzene (DCB) which enable high concentration stable dispersion of free standing mono or few layer nanosheet. The functionalized MoS<sub>2</sub> nanosheet was further utilized for the fabrication of solution processed 0D-2D hybrid of CuInS<sub>2</sub> and MoS<sub>2</sub> nanosheet. The photophysical and photoconductive studies confirm efficient charge separation and transfer occurs from CIS QDs to MoS<sub>2</sub> NS.

In **Chapter VII**, we demonstrated the enhancement in power conversion efficiency (*PCE*) of organic solar cells by incorporation of functionalized 2D-MoS<sub>2</sub> NS as an additional charge transporting material. The enhancement in *PCE* of ternary solar cells arises due to the synergic enhancement in exciton dissociation and improvement in both electrons and holes transport through the active layer of the solar cells.

**Chapter VIII** summarizes the results presented in the thesis highlighting the role of elongated shape nanocrystals and hybrid nanostructure on the exciton dissociation, charge transport in optoelectronic devices. In the future, hybrid nanomaterials composed of light-harvesting components of QDs and transporting channel of 1D or 2D network can be explored for enhanced performance of optoelectronics devices.

# सार

कोलायडल सेमिकंडक्टर नेनोक्रिस्टल्स ऑर क्वांटम डॉट्स हॅव बीन वाइडली इन्वेस्टिगेटेड जीरो-डाइमेंशनल (0डी) नेनोमटीरियल्स फॉर पासिबल अप्लिकेशन इन सल्यूशन प्रोसेस्ड ऑप्टोएलेक्ट्रॉनिक डिवाइसिस इयू टू इट्स शेप एंड साइज डिपेंडेंट ऑप्टिकल प्रॉपर्टीज़। दा यूनीक साइज एंड शेप डिपेंडेंट प्रॉपर्टीज़ ऑफ क्वांटम डॉट्स सच एज हाइ ऑप्टिकल अब्ज़ॉर्प्शन क्रॉस-सेक्शन, अ वाइडर अब्ज़ॉर्प्शन रेंज ट्यूनेबल फ्रॉम विज़िबल टू एन.आइ.आर. अचीवेबल बाइ वेरीयिंग पार्टिकल साइज एंड हाइ कॅरियर मोबिलिटी मेक इट एन आइडीयल कॅंडिडेट फॉर लाइट हार्वेस्टिंग कॉपोनेंट इन फोटोवोल्टेयिक डिवाइसिस। डेस्पाइट दा अबव मेन्षंड अड्वांटेजस, दा यूज ऑफ क्वांटम डॉट्स इन ऑप्टोएलेक्ट्रॉनिक अप्लिकेशन्स हॅज बीन लिमिटेड बाइ पुवर ट्रांसपोर्ट प्रॉपर्टीज़ अराइसिंग इयू टू इन्सुलेटिंग लिगेण्ड्स, इंटरपार्टिकल हॉप्स एंड अब्सेन्स ऑफ इंटरकनेक्टेड पकॉलेशन नेटवर्क फॉर चार्ज ट्रांसपोर्ट। फोटोवोल्टेयिक पर्फॉर्मेंस इन हाइब्रिड ओर्गेनिक-इनओर्गेनिक सिस्टम्स डिपेंड अपॉन दा टाइप एज वेल एज दा शेप ऑफ नेनोक्रिस्टल्स एंड दट टेट्रापॉड शेपड नेनोक्रिस्टल शोज़ बेटर डिवाइस पर्फॉर्मेंस देन क्वांटम डॉट्स एंड नेनोरोड्स। इन ऑर्डर टू इंप्रूव दा चार्ज सेपरेशन एंड इलेक्ट्रान ट्रांसपोर्ट, सेमिकंडक्टर क्वांटम डॉट्स केन बी कौजुगेटेड विध हाइ मोबिलिटी नेटवर्क ऑफ 1डी नेनोस्ट्रक्चर सच एज सिंगल-वॉल्ड कार्बन नेनोट्यूब (SWCNT) ऑर विध 2डी नेनोस्ट्रक्चर ऑफ ग्राफीन एंड ट्रॉन्जिशन मेटल डाइचालकोजनाइड्स। दस, ए हाइब्रिड कॉबिनेशन (0डी-1डी) ऑफ दा टाइप क्वांटम डॉट्स/SWCNT एंड (0डी-2डी) केन प्रोवाइड दा अड्वांटेज ऑफ इनक्रीज्ड फोटॉन अब्ज़ॉर्प्शन/एक्सिटन जेनरेशन ओब्टेंड बाइ दा क्वांटम डॉट्स एंड हाइ चार्ज मोबिलिटी बाइ दा 1डी SWCNT एंड 2डी ट्रॉन्जिशन मेटल डाइचालकोजनाइड्स, टू प्रॉपर्टीज़ विच आर वेरी यूज्फुल इन दा डेवेलपमेंट ऑफ क्वांटम डॉट्स बेस्ड ऑप्टोएलेक्ट्रॉनिक डिवाइसिस।

दा प्रेज़ेंट थीसिस ईज मेन्ली फोकस्ड ऑन दा सिंथेसिस ऑफ फोटोएक्टिव क्वांटम डॉट्स एंड इट्स हाइब्रिड नेनोस्ट्रक्चर्स (0डी क्वांटम डॉट्स, 0डी-1डी हाइब्रिड ऑफ क्वांटम डॉट्स डेकरेटेड SWCNT एंड 0डी-2डी हाइब्रिड्स ऑफ क्वांटम डॉट्स डेकरेटेड MoS<sub>2</sub> नेनोशीट) टू प्रमोट चार्ज सेपरेशन एंड एनहॅन्स्ड चार्ज ट्रांसपोर्ट फॉर एफीशियेंट ऑप्टोएलेक्ट्रॉनिक डिवाइसिस. दा डीटेल्ड प्लान ऑफ वर्क ईज एज फॉलोस:

चेप्टर वन ऑफ दा थीसिस ईज डिवोटेड टुवर्ड्स दा एक्सटेन्सिव लिटरेचर सर्वे ऑन पास्ट एंड प्रेज़ेंट रिसर्च वर्क ऑफ क्वांटम डॉट्स एंड इट्स हाइब्रिड नेनोस्ट्रक्चर बेस्ड ऑप्टोएलेक्ट्रॉनिक डिवाइसिस. इट समराइजिस दा जनरल रिव्यू ऑन वेरियस मेथड फॉर दा एनहॅन्समेंट इन दा

पर्फॉर्मन्स ऑफ ऑप्टॉयेलेक्ट्रॉनिक डिवाइसिस बाइ इंप्रूव्ड चार्ज सेपरेशन एंड ट्रांसपोर्ट. दिस चेप्टर इंट्रोड्यूस दा रीडर अबाउट दा रॅशनेल एंड ऑब्जेक्टिव्स ऑफ दा प्रेज़ेंट रिसर्च वर्क।

मेथड्स यूज़्ड फॉर दा सिंथेसिस ऑफ क्वांटम डॉट्स एंड देयर हाइब्रिड नेनोस्ट्रक्चर आर डिस्क्रीब्ड इन चेप्टर टू। दा डीटेल्ड प्रोसेस फॉर दा फॅब्रिकेशन ऑफ सल्यूशन प्रोसेस्ड ऑप्टॉयेलेक्ट्रॉनिक डिवाइसिस सच एज़ सोलर सेल्स एंड फोटोकंडक्टिव डिवाइसिस आर डिस्क्रीब्ड। ब्रीफ अकाउंट्स ऑफ दा टेक्नीक्स यूज़्ड टू करेक्टराइज़ दा न्यूली सिंथेसाइज़्ड मेटीरियल्स आर प्रोवाइडेड।

इन चेप्टर थ्री, वी प्रेज़ेंट दा एफेक्टिव एनहॅन्समेंट ऑफ एक्सिटन डिसोसियेशन एंड इलेक्ट्रान ट्रांसपोर्ट इन दा एक्टिव लेयर ऑफ ऑर्गेनिक सोलर सेल्स, बाइ इनकॉर्पोरेशन ऑफ टेट्रापाँड CdSe नेनोक्रीस्टल। वी ओब्ज़र्व्ड दट दा ओपन सर्किट वोल्टेज ऑफ टर्नरी ब्लेंड्स बेस्ड हाइब्रिड डिवाइसिस डिपेंड अपॉन कॉन्संट्रेशन ऑफ CdSe टेट्रापाँड्स। दा ओपन सर्किट वोल्टेज ग्रेजुयली इनक्रीजस विध दा इनक्रीसिंग कॉन्संट्रेशन ऑफ CdSe टेट्रापाँड्स इन टर्नरी ब्लेंड्स। दा इनक्रीज इन ओपन सर्किट वोल्टेज विध CdSe टेट्रापाँड्स मे बी ड्यू टू एनहॅन्सड कॅरियर लाइफ टाइम ड्यू टू क्रियेशन ऑफ न्यू इंटरफेशियल एनर्जी लेवल इंड्यूसड बाइ CdSe टेट्रापाँड्स।

इन चेप्टर फोर, वी हेव सिंथेसाइज़्ड आ सीरीज़ ऑफ डिफरेंट साइज़ एंड नियर्ली मोनोडिस्पर्स Ag<sub>2</sub>S क्वांटम डॉट्स बाइ यूज़िंग थायोएसिटामाइड एज़ आ सल्फर सोर्स अट आ रिलेटिवली लोवर टेंपरेचर (< 100 °C). आ हाइब्रिड सोलर सेल बेस्ड ऑन ब्लेंड्स ऑफ पॉली (3-हेक्साइलथायोफीन) एंड Ag<sub>2</sub>S क्वांटम डॉट्स वर फॅब्रिकेटेड एंड टेस्टेड फॉर फोटोवोल्टेयिक अप्लिकेशन।

इन चेप्टर फाइव, आ फोटोएक्टिव हाइब्रिड नेनोस्ट्रक्चर बेस्ड ऑन जीरो डाइमेन्शन (0डी) लाइट हार्वेस्टिंग कॉपोनेंट ऑफ CuInS<sub>2</sub> क्वांटम डॉट्स एंड वन-डाइमेन्शनल (1डी) ट्रांसपोर्टिंग चैनल ऑफ सिंगल-वॉल्ड कार्बन नेनोट्यूब (SWCNT) वाज़ सिंथेसाइज़्ड बाइ हाइड्रोफोबिक इंटरैक्शन। दा फोटोफिज़िकल स्टडीज़ एंड एलेक्ट्रिकल कॅरेक्टरिस्टिक्स ऑफ हाइब्रिड विध होल ट्रांसपोर्टिंग पॉलिमर डेमॉन्स्ट्रेटेड एनहॅन्सड चार्ज सेपरेशन एंड ट्रान्सफर विल अकर फ्रॉम क्वांटम डॉट्स टू कार्बन नेनोट्यूब।

इन चेप्टर सिक्स, वी प्रेज़ेंट लिगेंड असिस्टेड एक्सफोलीयेशन ऑफ MoS<sub>2</sub> नेनोशीट इन नॉन-पोलर ऑर्गेनिक सॉल्वेंट 1,2 डाइक्लोरोबेन्ज़ीन विच एनेबल हाइ कॉन्संट्रेशन स्टेबल डिसपरशन ऑफ फ्री स्टैंडिंग मोनो ओर फ्यू लेयर ननोशीट। दा फंक्शनलाइज़्ड MoS<sub>2</sub> नेनोशीट वाज़ फर्दर यूटिलाइज़्ड फॉर दा फॅब्रिकेशन ऑफ सल्यूशन प्रोसेस्ड 0डी-2डी हाइब्रिड ऑफ CuInS<sub>2</sub> एंड

MoS<sub>2</sub> नेनोशीट. दा फोटोफिज़िकल एंड फोटोकंडक्टिव स्टडीज़ कन्फर्म एफीशियेंट चार्ज सेपरेशन एंड ट्रांसफर अकर्स फ्रॉम CuInS<sub>2</sub> क्वांटम डॉट्स टू MoS<sub>2</sub> नेनोशीट।

इन चेप्टर सेवेन, वी डेमॉन्स्ट्रेटेड दा एनहॅन्समेंट इन पॉवर कन्वर्षन एफीशियेन्सी ऑफ ऑर्गेनिक सोलर सेल्स बाइ इनकॉर्पोरेशन ऑफ फंक्शनलाइज़्ड 2डी-MoS<sub>2</sub> नेनोशीट एज़ अन अडीशनल चार्ज ट्रांसपोर्टिंग मेटीरियल। दा एनहॅन्समेंट इन पॉवर कन्वर्षन एफीशियेन्सी ऑफ टर्नरी सोलर सेल्स अराइज़स इयू टू दा सिनर्जिक एनहॅन्समेंट इन एक्सिटन डिसोसियेशन एंड इंप्रूवमेंट इन बोथ इलेक्ट्रॉन्स एंड होल्स ट्रांसपोर्ट थ्रू दा एक्टिव लेयर ऑफ दा सोलर सेल्स।

चेप्टर एट समराइज़िस दा रिज़ल्ट्स प्रेज़ेंटेड इन दा थीसिस हाइलाइटिंग दा रोल ऑफ इलॉगेटेड शेप नेनोक्रीस्टल्स एंड हाइब्रिड नेनोस्ट्रक्चर्स ऑन दा एक्सिटन डिसोसियेशन, चार्ज ट्रांसपोर्ट इन ऑप्टॉयेलेक्ट्रॉनिक डिवाइसिस इन दा फ्यूचर, हाइब्रिड नेनोमटीरियल कंपोज्ड ऑफ लाइट-हार्वैस्टिंग कॉपोनेंट्स ऑफ क्वांटम डॉट्स एंड ट्रांसपोर्टिंग चैनल ऑफ 1डी ओर 2डी नेटवर्क केन बी एक्सप्लोर्ड फॉर एनहॅन्सड पर्फॉर्मेंस ऑफ ऑप्टॉयेलेक्ट्रॉनिक डिवाइसिस।

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# Glossary of Symbols and Abbreviations

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OSCs	Organic Solar Cells
BHJ	Bulk-heterojunction
PCE	Power conversion efficiency
EQE	External quantum efficiency
HOMO	Highest occupied molecular orbital
LUMO	Lowest unoccupied molecular orbital
CB	Conduction band
VB	Valence band
MoO <sub>3</sub>	Molybdenum oxide
TMDs	Transition metal dichalcogenides
QDs	Quantum dots
NS	Nanosheets
NCs	Nanocrystals
TPs	Tetrapods
0D	Zero-dimension
1D	One-dimension
2D	Two-dimension
ZnO	Zinc oxide
CNTs	Carbon nanotubes
NCNTs	Nitrogen doped carbon nanotubes

GO	Graphene oxide
rGO	Reduced graphene oxide
MoS <sub>2</sub>	Molybdenum disulfide
Ag <sub>2</sub> S	Silver sulfide
CuInS <sub>2</sub> , CIS	Copper indium sulfide
ITO	Indium tin oxide
PEDOT:PSS	Poly-(3,4-ethylenedioxythiophene): poly(styrenesulfonate)
P3HT	Poly(3-hexylthiophene)
PTB7	Poly({4,8-bis[(2-ethylhexyl)oxy]benzo[1,2-b:4,5-b']dithiophene-2,6-diyl}{3-fluoro-2-[(2-ethylhexyl)carbonyl]thieno[3,4-b]thiophenediyl})
PCDTBT	Poly[N-9'-heptadecanyl-2,7-carbazole-alt-5,5-(4',7'-di-2-thienyl-2',1',3'-benzothiadiazole)], Poly[[9-(1-octylnonyl)-9H-carbazole-2,7-diyl]-2,5-thiophenediyl-2,1,3-benzothiadiazole-4,7-diyl-2,5-thiophenediyl]
MDMO-PPV	Poly[2-methoxy-5-(3',7'-dimethyloctyloxy)-1,4-phenylenevinylene]
PCPDTBT	Poly[2,6-(4,4-bis-(2-ethylhexyl)-4H-cyclopenta [2,1-b;3,4-b']dithiophene)-alt-4,7(2,1,3-benzothiadiazole)]
PC <sub>61</sub> BM, PC <sub>60</sub> BM	[6,6]-phenyl-C <sub>61</sub> butyric acid methyl ester
PC <sub>71</sub> BM	[6,6]-phenyl-C <sub>71</sub> butyric acid methyl ester
ICBA	Indene-C <sub>60</sub> bisadduct
EDAX	Energy dispersive x-ray analysis
HRTEM	High resolution transmission electron microscope
AFM	Atomic force microscopy

XRD	X-ray diffraction
SEM	Scanning electron microscope
XPS	X-ray photoelectron spectroscopy
UPS	Ultra violet photoelectron spectroscopy
UV-vis	Ultraviolet-visible
PL	Photoluminescence
TRPL	Time-resolved Photoluminescence
TCSPC	Time correlated single photon counts
AM	Air mass
ITO	Indium tin oxide
Ag	Silver
Al	Aluminum
Au	Gold
V	Voltage
J-V	Current density-Voltage
J <sub>sc</sub>	Short-circuit current density
V <sub>oc</sub>	Open-circuit voltage
FF	Fill factor
μ	Mobility
nm	nanometer
M	Molar
cm	centimeter

mW	milli-watt
eV	Electron-volt
$\mu$ L	microliter
nm	nanometer
mL	milliliter
Hz	Hertz
Å	angstrom
°C	degree centigrade
v	frequency
%	percent
ns	nanosecond