

**UNIVERSITY GRANTS COMMISSION
BAHADUR SHAH ZAFAR MARG
NEW DELHI-110 002**

Final Report of the work done on the Major Research Project.

1. Project report No. 1st/2nd/Final: Final
2. UGC Reference No: F. -43-174/2014(SR), dated 17.08.2015
3. Period of Report from : 1st July, 2015 to 30st June, 2018.
4. Title of research project: Electronic Structure of Functionalized Semiconductor Nanoparticles
5. Dept. and University where work is progressed: Dept. of Chemistry, Visva-Bharati, West-Bengal.
6. Effective date of starting of the project: 17th August, 2015
7. Grant approved and expenditure incurred during the period of the report:
 - a) Total amount approved Rs. 9,80,000/-
 - b) Total expenditure Rs. 9,80,000 /-
8. Report of the work done:
 - a) Brief objective of the project:

To study the electronic structure of porphyrin functionalized semiconductor nanoparticles with a goal to understand the efficacy of this hybrid nanostructures for use in solar cells

To study the electronic structure of fullerene/carbon nanotube functionalized semiconductor nanostructures

To study the electronic structure of self-assembly of zero-dimensional Cd-Chalcogenide clusters functionalized with bi-functional covalent linkers to understand the feasibility of creating an organized nanocluster-ligand assemblies.
 - b) Work done so far and results achieved and publication if any, resulting from the work(Give details of the title of the papers and name of the journals in which it has been published or accepted for publication): Please see Annexure-I for work done

Publication:

(i) **B. Rajbanshi and P. Sarkar** "Optimizing the Photovoltaic Properties of CdTe Quantum Dot-Porphyrin Nanocomposites: A Theoretical Study", **J. Phys. Chem C**, **120**, 17878, 2016.

(ii) **B. Rajbanshi and P. Sarkar** "Is the Metallic Phosphorus Carbide (β_0 -PC) Monolayer Stable? An Answer from a Theoretical Perspective", **J. Phys. Chem Letts.** **8**, 747, 2017.

(iii) **B. Rajbanshi, M. Kar, P. Sarkar and P. Sarkar**, " Phosphorene quantum dot-fullerene nanocomposites for solar energy conversion: An unexplored inorganic-organic nanohybrid with novel photovoltaic properties", **Chem. Phys. Letts.** **685**, 16, 2017.

(iv) **S. Biswas, A. Pramanik, S. Pal and P. Sarkar**, " A Theoretical Perspective on the Photovoltaic Performance of S,N- Heteroacenes: An Even-Odd Effect on the Charge Separation Dynamics", **J. Phys. Chem. C**, **121**, 2574, 2017.

(v) **C. Chakravarty, B. Mandal, P. Sarkar**, " Bis(dithioline)-Based Metal-Organic Frameworks with Superior Electronic and Magnetic Properties: Spin Frustration to Spintronics and Gas Sensing", **J. Phys. Chem. C**, **120**, 23807, 2017

c) Has the progress been according to original plan of work and towards achieving the objective, if not, state reasons

NA

d) Please indicate the difficulties, if any experienced in implementing the project

No Difficulties

e) If the project has not been completed, please indicate the approximate time by which it is likely to be completed .

NA

f) If the project has been completed, please enclose a summary of the findings of the Study:

By using density functional method, an exhaustive theoretical study of a novel configuration for dye sensitized solar cell (DSSC) based on TPP-CdTeQD and ZnTPP-CdTeQD nanocomposites is presented. The results indicate that the nanocomposites composed of simple TPP and CdTeQD are not so suitable for DSSC application as they are devoid of any charge separation, except for a few particular sized QDs. The substitution at the para-position of phenyl ring of the porphyrin molecule by organic functionalizing groups can overcome such an unpleasant situation. The substitution with either strong electron donating ($-NH_2$) or withdrawing groups ($-NO_2$) can yield charge separation even for the very

small QD, whereas weak/mild functionalizing groups ($-OCH_3$ or $-COOH$) can do so for larger QDs. However, if the starting porphyrin is ZnTPP instead of TPP, then, whatever may be the size of the QD, there will be charge separation between ZnTPP and CdTeQD in the axially coordinated nanocomposites. Moreover, as the size of the QD in ZnTPP-CdTeQD nanocomposites increases, the difference between the LUMO of the QDs and LUMO of the ZnTPP, which is key for dictating the dynamics of electron transfer, starts to increase continuously. So, one could expect a faster electron transfer rate for a larger CdTeQD as compared to a smaller one. Such observation is quite contrary to our previous studies, where smaller QDs are supposed to show faster electron transfer. Hence, ZnTPP-CdTeQD nanocomposites open a scope of ease to the experimentalists for the application in DSSCs. Based on the qualitative idea we have ultimately concluded that the ZnTPP-CdTeQD nanocomposites will show higher performance for light harvesting devices with moderate size of QD, rather than too big or too small one

The covalently linked (by both amide and ester linkage) 1D-linear assembled superstructure containing large number of CdTe QDs will show very high photoelectric conversion efficiency and it increases with increasing the size of CdTe QDs in assembly. Another important observation is that we can achieve 1D semiconductor with different size of band gaps by varying the size of the QDs and by varying the functional group of linkers in assembly, which may find application in electronic devices. The excellent tunability of the optoelectronic properties of QDs assembly has become one of the most attractive properties in its design, allowing their harnessing of different energy solar photons.

- g) Any other information which would help in evaluation of this work done of the project. At the completion of the project, the final report should indicate the output, such as (a) Manpower trained, (b) other impact, if any

Manpower Trained: One fellow obtained Ph. D. degree and He is now doing Postdoctoral research in USA.

अग्रेषित
Forwarded

[Signature]

अध्यक्ष/Principal
शिक्षा-भवन/SIKSHA-BHAVANA
(विज्ञान-संस्थान)/(Institute of Science)
विश्वभारती, शान्तिनिकेतन
Visva-Bharati, Santiniketan

Pranab Sarkar 14/09/18
Principal Investigator
Prof. Dr. Pranab Sarkar
Department of Chemistry
Visva-Bharati
Santiniketan - 731235
P.I. of UGC Sponsored Project
F. No. 43-174/2014 (SR)

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[Signature]

Head
Department of Chemistry
Visva-Bharati
Santiniketan - 731235

Registrar

[Signature]
कुलसचिव (कार्यवाहक)
विश्वभारती
Registrar (Acting)
Visva-Bharati

Annexure-V
UNIVERSITY GRANTS COMMISSION
BAHADUR SHAH ZAFAR MARG
NEW DELHI-110 002

STATEMENT OF EXPENDITURE IN RESPECT OF MAJOR RESEARCH PROJECT
UNDER THE SCHEME SUPPORT OF RESEARCH IN MAJOR RESEARCH
PROJECT

1. Name of the Principal Investigator : Pranab Sarkar
2. Dept. of University/College : Dept. of Chemistry, Visva-Bharati
3. UGC approved No. & date : F. -43-174/2014(SR), dated 17.08.2015
4. Title of the Research Project : Electronic Structure of Functionalized Semiconductor Nanoparticles
5. Effective date of starting the project : 17.08.2015
6. (a) Period of expenditure: From 17.08.2015 to 30.06.18
(b) Details of expenditure:

S. No.	Item	Amount (Total) (Rs.)	Approved	Expenditure incurred (Rs.) (Between 17.08.2015-30.06.2018)
1.	Books & Journals	Nil		NA
2.	Contingency	Nil		NA
3.	Equipment	9,80,000/-		9,80,000/-
4.	Field work &	Nil		NA

	Travel		
5.	Overhead Charges	Nil	Nil
			Total Rs. 9,80,000/-

(c) Staff: Date of Appointment: NA

Sl. No.	Amount Approved	Expenditure Incurred
	Nil	NA

It is certified that the grant of Rs. 9,80,000/- (Rupees Nine lakhs eighty thousand only) received from the University Grants Commission under the scheme of support for Major Research Project entitled Electronic Structure of Functionalized Semiconductor Nanoparticles vide UGC letter No. F. -43-174/2014(SR), dated 17.08.2015 has been fully utilized for the purpose for which it was sanctioned and in accordance with the terms and conditions laid down by the University Grants Commission.

Pranab Sarkar 14/09/18
Signature of P. I.

Prof. Dr. Pranab Sarkar
Department of Chemistry
Visva-Bharati
Santiniketan - 731235
P.I. of UGC Sponsored Project
F. No. 43-174/2014 (SR)

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[Signature]

Signature of the Principal
अध्यक्ष/Principal
शिक्षा-भवन/SIKSHA-BHAVANA
(विज्ञान-संस्थान)/(Institute of Science)
विश्वभारती, शान्तिनिकेतन
Visva-Bharati, Santiniketan

[Signature]
Signature of the Head of the department

Head
Department of Chemistry
Visva-Bharati
Santiniketan - 731235

[Signature]
Signature of the Accounts Officer

Accounts Officer / Joint Registrar
Visva-Bharati, Santiniketan

[Signature]
18/09/18

[Signature]
Signature of the Registrar

कुलसचिव (अभ्यर्थक)
विश्वभारती
Registrar (Acting)
Visva-Bharati

Annexure-VI
UNIVERSITY GRANTS COMMISSION
BAHADUR SHAH ZAFAR MARG
NEW DELHI-110 002

UTILISATION CERTIFICATE

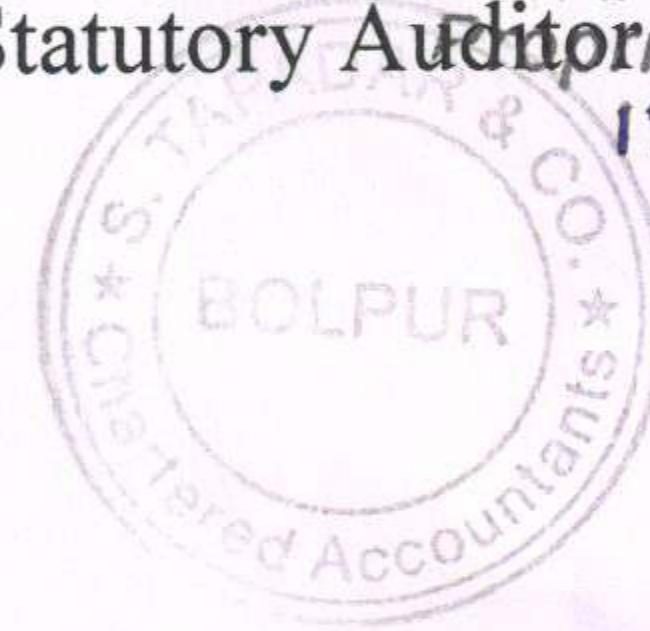
Certified that the grant of Rs. 9,80,000/- (Nine lakhs eighty thousand only) received from the University Grants Commission under the scheme of support for major research project entitled "Electronic Structure of Functionalized Semiconductor Nanoparticles" vide UGC letters no F. -43-174/2014(SR), dated 17.08.2015, a sum of Rs. 9,80,000/- (Nine lakhs eighty thousand) has been utilized for the purpose which it was sanctioned and in accordance with the terms and conditions laid down by the University Grants Commission.

Pranab Sarkar 14/9/18
Signature of Principal
Investigator
Dr. Pranab Sarkar
Department of Chemistry
Visva-Bharati
Santiniketan - 731235
P.I. of UGC Sponsored Project
F. No. 43-174/2014 (SR)

[Signature] 14/9/18
Head
Department of Chemistry
Visva-Bharati
Santiniketan - 731235

[Signature] 14/9/18
Registrar
कुलसचिव (कार्यवाहक)
विश्वभारती
Registrar (Acting)
Visva-Bharati
[Signature] 14/9/18
Accounts Officer / Joint Registrar
Visva-Bharati, Santiniketan

For S. TAPADAR & CO.
Chartered Accountants
[Signature]
S. TAPADAR, F.C.A.
Statutory Auditor
15th July, 2018



M. No. - 057332

अग्रेषित
Forwarded

[Signature] 15/9
अध्यक्ष / Principal
शिक्षा-भवन / SIKSHA-BHAVANA
(विज्ञान-संस्थान) / (Institute of Science)
विश्वभारती, शान्तिनिकेतन
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