Curriculum Vitae

Brief Profile:

I have done my doctoral research (2014) under the supervision of Prof. Pranab Sarkar at Department of Chemistry, Visva-Bharati, India. In this period, we pursued the state-of-the-art theoretical approach to explore the electronic structure of semiconductor nanomaterials. The SCC-DFTB method is used which has already been successfully applied to simulate large systems quantum-mechanically. We developed the set of parameters of different systems within this method. We have modelled various hybrid nanostructures to tune their electronic properties for the possible use in optoelectronic devices. The current transport phenomenon of various carbon based nanostructures are also investigated by utilizing the NEGF technique within the DFT. We have discussed the negative differential resistance behavior of different doped and defective graphene nanoribbons for technological importance.

During my postdoc with Prof. Michal Otyepka at RCPTM in Palackỳ University, Olomouc, Czech Republic, we have studied the absorption properties of carbon dots using TDDFT. We have investigated the optoelectronic properties of multilayer carbon dot models which are important in wide range of potential applications.

In my recent postdoc at Kent State University, Kent, Ohio, United States with Prof. Barry D. Dunietz, we employed the advanced Quantum Chemical tools to investigate the excited states properties of molecular systems. The design principles for achieving optimal photo-emission in organic materials are our important field of research for the next generation OLED applications. We have also systematically explored a new approach for designing the organic materials with enhanced charge mobilities used in the fabrication of efficient solar cells.

The aim of our future research is the computational modelling of advanced materials for the optoelectronic applications. In this regard, we are keen to study the electronic, optical and transport properties of various inorganic nanomaterials, carbon nanostructures, π-conjugated organic molecules and related nanoscale systems. Our future research plan also includes the understanding of the energy transfer and charge transfer processes involved in the various organic photo systems.

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5. Field(s) of Specialization:
Physical Chemistry, Theoretical & Computational Chemistry,
Electronic Structure of Materials.

6. Employment Profile

Job Title	Employer	From	To
Assistant Professor	National Institute of Technology, Tiruchirappalli, India	2018	onwards
Post-Doctoral Fellow	Kent State University, United States	2016	2017
Post-Doctoral Fellow	RCPTM, Palackỳ University, Czech Republic	2014	2015

7. Academic Qualifications:

Examination	Board / University	Year	Division/ Grade	Subjects
Ph.D.	Visva-Bharati	2014		Chemistry
M.Sc.	Visva-Bharati	2008	1st	Chemistry (Spcl: Physical Chemistry)
B.Sc.	Visva-Bharati	2006	1st	Chemistry (H), Mathematics, Physics

8. Awards, Associateships etc.

Year of Award	Name of the Award	Awarding Organization
2011	One of the Best Poster award	IIT, Guwahati (ICANN-2011)
2008	Lecturership Award	CSIR-UGC (NET)

9. Fellowships

Year of Award	Name of the Fellowship	Awarding Organization	From (Month/Year)	To (Month/Year)
2011	Senior Research Fellowship	CSIR	Jan, 2011	Dec, 2013
2008	Junior Research Fellowship	CSIR	Jan, 2009	Dec, 2010

10. Participation in Workshops/ Symposia/ Conferences/ Colloquia /Seminars/ Schools etc. (mentioning the role)

Date (s)	Title of Activity	Level of Event (International/ National/ Local)	Role (Participant/ Speaker/ Chairperson, Paper presenter, Any other)	Event Organized by	Venue
Feb, 2015	6th European Symposium on Computing Π-Conjugated Compounds	International	Speaker	Department of Physical Chemistry, Palackỳ University	Olomouc, Czech Republic
Mar, 2014	National Seminar on Recent Advances in Chemistry	National	Poster presenter	Department of Chemistry, Visva-Bharati	Santiniketan, India
Dec, 2012	International Workshop on Nanomaterials (IWoN): Engineering Photon and Phonon Transport	International	Poster presenter	Department of Physics, Jadavpur University	Kolkata, India
Dec, 2011	International Conference on Advanced Nanomaterials and Nanotechnology (ICANN-2011)	International	Poster presenter	Department of Physics and Center for Nanotechnology, Indian Institute of Technology, Guwahati	Guwahati, India

11. Academic Foreign Visits

Country	Duration of Visit	Programme
United States	Feb, 2016 – Dec, 2017	Postdoc
Czech Republic	Aug, 2014 – Jul, 2015	Postdoc

12. Publications

(A) Refereed Research Journals:

Author(s)	Title of Paper	Journal	Volume (No.)	Page numbers	Year	Impact Factor of the Journal (Optional)
S. Sarkar, J. D. Protasiewicz and B. D. Dunietz.	Controlling the Emissive Activity in Heterocyclic Systems Bearing C═P Bonds	J. Phys. Chem. Lett.	9	3567-3572	2018	9.353
B. Maiti, A. Schubert, **S. Sarkar,** S. Bhandari, K. Wang, Z. Li, E. Geva, R. J. Twieg, and B. D. Dunietz.	Enhancing Charge Mobilities in Organic Semiconductors by Selective Fluorination: A Design Approach Based on a Quantum Mechanical Perspective.	Chemical Science	8	6947-6953	2017	8.668
S. Sarkar, H.P.Hendrickson, D.Lee, F.Devine, J.Jung, E.Geva, J.Kim, and B.D.Dunietz.	Phosphorescence in Bromobenzaldehyde Can Be Enhanced Through Intramolecular Heavy Atom Effect.	J. Phys. Chem. C	121	3771-3777	2017	4.536
S. Sarkar, S.Saha, S.Pal, and P.Sarkar.	Exploring the Electronic Structure of Nanohybrid Materials for Their Application in Solar Cell.	Chemical Modelling (Invited Book Chapter), Royal Society of Chemistry	13	27-71	2017	
B. Rajbanshi, **S. Sarkar**, B. Mandal and P. Sarkar.	Energetic and Electronic Structure of Penta-Graphene Nanoribbons	Carbon	100	118-125	2016	6.337
S. Sarkar, M.Sudolska, M.Dubecky, C.J.Reckmeier,	Graphitic Nitrogen Doping in Carbon Dots Causes Red-Shifted Absorption	J. Phys. Chem. C	120	1303-1308	2016	4.536

A.L.Rogach, R.Zboril and M.Otyepka.						
R. Sarkar, **S. Sarkar,** A. Pramanik, P. Sarkar and S. Pal.	Isoelectronically Doped CdSe/Te Nanoalloys as Alternative Solar Cell Materials: Insight from Computational Analysis	RSC Advances	6	86494-86501	2016	3.108
S. Sarkar, A.Pramanik, and P.Sarkar.	Quantum Transport Behavior of Ni-Based Di-nuclear Complexes in Presence of Zigzag Graphene Nanoribbon as Electrode	Chem. Phys.	478	173-177	2016	1.767
M. Sudolska, M. Dubecky, **S. Sarkar,** C. J. Reckmeier, R. Zboril, A. L. Rogach and M. Otyepka.	Nature of Absorption Bands in Oxygen-Functionalized Graphitic Carbon Dots	J. Phys. Chem. C	119	13369-13373	2015	4.536
B.Rajbanshi, **S. Sarkar** and P.Sarkar.	The Electronic and Optical Properties of $MoS_{2(1-x)}Se_{2x}$ and $MoS_{2(1-x)}Te_{2x}$ Monolayers	Phys. Chem. Chem. Phys.	17	26166-26174	2015	4.123
B. Mandal, **S. Sarkar** and P. Sarkar	Theoretical Studies on Understanding the Feasibility of Porphyrin Sensitized Graphene Quantum Dot Solar Cell	J. Phys. Chem. C	119	3400-3407	2015	4.536
A.Pramanik, **S. Sarkar**, S.Pal and P.Sarkar	Pentacene-Fullerene Bulk-Heterojunction Solar Cell: A Computational Study	Phys. Lett. A	379	1036-1042	2015	1.772
S. Sarkar, B. Rajbanshi and P. Sarkar	Understanding the Electronic Structure of CdSe Quantum Dot Fullerene(C60) Hybrid Nanostructure for Photovoltaic Applications	J. Appl. Phys.	116	114303	2014	2.068
B.Mandal, **S. Sarkar**,	Doped Defective Graphene	RSC Advances	4	49946-49952	2014	3.108

A.Pramanik and P.Sarkar	Nanoribbon-A New Class of Materials with Novel Spin Filtering Properties.					
B. Rajbanshi, **S. Sarkar** and P. Sarkar	Band Gap Engineering of Graphene-CdTe Quantum Dot Hybrid Nanostructures.	J. Mater. Chem. C	2	8967-8975	2014	5.256
A. Pramanik, B. Mandal, **S. Sarkar** and P. Sarkar.	Effect of Edge States on the Transport Properties of Pentacene-Graphene Nanojunctions.	Chem. Phys. Lett.	597	1-5	2014	1.815
S. Sarkar, S.Saha, S.Pal and P.Sarkar	Electronic Structure and Band Gap Engineering of CdTe Nanotubes and Designing the CdTe Nanotube-Fullerene Hybrid Nanostructures for Photovoltaic Applications	RSC Advances	4	14673-14683	2014	3.108
S. Saha, **S. Sarkar,** S.Pal and P.Sarkar	Ligand Mediated Tuning of the Electronic Energy Levels of ZnO Nanoparticles.	RSC Advances	3	532-539	2013	3.108
B.Mandal, **S. Sarkar** and P.Sarkar	Energetics and Electronic Structure of Encapsulated Graphene Nanoribbons in Carbon Nanotube.	J. Phys. Chem. A	117	8568-8575	2013	2.847
S.Saha, **S. Sarkar**, S.Pal, and P.Sarkar.	Tuning the Energy Levels of ZnO/ZnS Core/Shell Nanowire to Design an Efficient Nanowire-Based Dye-Sensitized Solar Cell.	J. Phys. Chem. C	117	15890-15900	2013	4.536
S. S. Mati, **S. Sarkar**, S. Rakshit, A. Sarkar and S. C. Bhattacharya	Probing the Spectral Response of a New Class of Bioactive Pyrazoline Derivative in Homogeneous Solvents and Cyclodextrin Nanocavities: A	RSC Advances	3	8071-8082	2013	3.108

	Spectroscopic Exploration Appended by Quantum Chemical Calculations and Molecular Docking Analysis					
B.Mandal, **S. Sarkar**, A.Pramanik and P.Sarkar	Pure Carbon-Based Schottky Diode, an Implication of Stretched Carbon Nanowire	J. Appl. Phys.	114	173701-173707	2013	2.068
B.Mandal, **S. Sarkar**, A.Pramanik and P.Sarkar	Theoretical Prediction of a New Two-Dimensional Carbon Allotrope and NDR Behaviour of its One-Dimensional Derivatives.	Phys. Chem. Chem. Phys.	15	21001-21006	2013	4.123
S.S.Mati, **S. Sarkar**, P. Sarkar and S.C.Bhattacharya	Explicit Spectral Response of the Geometrical Isomers of a Bio-Active Pyrazoline Derivative Encapsulated in β-Cyclodextrin Nanocavity: A Photophysical and Quantum Chemical Analysis.	J. Phys. Chem. A	116	10371-10382	2012	2.847
S. Sarkar, S. Pal and P. Sarkar	Electronic Structure and Band Gap Engineering of CdTe Semiconductor Nanowires	J. Mater. Chem.	22	10716-10724	2012	5.914
B.Mandal, **S. Sarkar**, A.Pramanik and P.Sarkar	Electronic Structure and Transport Properties of Sulfur Passivated Graphene Nanoribbons	J. Appl. Phys.	112	113710-113715	2012	2.068
S.Pal, **S. Sarkar**, S.Saha and P.Sarkar	Size-Dependent Electronic Structure of Semiconductor Nanoparticles.	Chemical Modelling: Applications and Theory (Invited Book Chapter),	9	135-167	2012	

		Royal Society of Chemistry				
S. Sarkar, S. Saha, S. Pal and P. Sarkar.	Electronic Structure of Thiol-Capped CdTe Quantum Dots and CdTeQD-Carbon Nanotube Nanocomposites.	J. Phys. Chem. C	116	21601-21608	2012	4.536
B. Mandal, **S. Sarkar,** and P. Sarkar	Exploring the electronic structure of graphene quantum dots	J. Nanopart. Res.	14	1317	2012	2.020
A.Pramanik, **S. Sarkar** and P.Sarkar.	Doped GNR p-n Junction as High Performance NDR and Rectifying Device.	J. Phys. Chem. C	116	18064-18069	2012	4.536
S. Sarkar, S. Pal, P. Sarkar, A. L. Rosa and Th. Frauenheim.	Self-Consistent-Charge Density-Functional Tight-Binding Parameters for Cd-X (X=S,Se,Te) Compounds and Their Interaction with H,O,C,and N.	J. Chem. Theory Comput.	7	2262-2276	2011	5.245

(B) Conferences/Workshops/Symposia Proceedings

Author(s)	Title of Abstract/ Paper	Title of the Proceedings	Page numbers	Conference Theme	Venue	Year

(C) Books & Monographs

Author(s)	Title of Book/Monograph	Name of Publishers	Year of Publication	ISSN/ISBN Number