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Visva-Bharati, Santiniketan

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RESEARCH EXPERIENCE

❖ **Visva-Bharati**
Department of Chemistry
Assistant Professor

Santiniketan, India
Dec, 2020 - present

❖ **University of Massachusetts**
Department of Chemical Engineering
Postdoctoral Associate
Advisor: Dr. Peng Bai

Amherst, USA
Aug, 2020 - Dec, 2020

- Computational heterogeneous catalysis
- Plastic degradation
- Li-ion battery

❖ **University of South Carolina**
Department of Chemical Engineering
Postdoctoral Associate
Advisor: Dr. Andreas Heyden, Professor

Columbia, USA
Jan, 2018 - Aug, 2020

- Computational heterogeneous catalysis for energy conversion
- Catalyst search, active site identification, TS calculation using NEB and dimer methods
- Reaction mechanism investigations
- Microkinetic Modeling for kinetic data analysis
- Quantifying the solvation effects on reaction (implicit solvation using COSMO and COSMO-RS models).

❖ **Visva-Bharati**
Department of Chemistry
Senior and Junior Research Fellow
Advisor: Dr. Pranab Sarkar, Professor

Santiniketan, India
Oct, 2012 - Dec, 2017

- First-principles calculations on the stability and electronic structure of newly proposed Carbon, Phosphorous-based periodic nanostructures.
- DFT calculations of electronic, optical, transport and photovoltaic properties of inorganic nanostructures, carbon nanostructures and related nanoscale systems.
- Computational modelling of nanocomposites for the improvement of solar energy harvesting device performance using self-consistent charge density-functional tight-binding (SCC-DFTB) method.

RESEARCH GRANTS

❖ The Start-up Research Grant (SRG)

(Sanction number: SRG/2022/000215 dated 13.09.2022)

Science and Engineering Research Board (SERB)

Project Title: “*Quantum Mechanical Investigation of Olefin Metathesis Over Supported Metal Oxide Catalysts: A Step Towards Advanced Plastic to Fuel Conversion*”

Total Budget: 32 L

Duration: 2 yrs.

❖ Empowerment and Equity Opportunities for Excellence in Science (EMEQ)

(File no EEQ/2022/000312)

Science and Engineering Research Board (SERB)

Project Title: “*Quantum Mechanical Exploration of Alkanes to Alkenes Formation via Catalytic Dehydrogenation and Oxidative Dehydrogenation Over Metal and Metal Oxide Catalysts: A New Initiative to Convert Plastics into Fuel*”

Total Budget: 41 L

Duration: 3 yrs.

EDUCATION

PhD Visva-Bharati, Santiniketan, India

December 2017

Department of Chemistry

Thesis: “Studies on The Electronic Structure of Some Graphene-, Phosphorene-, and Metal Chalcogenide- Based Nanomaterials of Contemporary Interest”

Advisor: Dr. Pranab Sarkar, Professor

MSc Visva-Bharati, Santiniketan, India

July 2012

Department of Chemistry, Specialization: Physical Chemistry

BSc Visva-Bharati, Santiniketan, India

December 2010

Department of Chemistry

Majored in Chemistry and minored in Mathematics, Physics

FELLOWSHIP AND AWARDS

- Rajeev Gandhi National Fellowship (RGNF)** 2012-2017
Senior and Junior Research Fellowship sponsored by University Grant Commission (UGC), New Delhi, India.
- National Eligibility Test (NET)** June 2013
Qualified joint CSIR-UGC NET and secured 0078/0823 rank in the subject CHEMICAL SCIENCES under UGC fellowship scheme, India.
- Graduate Aptitude Test for Engineers (GATE)** 2012
All India 1311th rank in Chemistry.

PUBLICATIONS

Journal Publications

- ❖ C Fricke, **B Rajbanshi**, EA Walker, G Terejanu, A Heyden, “Propane Dehydrogenation on Platinum Catalysts: Identifying the Active Sites through Bayesian Analysis”, **ACS Catalysis**, 2022, 12 (4), 2487-2498.
<https://pubs.acs.org/doi/abs/10.1021/acscatal.1c04844>
- ❖ H Yang, K Tay, Y Xu, **B Rajbanshi**, S Kasani, J Bright, J Boryczka, C Wang, P Bai, and N Wu, “Nitrogen-Doped Lithium Lanthanum Titanate Nanofiber-Polymer Composite Electrolytes for All-Solid-State Lithium Batteries”, **Journal of The Electrochemical Society**, 2021, 168 (11), 110507.
<https://iopscience.iop.org/article/10.1149/1945-7111/ac30ad/meta>
- ❖ **B Rajbanshi**, W Yang, A Yonge, S K Kundu, C Fricke, and A Heyden, “Understanding the mechanism of the catalytic hydrodeoxygenation of propanoic acid over a Cu (111) surface,” **The Journal of Physical Chemistry C**, 2021, 125 (35), 19276-19293.
<https://pubs.acs.org/doi/abs/10.1021/acs.jpcc.1c05240>
- ❖ **B Rajbanshi**, S Saha, C Fricke, S C Ammal, and A Heyden, “Oxidative Dehydrogenation of Propane on the Oxygen Adsorbed Edges of Boron Nitride Nanoribbons,” **Catalysis Science & Technology**, 2020, 10, 5181-5195.
<https://pubs.rsc.org/no/content/articlelanding/2020/cy/d0cy01031f/unauth#!divAbstract>
- ❖ K Abdelfatah, W Yang, V Solomon, **B Rajbanshi**, A Chowdhury, M Zare, S Kundu, A Yonge, A Heyden, and G Terejanu, “Prediction of transition state energies of hydrodeoxygenation reactions on transition metal surfaces based on machine learning,” **J. Phys. Chem. C**, 2019, 123, 29804-29810.

<https://pubs.acs.org/doi/abs/10.1021/acs.jpcc.9b10507>

- ❖ M Kar, **B Rajbanshi**, R Sarkar, S Pal, P Sarkar, “Periodically-Ordered One and Two Dimensional CdTe QD Superstructures: A Path Forward in Photovoltaics,” *Phys. Chem. Chem. Phys.*, 2019, 21, 19391-19402.
<https://pubs.rsc.org/am/content/articlelanding/2019/cp/c9cp03529j/unauth#!divAbstract>
- ❖ M Kar, **B Rajbanshi**, S Pal, P Sarkar, “Engineering the electronic structure of tin sulfide nanoribbons: A computational study,” *J. Phys. Chem. C*, 2018, 122 (10), 5731-5741.
<https://pubs.acs.org/doi/abs/10.1021/acs.jpcc.7b11453>
- ❖ **B Rajbanshi**, M Kar, P Sarkar, P Sarkar, “Phosphorene quantum dot-fullerene nanocomposites for solar energy conversion: An unexplored inorganic-organic nanohybrid with novel photovoltaic properties,” *Chem. Phys. Lett.*, 2017 685, 16-22.
<https://www.sciencedirect.com/science/article/abs/pii/S0009261417307030>
- ❖ **B Rajbanshi**, P Sarkar, “Is the Metallic Phosphorus Carbide (β_0 -PC) Monolayer Stable? An Answer from a Theoretical Perspective,” *J. Phys. Chem. Lett.*, 2017, 8 (4), 747-754.
<https://pubs.acs.org/doi/abs/10.1021/acs.jpcclett.6b02986>
- ❖ **B Rajbanshi**, P Sarkar, “Optimizing the Photovoltaic Properties of CdTe Quantum Dot-Porphyrin Nanocomposites: A Theoretical Study,” *J. Phys. Chem. C*, 2016, 120 (32), 17878-17886.
<https://pubs.acs.org/doi/abs/10.1021/acs.jpcc.6b04662>
- ❖ **B Rajbanshi**, S Sarkar, B Mandal, P Sarkar, “Energetic and electronic structure of penta-graphene nanoribbons,” *Carbon*, 2016, 100, 118-125.
<https://www.sciencedirect.com/science/article/abs/pii/S0008622316300148>
- ❖ **B Rajbanshi**, S Sarkar, P Sarkar, “The electronic and optical properties of $\text{MoS}_{2(1-x)}\text{Se}_{2x}$ and $\text{MoS}_{2(1-x)}\text{Te}_{2x}$ monolayers,” *Phys. Chem. Chem. Phys.*, 2015, 17 (39), 26166-26174.
<https://pubs.rsc.org/am/content/articlelanding/2015/cp/c5cp04653j/unauth#!divAbstract>
- ❖ S Sarkar, **B Rajbanshi**, P Sarkar, “Understanding the electronic structure of CdSe quantum dot-fullerene (C60) hybrid nanostructure for photovoltaic,” *J. Appl. Phys.*, 2014, 116 (11), 114303.
<https://aip.scitation.org/doi/abs/10.1063/1.4895775>
- ❖ **B Rajbanshi**, S Sarkar, P Sarkar, “Band gap engineering of graphene-CdTe quantum dot hybrid nanostructures”, *J. Mater. Chem. C*, 2014, 2 (42), 8967-8975.

<https://pubs.rsc.org/en/content/articlelanding/2014/tc/c4tc01735h/unauth#!divAbstract>

Oral Presentation

- ❖ A Heyden and **B Rajbanshi**, “Oxidative Dehydrogenation of Propane on Boron Nitride Catalyst: A Computational Investigation of Active Site as well as Involved Mechanism using Boron Nitride Nanoribbons,” **Accepted abstract**, 2019 AIChE annual meeting, November 10-15, 2019, Orlando, FL, USA.
<https://aiche.confex.com/aiche/2019/meetingapp.cgi/Paper/562311>

Poster Presentations

- ❖ **B Rajbanshi**, P Sarkar, “Is the Metallic Phosphorus Carbide (β_0 -PC) Monolayer Stable? An Answer from Theoretical Perspective,” 15th Indian Theoretical Chemistry Symposium, December 14th-17th, 2016, University of Hyderabad, Hyderabad, India.
- ❖ **B Rajbanshi**, P Sarkar, “Optimizing the Photovoltaic Properties of CdTe Quantum Dot-Porphyrin Nanocomposites,” Condense Matter Days, August 27th-29th, 2015, Department of Physics, Visva-Bharati, Santiniketan, India.
- ❖ **B Rajbanshi**, S Sarkar, P Sarkar, “Band gap engineering of graphene-CdTe quantum dot hybrid nanostructures,” Theoretical Chemistry Symposium, 18th-21st December, 2014, CSIR-National Chemical Laboratory, Pune, India.