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RESEARCH EXPERIENCE

❖ **Visva-Bharati** — Santiniketan, India
Department of Chemistry — Dec, 2020 - present
Assistant Professor

❖ **University of Massachusetts** — Amherst, USA
Department of Chemical Engineering — Aug, 2020 - Dec, 2020
Postdoctoral Associate
Advisor: Dr. Peng Bai

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

❖ **University of South Carolina** — Columbia, USA
Department of Chemical Engineering — Jan, 2018 - Aug, 2020
Postdoctoral Associate
Advisor: Dr. Andreas Heyden, Professor

- 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** — Santiniketan, India
Department of Chemistry — Oct, 2012 - Dec, 2017
Senior and Junior Research Fellow
Advisor: Dr. Pranab Sarkar, Professor

- 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. (Completed)

❖ **Empowerment and Equity Opportunities for Excellence in Science (EMEQ)**
(File no EEQ/2022/000312 dated 14.02.2023)
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. (Ongoing)

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

- A Pramanik, S Ghoshal, S Biswas, **B Rajbanshi**, P Sarkar, "Accurate Determination of Materials Properties: Role of Electron Density", Electron Density: Concepts, Computation and DFT Applications, 2024, 329-353. https://doi.org/10.1002/9781394217656.ch18

- W Yang, KE Abdelfatah, SK Kundu, **B Rajbanshi**, GA Terejanu, A Heyden, "Machine learning accelerated first-principles study of the hydrodeoxygenation of propanoic acid", **ACS Catalysis**, 2024, 14 (13), 10148-10163 https://doi.org/10.1021/acscatal.4c01419

- AV Le, **B Rajbanshi**, RF Lobo, P Bai, "Mechanistic study of heterogeneous propene metathesis on WO_x/SiO_2 catalysts", **Journal of Catalysis**, 2023, 427, 115117. https://doi.org/10.1016/j.jcat.2023.115117

- 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.jpclett.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 $MoS_{2(1-x)}Se_{2x}$ and $MoS_{2(1-x)}Te_{2x}$ 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.