Swastika Banerjee

Curriculum Vitae

Room 216, Block A
Department of Chemistry
IIT Roorkee
✉ *sbanerjee@cy.iitr.ac.in*

Professional Experience

Mar, 2022 - Present **Assistant Professor**, *Department of Chemistry*, IIT Roorkee, India.

Aug, 2021 - Mid-Mar, 2022 **Postdoctoral Associate**, *University of Luxembourg.*

Mar, 2019 - July, 2021 **Postdoctoral Associate**, *University of California San Diego, USA.*

Jul, 2017 - Feb, 2019 **Postdoctoral Researcher & Affiliate**, *Lawrence Berkeley National Laboratory, USA*, Shenzhen University, China.

Jan, 2017 - Jun, 2017 **Research Associate**, *Jawaharlal Nehru Center For Advanced Scientific Research, Bangalore, India.*

Nov, 2016 - Dec, 2016 **Visiting Scientist**, *Institute of Semiconductors, Chinese Academy of Science, Beijing, China.*

Education

2011 - 2017 **PhD**, *Jawaharlal Nehru Center For Advanced Scientific Research, Bangalore.*

2009 - 2011 **Master of Science**, *Department of Chemistry, Indian Institute of Technology Kharagpur*, CGPA: 9.1/10, ***IIT Rank: 3rd***.

2006 - 2009 **Bachelor of Science**, *Subject: Chemistry(Hons), Physics, Mathematics*, The University of Burdwan, India, 77.75 %, ***University Rank: 1st***.

Research Interests

- Role of Non-Local Many Body Dispersion Interactions on Materials' properties
- Electrochemistry and Interfacial phenomena
- Energy Storage focusing on Battery Materials Research
- Non-Adiabaticity in Chemical Reactions
- Thermoelectric property of Nanostructures
- First-principles electronic structure theory
- Algorithmic development for large scale simulation
- Creating Materials Data Infrastructure & Developing Materials Informatics

Research Experience

My prior research endeavor aimed to advance the materials engineering and understanding the electrochemical, chemical and transport properties through theory/computation. Computational method development includes Boltzmann Transport Equation coupled with Density Functional Theory, Non-Adiabatic Molecular Dynamics, Data-driven materials discovery and Machine Learning Molecular Dynamics for large scale simulation. These powerful tools have been utilized to target critical materials problems in the field of sustainable energy technology gaining momentum globally, namely, the electrochemical energy storage focusing on battery materials research and the solar energy conversion.

- **Designing Framework for Super-ionic Conduction of Alkali metals, a Principal Component for All-Solid-State-Battery:** Primary goal of my research is to target critical materials problems in the field of battery energy storage. Specifically, Lithium superionic conductors (LSCs) are of major importance as solid electrolytes for next-generation all-solid-state ion batteries (ASSBs). We have utilized **automated computation using first principles DFT and molecular dynamic simulation coupled with machine learning potential** based approaches to design new materials with enhancement in multiple properties for battery applications, including (i) principles to design anionic framework to achieve faster Na-conduction; (ii) Entropy-enhanced glass ceramics as a novel space of LSCs; (iii) Motif-based designing of Li/Na SEs that can potentially achieve a superior balance of stability, conductivity and compatibility with electrode compared to current liquid electrolyts.

- **Electrode for Rechargeable Alkali-ion Batteries, Focusing on Designing Insertion-Type Anode for Li and Post-Li Electrochemical Cell:** We have leveraged an array of computational techniques, such as, first principles **DFT and molecular dynamic** simulations for understanding the intercalation chemistry to design electrode materials for Li/Na/Mg-ion batteries.

- **Excited State Dynamics of Electron/hole and Non-adiabaticity:** We are interested in understanding the excited (hot) carrier dynamics in hybrid perovskites using a newly developed **Non-Adiabatic Molecular Dynamics** method. In this approach, the nuclear trajectory is based on Born–Oppenheimer ground state molecular dynamics, which is then followed by the evolution of carrier wave function including the detailed balance and decoherence effects.

- **Electronic Structure and Electron-Hole Transport with a Focus on Transport and Trapping of Charge Carriers in Semiconductors:** We have focused on the electron/hole transport behavior in layered semiconductors relevant to their application in transport devices using Boltzmann transport theory coupled with Density functional theory.
  Overall, being a theoretical/computational chemist, I have been fascinated to balance both the implementation of new method and exploring new parameters for smart materials design.

Selected key references:

- E. Wu, *et al.* **Nat. Commun.**, 12, 1256 (2021), *Equal first author
- S. Patel *et al.* **Chem. Mater.**, 33, 4, 1435–1443 (2021) *Equal first author
- A. Van der Ven *et al.* **Chem. Rev.**, 120, 14, 6977–7019 (2020)
- S. Banerjee *et al.* **J. Chem. Phys.**, 152 (9), 091102 (2020)
- S. Banerjee *et al.* **Chem. Mater.**, 31 (18), 7265-7276 (2019)
- S. Banerjee *et al.* **Phys. Chem. Chem. Phys**, 19 (32), 21282-21286 (2017)
- S. Banerjee *et al.* **Phys Chem. Chem. Phys.**, 18 (24), 16345-16352 (2016)
- S. Banerjee *et al.* **Chem. Commun.**, 52, 8381-8384 (2016)
- S. Banerjee *et al.* **J. Mater. Chem. A**, 4, 5517-5527 (2016)
- S. Banerjee *et al.* **J. Mater. Chem. A**, 2, 3856-3864 (2014)
- S. Banerjee *et al.* **Nanoscale**, 6 (22), 13430-13434 (2014)

Theoretical models & methods

- Non-adiabatic Molecular Dynamics & Boltzmann Transport Formalism
- Density Functional Theory (DFT) & Density Functional Perturbation Theory (DFPT)
- Conceptual Density Functional Theory based reactivity descriptors (Local, Non-local and Global)
- Time-Dependent Density Functional Theory (TDDFT)
- Data-driven materials design & analysis : Materials Project/Pymatgen,
- Classical and *ab-initio* molecular dynamics simulations

Experience with Home-grown code

Python Materials Genomics (pymatgen) materials analysis package, PWmat: Plane Wave Density Functional Theory Simulations Based on GPU, Fortran-90 code for implementation of Boltzmann Transport Formalism

DFT-based Packages

VASP, Quantum Espresso, SIESTA, CP2K, Gaussian (g03/g09), GROMACS and LAMMPS

Professional service as Journal reviewer

Angewandte Chemie, Chemistry of Materials, ACS Applied Energy Materials, Physical Chemistry Chemical Physics, Cell-Matter, Chem, Joule, Nature Communications

Selected Workshops/Conferences/Schools Attended

- MRS Fall Meeting & Exhibit, Boston, Massachusetts, USA, Dec-2021
- LINO19 "69th Lindau Nobel Laureate Meeting", Lindau, Germany, Jul-2019
- Post-doctoral Research Career Symposium, Lawrence Berkeley National Laboratory, USA, Jun-2018
- MRS Spring Meeting & Exhibit, Phoenix, Arizona, USA, April-2018
- Gordon Research Conference, Ventura, California, USA, Feb-2015. (Presented a poster)
- Faraday Discussion, University of Cambridge, Cambridge, UK, Sep-2013 (Presented a poster)
- "Chemical Frontiers-2015", Goa, India, Aug-2015. (poster and oral)
- "Light on Molecular Functional Materials", at JNCASR, Bangalore, Mar-2015.(Presented Poster)
- "MD@50" at JNCASR, Bangalore, Aug-2014. (Presented a poster)
- "Theoretical Chemistry Symposium", IISER-Pune, Dec-2014. (Presented a poster)
- "Directions in Materials Science", JNCASR, Bangalore, Nov-2013. (Presented a poster)
- "Molecular Material"s, IISc, Bangalore, Jul-2013.(Presented a poster)
- "Training Session on Intel Cluster Software Tools", JNCASR, Bangalore, India, Sep-2012
- "High Performance Computing Sciences and Engineering", JNCASR, Bangalore, Oct-2011

Awards/Scholarships/Fellowships/Achievements

2021: Ramanujan Fellowship (declined)
2021: Alexander von Humboldt Fellowship for Postdoctoral Researcher (declined)
2017: National Key R & D Program of China (Grant No. 2016YFB0700700)
2017: National Natural Science Foundations of China (Grant No. 11774239)
2016: Fellowship by Chinese Academy of Science (CAS) ***Visiting Scientist***
2015: ***International Travel Grant*** by Science and Engineering Research Board (SERB)
2015: ***Best Poster Award,*** "Chemical Frontiers", Aug-2015, Goa
2014: ***Best Poster Award,*** "Theoretical Chemistry Symposium", Dec-2014, IISER, Pune
2014: ***Best Poster Award,*** "Winter School on Frontiers in Materials", Dec-2014, JNCASR
2013: ***Best Poster Award,*** "STCC-FC", Jun-2013, Bharathidasan University, Tiruchirappalli
2011-2016: ***National Eligibility Test (NET) for Research Fellowship***
2011: ***Graduate Aptitude Test in Engineering (GATE)-2011 (All India Rank 16)***
2010-2011: Indian Institute of Technology-Kharagpur ***Merit Scholarship***
2010: Qualified Joint Admission test for M.Sc. ***(JAM)-2009***
2010: ***Jawaharlal Nehru Memorial Award*** *for First rank in The University of Burdwan*

Patents

1. "Novel chlorine-based sodium solid electrolyte", ***Swastika Banerjee***, Erik Wu, Hanmei Tang, Abhik Banerjee, Ying Shirley Meng, and Shyue Ping Ong, Submitted as **US patent** (2021), Application No. **SD2020-098-1**, **MD Ref. UCSD.20098PR**

Publications

1. "Role of Critical Oxygen Concentration in the β-$Li_3PS_{4-x}O_x$ Solid Electrolyte", ***Swastika Banerjee***, H.C. Manas Likhit and Shyue Ping Ong, **ACS Applied Energy Materials**, 5, 1, 35 (2022).
2. "Bridging the Gap Between Simulated and Experimental Ionic Conductivities in Lithium Superionic Conductors", Ji Qi, ***Swastika Banerjee***, Yunxing Zuo, Chi Chen, Zhuoying Zhu, H.C. Manas Likhit and Shyue Ping Ong, **Materials Today Physics**, 21, 100463 (2021).
3. "An Electrochemically-Stable Cathode-Solid Electrolyte Composite for Long-Cycle-Life Solid-State Sodium-ion Batteries", Erik Wu*, ***Swastika Banerjee***, Hanmei Tang*, Peter M Richardson, Jean-Marie Doux, Ji Qi, Zhuoying Zhu, Antonin Grenier, Yixuan Li, Enyue Zhao, Grayson Deysher, Han Nguyen, Ryan Stephens, Guy Verbist, Karena W Chapman, Raphaële J Clément, Abhik Banerjee, Ying Shirley Meng, and Shyue Ping Ong, **Nat. Commun.**, 12, 1256 (2021) *Equal first author
4. "Tunable Lithium Transport in Mixed-Halide Argyrodite", Sawan K. Patel*, ***Swastika Banerjee***, Haoyu Liu, Pengbo Wang, Po-Hsiu Chien, Xuyong Feng, Jue Liu, Shyue Ping Ong, Yan-Yan Hu, **Chem. Mater.**, 33, 4, 1435–1443 (2021) *Equal first author
5. "Effect of conjugation on the vibrational modes of a carbon nanotube dimer", Deepa Sharma, ***Swastika Banerjee***, Swapan K.Pati and Neena Jaggi, **Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy** , 246, 118985 (2021).
6. "Rechargeable Alkali-Ion Battery Materials: Theory and Computation", Anton Van der Ven, Zhi Deng, ***Swastika Banerjee*** and Shyue Ping Ong, **Chem. Rev.** 120 (14), 6977 (2020)
7. "The effects of interstitial iodine in hybrid perovskite hot carrier cooling: A non-adiabatic molecular dynamics study", ***Swastika Banerjee***, Jun Kang, Xiuwen Zhang, Lin-Wang Wang, **J. Chem. Phys.** 152 (9), 091102 (2020)
8. "Motif-Based Design of an Oxysulfide Class of Lithium Superionic Conductors: Toward Improved Stability and Record-High Li-Ion Conductivity", ***Swastika Banerjee****, Xiuwen Zhang and Lin-Wang Wang, **Chem. Mater.** 31 (18), 7265-7276 (2019) *Corresponding author and first author
9. "Designing a porous-crystalline structure of β-Ga_2O_3: a potential approach to tune its opto-electronic properties", ***Swastika Banerjee***,* Xiangwei Jiang, Lin-Wang Wang, **Phys. Chem. Chem. Phys.** 20, 14, 9471-9479 (2018) *Corresponding author and first author
10. "Regulation of transport properties by polytypism: a computational study on bilayer MoS_2",***Swastika Banerjee***, Jaehong Park, Cheol Seong Hwang, Jung-Hae Choi, Seung-Cheol Lee and Swapan K. Pati, **Phys. Chem. Chem. Phys.**, 19, 21282 (2017)
11. "Nanoscale Stabilization of Nonequilibrium Rock Salt BiAgSeS: Colloidal Synthesis and Temperature Driven Unusual Phase Transition", Satya Narayan Guin, ***Swastika Banerjee***, Dirtha Sanyal, Swapan K. Pati and Kanishka Biswas, **Chem. Mater.** 29, 3769-3777 (2017)
12. "Synthetically Tuned Structural Variations in Ce_2PdGe_3 Towards Magnetic Exchange Bias and other Physical Properties",Sumanta Sarkar, ***Swastika Banerjee***, Pramod Halappa, Deepti Kalsi, Swapan K. Pati, Somnath Ghara, A. Sundaresan, Ivan da Silva, Rajeev Rawat, Sudhindra Rayaprol, Boby Joseph and Sebastian C. Peter, **Inorg. Chem. Front.**, 4, 241 (2017)
13. "Black Phosphorus as Anode for Magnesium-ion Battery: The Significance of Mg-P Bond-synergy", ***Swastika Banerjee*** and Swapan K. Pati, **Chem. Commun.** 52, 8381-8384 (2016)
14. "First-principles Design of a Borocarbonitride based Anode for Superior Performance in Sodium-ion Battery and Capacitor", ***Swastika Banerjee***, Siam Khanthang Neihsial, and Swapan K. Pati, **J. Mater. Chem. A**, 4, 5517-5527 (2016)
15. "Origin of order-disordered phase transition and anomalous change of thermopower in $AgBiS_2$ Nanocrystals: A combined experimental and theoretical study", Satya N. Guin, ***Swastika Banerjee***, Dirtha Sanyal, Swapan K. Pati and Kanishka Biswas, **Inorg. Chem.** 55 (12), 6323-6331 (2016)
16. "Charge-transport anisotropy in black phosphorus: critical dependence on the number of layers",***Swastika Banerjee*** and Swapan K. Pati, **Phys. Chem. Chem. Phys.** 18, 16345-16352 (2016)
17. "$Eu_3Ir_2In_{15}$: A Mixed-Valent and Vacancy-Filled Variant of the $Sc_5Co_4Si_{10}$ Structure Type with

Anomalous Magnetic Properties" Sumanta Sarkar, ***Swastika Banerjee***, Rajkumar Jana, Ramesh Siva, Swapan K Pati, Mahalingam Balasubramanian, Sebastian C Peter, **Inorg. chem.**, 54 (22), 10855-10864 (2015)

18. "Surface-Mediated Extraction and Photoresponse Modulation of Bisphenol A Derivatives: A Computational Study" ***Swastika Banerjee*** and Swapan K. Pati, **ACS applied materials & interfaces**, 7 (43), 23893-23901 (2015)
19. "Criticality of Surface Topology for Charge-carrier Transport Characteristics in Two-Dimensional Borocarbonitrides: Design Principle of an Efficient Electronic Material" ***Swastika Banerjee*** and Swapan K. Pati, **Nanoscale**, 6, 13430-13434 (2014)
20. "Possible application of 2D-boron sheets as anode material in lithium ion battery: A DFT and AIMD study" ***Swastika Banerjee***, Ganga Periyasamy and Swapan K. Pati, **J. Mater. Chem. A**, 2, 3856-3864(2014).
21. "Formation Mechanism and Possible Stereo Control of Bisphenol A derivatives: A Computational Study" **Swastika Banerjee**, Ganga Periyasamy and Swapan K. Pati, **J. Phys. Chem. B**, 118, 9258-9262 (2014).
22. "Structural, optical and hydrogen adsorption properties of B_9/metal-B_9 clusters: A Density Functional Theoretical Study" ***Swastika Banerjee***, Ganga Periyasamy and Swapan K. Pati, **Phys. Chem. Chem. Phys.**, 15 , 8303-8310 (2013).
23. "Role of Lithium Decoration on Hydrogen Storage Potential" Sudip Pan, ***Swastika Banerjee***, Pratim Kumar Chattaraj, **J. Mex. Chem. Soc.** 56, 3, 229-240 (2012).