

Shweta Choudhary

PM Research Fellow

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Education

- 2022–present **PhD in Computational Chemistry**, Department of Chemistry, Indian Institute of Technology Roorkee, India
- 2020–2022 **Master of Science in Chemistry**, Department of Chemistry, Indian Institute of Technology Roorkee, India, CGPA: 8.88/10
- 2017–2020 **Bachelor of Science with honor in Chemistry**, Department of Chemistry, Gargi College, University of Delhi, India, CGPA: 9.23/10

Research Experience

- 2021–2022 **Graduate student**, “First-principle investigation for anode material for beyond Li-ion batteries, focusing on designing low-dimensional anodes for Na-ion batteries”, Indian Institute of Technology Roorkee, India

Advisor: **Prof. T. J. Dilip Kumar**

Publications

- 2025 **Choudhary, S.** & Banerjee, S. Ion coordination and migration mechanisms in alkali metal complex borohydride-based solid electrolytes. *Communications Chemistry* **8**, 123 (2025)
- 2025 Saroha, R., **Choudhary, S.**, Brahma, R. & Banerjee, S. Designing Superatomic (Li/Na/K)-Al-Sc Cluster Catalysts for Selective Electrochemical HER and NRR. *The Journal of Physical Chemistry C* **129**, 6562–6573 (2025)
- 2024 **Choudhary, S.**, Saroha, R. & Banerjee, S. Efficient Electron Injection into Graphullerene Enables Reversible NaC₂ Sodium Storage. *ACS Applied Materials & Interfaces* **16**, 50859–50869 (2024)
- 2023 Saini, V.[†], Krishankant[†], **Choudhary, S.**[‡], Gaur, A., Banerjee, S., Bagchi, V. & Venkatesh, V. Atomically Precise Copper Nanoclusters as a Potential Catalyst for the Electrochemical Oxygen Evolution Reaction. *Journal of Materials Chemistry A* **11**, 24754–24763 (2023) [‡]Second author
- 2022 **Choudhary, S.**, Duhan, N. & Kumar, T. D. Hydrogen Passivated β 12-Borophene Nanoribbon: A Propitious One-dimensional Metallic Anode for Sodium-ion Rechargeable Batteries. *Applied Surface Science* **606**, 154825 (2022)

Awards, Fellowships & Academic Achievements

- 2024 Best Poster Award, ChemDay 2024 at IIT Roorkee

- 2024 Best Poster Award, CRSI-ACS Early Career Researchers' Symposium 2024 at KIIT Bhubaneswar
- 2023 Prime Minister Research Fellowship (PMRF)
- 2022 Qualified Graduate Aptitude Test in Engineering (GATE)
- 2020 Qualified IIT- Joint Admission Test (JAM)

Experience with Theoretical Models, Methods & Packages

Models & methods	Density functional theory (DFT), density functional perturbation theory (DFPT), nudged elastic band method (NEB), growing string method, classical and <i>ab initio</i> molecular dynamics simulations, Quasi-Harmonic Approximation
GUI and Python modules	Pymatgen, ASE, VASPKIT code, baderVis, VTST tools, VESTA, VMD, sumo, pyband, Aimstools, GIMS, Phonopy, aimsChain
DFT-based Packages	VASP, FHI-aims, FHI-vibes, i-PI, Gaussian, GaussView, Critic2, Material Studio, Avogadro, CP2K, and GROMACS
Technical skills	Anaconda, Python, Bash/Shell scripting, LaTeX
Architectures	Linux, Mac, Windows

Workshops, Presentations & Conferences

- Jan 2025 **Evolution of Electronic Structure Theory & Experimental Realization (EESTER)**, SRM Institute of Science and Technology & IIT Madras. (Attended workshop & Presented poster)
- Dec 2024 **Conference on Advances in Chemistry for Energy and Environment (CACEE)**, TIFR Mumbai. (Presented poster)
- Nov 2024 **Research Scholar's Day-ChemDay**, Department of Chemistry, IIT Roorkee. (Received best poster award)
- Oct 2024 **CRSI-ACS Early Career Researchers' Symposium**, KIIT Bhubaneswar. (Received best poster award)
- Jan 2024 **International Conference on Functional Materials**, IIT Kharagpur. (Presented poster)

Referees

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