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 Ropar*, 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 Ropar, India

Advisor: **Dr. T. J. Dhilip 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 β12-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 *ab initio* 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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