Shweta Choudhary

Prime Minister Research Fellow

Personal Details

Date of Birth	13 Nov 1999
Nationality	Indian
Address	Department of Chemistry, Indian Institute of Technology Roorkee, Haridwar-247667, Uttarakhand, India
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Area of research	Computational chemistry

Education

Dec 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: **Prof. 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 super-atomic (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 NaC_2 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. & Dhilip Kumar, T. J. Hydrogen passivated β_{12}-borophene nanoribbon: a propitious one-dimensional metallic anode for sodium-ion rechargeable batteries. *Applied Surface Science* **606,** 154825 (2022)

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)

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

Referees

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