Sk Mujaffar Hossain, Ph.D.

Computational Materials Science & Quantum Computing

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Research Vision

I am a computational materials scientist with research interests spanning electronic structure, energy storage materials, and quantum simulation. My doctoral and postdoctoral training have equipped me with a unique blend of DFT, quantum chemistry, and quantum computing skills. I thrive in collaborative environments that connect computation with experimental insight, and I seek a research opportunity to expand this integration further..

Employment History

2024 – present — **R&D Post Doctoral Fellow,** Indo-Korea Science and Technology (IKST) Center Bengaluru, India.

2022 – 2024 — **Research Associate (RA),** Research Institute of Sustainable Energy (RISE) TCG CREST, Kolkata, India.

2015 – 2016 — **Junior Research Fellow (JRF)**, Indian Institute of Technology Bombay (IITB), India

Education

2016 – 2022 — **Ph.D., Computational Chemistry,** IISER Pune, India.
Thesis title: *Combined Theoretical and Experimental Studies of Some Antiperovskite Systems and their Energy Applications.*
Advisor: *Prof. Satish Ogale and Dr. Prasenjit Ghosh*

2012 – 2014 — **M.Sc. Physics,** Presidency University, Kolkata, India.
Thesis title: *A study of the electronic properties of graphene allotropes and its extended defects.*
Advisor: *Late Emeritus Prof. Abhijit Mookerjee*

2009 – 2012 — **B.Sc. Physics,** Vidyasagar University, West Midnapre, India.

Skills

Technical Programming — Python, Bash, Fortran90, LaTeX, Git, Conda, Jupyter, Shell scripting.

Quantum Simulation — Qiskit, Qiskit Nature, VQE, qEOM, QPE, SQD, Qubit mappings: JW, BK, Parity, Active Space Modeling, Quantum ML.

Skills (continued)

Computational Chemistry — VASP, Quantum ESPRESSO, Phonopy, BoltzTrap2, PySCF, Gaussian16, SIESTA, GROMACS, QuantumATK, Visualization: VESTA, XCrySDen, VMD, Chimera, Ovito, and etc.

Machine Learning & Data Analysis — Scikit-learn, PyTorch, Matminer, Pymatgen, XenonPy; Feature engineering, Model building, Property prediction, Explainability, NumPy, Pandas, Matplotlib, Seaborn, Origin, Xmgrace.

Scientific Communication — Manuscript writing, Data visualization, graphical abstract design, Tools: ChemDraw, Inkscape, Blender, ChemCraft.

Languages — English (fluent), Bengali (native), Hindi (fluent)

Research Publications

Preprints and Submitted Manuscripts

To view recently submitted & published work please click here.

Journal Articles

1. T. Ghogare, I. Patil, **Sk Mujaffar Hossain**, *et al.*, "Earth-abundant 3d-transition metal metasilicates as effective electrocatalysts for alkaline her: Cuznsio3 outperforms cusio3 and znsio3," *ChemSusChem*, vol. 18, no. 9, e202402043, 2025. DOI: 10.1002/cssc.202402043.
2. **S. M. Hossain**, N. A. Koshi, S.-C. Lee, G. Das, and S. Bhattacharjee, "Integrating density functional theory with deep neural networks for accurate voltage prediction in alkali-metal-ion battery materials," *Small Methods*, e02076, 2025. DOI: 10.1002/smtd.202502076.
3. R. Godbole, S. Hiwase, **Sk Mujaffar Hossain**, *et al.*, "Light element (b, n) co-doped graphitic films on copper as highly robust current collectors for anode-free li metal battery applications," *Applied Physics Reviews*, vol. 11, no. 3, 2024. DOI: 10.1063/5.0208785.
4. **Sk Mujaffar Hossain**, N. Kumar, B. Debnath, and S. Ogale, "Core–shell cu1- x nco3- y/a-cufeco antiperovskite as high-performance anode for li-ion batteries," *Journal of Physics: Energy*, vol. 6, no. 1, p. 015 008, 2024. DOI: 10.1088/2515-7655/ad08d9.
5. B. Debnath, S. Singh, **Sk Mujaffar Hossain**, S. Krishnamurthy, V. Polshettiwar, and S. Ogale, "Visible light-driven highly selective co2 reduction to ch4 using potassium-doped g-c3n5," *Langmuir*, vol. 38, no. 10, pp. 3139–3148, 2022. DOI: 10.1021/acs.langmuir.1c03127.
6. B. Debnath, **Sk Mujaffar Hossain**, A. Sadhu, S. Singh, V. Polshettiwar, and S. Ogale, "Construction of a 2d/2d g-c3n5/nicr-ldh heterostructure to boost the green ammonia production rate under visible light illumination," *ACS Applied Materials & Interfaces*, vol. 14, no. 32, pp. 37 076–37 087, 2022. DOI: 10.1021/acsami.2c03758.

7. A. Biswas, A. Sengupta, **Sk Mujaffar Hossain**, *et al.*, "Growth, properties, and applications of pulsed laser deposited nanolaminate ti_3alc_2 thin films," *Phys. Rev. Applied*, vol. 13, no. 1, p. 044 075, 2020. DOI: 10.1103/PhysRevApplied.13.044075.

8. K. Roy, V. Chavan, **Sk Mujaffar Hossain**, *et al.*, "Fe3snc@ cnf: A 3 d antiperovskite intermetallic carbide system as a new robust high-capacity lithium-ion battery anode," *ChemSusChem*, vol. 13, no. 1, pp. 196–204, 2020. DOI: 10.1002/cssc.201902508.

Miscellaneous Experience

Awards and Achievements

2016 — **MHRD Fellowship**, Ph.D. doctoral fellowship grant from Ministry of Human Resource and Development (MHRD), Govt. of India.

2020 — **Teaching assistant award**, for winter school on "Electronic Structure and Molecular Dynamics Simulations"

2002-2008 — **Merit-Cum Means Scholarship**, Government of West Bengal from class VI-XII

Certification

2025 — **Certified Quantum Computing**. Quantum Computing course jointly conducted by C-DAC and IIT Roorkee, with support from the Ministry of Electronics and Information Technology (MeitY), Government of India.

Teaching Experience

2018 — **Teaching Assistant**, Chemical Principle I Course (CHM101), IISER Pune.

Teaching Assistant, Computational Modelling Course (CMC101), IISER Pune.

2019 — **Teaching Assistant**, Chemical Principle II Course (CHM102), IISER Pune.

Teaching Assistant, Principles of Physical Chemistry Course (CH1213), IISER Pune.

Conferences, Workshops, and Schools

2025 — **Talk:** Korea–India Research Joint Workshop — Kookmin University and KIST, Seoul, South Korea (8–25 May 2025).

Poster: International Conference on Sustainable Batteries - TCG CREST, Kolkata, India (24-27 Feb 2025). [**Receive best poster award**]

Participant: International School on Modelling and Simulations of Materials — JNCASR, Bengaluru, India (20–22 Jan 2025).

2021 — **Participant:** COMSOL Multiphysics — Intensive Online Training Course.

Conferences, Workshops, and Schools (continued)

2020 **Participant:** EESTER-2020 — Evolution of Electronic Structure Theory & Experimental Realization, IIT Madras, Chennai, India.

Participant: Winter School on Electronic Structure and Molecular Dynamics Simulation — Kathmandu University, Nepal.

2018 **Talk:** "Machine Learning in Materials Science" — Departmental Seminar, IISER Pune, India.

Participant: EESTER-2018 — Evolution of Electronic Structure Theory & Experimental Realization, SRM University, Chennai, India.

References

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