

Sk Mujaffar Hossain, Ph.D.

Computational Materials & Quantum Computations

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Research Vision

I am a computational materials scientist integrating first-principles electronic structure methods, materials-focused machine learning, and near-term quantum algorithms to address computational bottlenecks in energy materials and excited-state chemistry. My research spans density functional theory, quantum chemistry, and variational quantum simulation, with emphasis on active-space design, methodological rigor, and reproducible workflows. I focus on problems where classical approaches become computationally intensive or opaque, and where hybrid classical-quantum strategies may offer scalable alternatives. I seek to advance this integration further by developing coherent frameworks that connect predictive modeling, algorithmic innovation, and experimentally relevant materials systems.

Employment History

- 2024 – present **R&D Post Doctoral Fellow**, Indo-Korea Science and Technology (IKST) Center Bengaluru, India.
Research focus: Integration of density functional theory, materials-focused machine learning, and quantum algorithms (VQE-qEOM, SQD) for materials and molecules.
- 2022 – 2024 **Research Associate (RA)**, Research Institute of Sustainable Energy (RISE) TCG CREST, Kolkata, India.
Research focus: First-principles modeling and machine learning for alkali-ion battery materials, including high-throughput descriptor development and voltage prediction frameworks.
- 2015 – 2016 **Junior Research Fellow (JRF)**, Indian Institute of Technology Bombay (IITB), India
Research focus: Electronic structure calculations and materials modeling using density functional theory.

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 Midnapore, India.

Research Publications

Preprints and Submitted Manuscripts


🌐 [To view recently submitted manuscripts please click here.](#)

Journal Articles


- 1 **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*, eo2o76, 2026.
- 2 **S. M. Hossain**, S.-C. Lee, and S. Bhattacharjee, "Quantum simulations of battery electrolytes using variational quantum eigensolver, equation-of-motion, and sample-based diagonalization methods: Active-space design, dissociation, and excited states of lipf₆, napf₆, and fsi salts," *Advanced Quantum Technologies*, vol. 9, no. 2, e00871, 2026.
- 3 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.
- 4 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.
- 5 **Sk Mujaffar Hossain**, N. Kumar, B. Debnath, and S. Ogale, "Core-shell cu_{1-x} nco_{3-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.
- 6 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.
- 7 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.
- 8 A. Biswas, A. Sengupta, **Sk Mujaffar Hossain**, *et al.*, "Growth, properties, and applications of pulsed laser deposited nanolaminate ti₃alc₂ thin films," *Phys. Rev. Applied*, vol. 13, no. 1, p. 044 075, 2020.  DOI: 10.1103/PhysRevApplied.13.044075.
- 9 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.

Skills


Technical Programming

 Python, Bash, Fortran90, L^AT_EX, Git, Conda, Jupyter, Shell scripting.

Quantum Simulation

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

Computational Chemistry

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

Skills (continued)

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)

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).
	■ Participant: International School on Modelling and Simulations of Materials — JNCASR, Bengaluru, India (20–22 Jan 2025).
2021	■ Participant: COMSOL Multiphysics — Intensive Online Training Course.
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.


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

Miscellaneous Experience (continued)

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.

References


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