Sk Mujaffar Hossain, Ph.D.

Computational Materials Science & Quantum Computing

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Research Vision

I am a computational materials scientist integrating first-principles electronic structure methods, materials-focused machine learning, and variational quantum algorithms to address computational bottlenecks in materials and molecular systems. My work spans density functional theory, quantum chemistry, and quantum simulation, with particular emphasis on active-space design, algorithmic benchmarking, and reproducible hybrid classical–quantum workflows. I focus on chemically and energetically relevant systems where conventional approaches become computationally intensive or lack interpretability, and where quantum-enhanced strategies may offer scalable alternatives. My research aims to develop coherent frameworks that unify predictive modeling, quantum algorithm development, and experimentally meaningful materials problems.

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 Midnapre, India.

Research Publications

Preprints and Submitted Manuscripts

To view recently submitted manuscripts please click here.

Journal Articles

1. **Sk Mujaffar Hossain** et al. "Integrating Density Functional Theory with Deep Neural Networks for Accurate Voltage Prediction in Alkali-Metal-Ion Battery Materials". In: *Small Methods* (2026), e02076. DOI: 10.1002/smtd.202502076.
2. **Sk Mujaffar Hossain**, Seung-Cheol Lee, and Satadeep 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 $LiPF_6$, $NaPF_6$, and FSI Salts". In: *Advanced Quantum Technologies* 9.2 (2026), e00871. DOI: 10.1002/qute.202500871.
3. Trupti Ghogare et al. "Earth-Abundant 3d-Transition Metal Metasilicates As Effective Electrocatalysts For Alkaline HER: CuZnSiO3 Outperforms CuSiO3 and ZnSiO3". In: *ChemSusChem* 18.9 (2025), e202402043. DOI: 10.1002/cssc.202402043.
4. Rhushikesh Godbole et al. "Light element (B, N) co-doped graphitic films on copper as highly robust current collectors for anode-free Li metal battery applications". In: *Applied Physics Reviews* 11.3 (2024). DOI: 10.1063/5.0208785.
5. **Sk Mujaffar Hossain** et al. "Core–shell Cu1- x NCo3- y/a-CuFeCo antiperovskite as high-performance anode for Li-ion batteries". In: *Journal of Physics: Energy* 6.1 (2024), p. 015008. DOI: 10.1088/2515-7655/ad08d9.
6. Bharati Debnath et al. "Visible Light-Driven Highly Selective CO2 Reduction to CH4 Using Potassium-Doped g-C3N5". In: *Langmuir* 38.10 (2022), pp. 3139–3148. DOI: 10.1021/acs.langmuir.1c03127.
7. Bharati Debnath et al. "Construction of a 2D/2D g-C3N5/NiCr-LDH heterostructure to boost the green ammonia production rate under visible light illumination". In: *ACS Applied Materials & Interfaces* 14.32 (2022), pp. 37076–37087. DOI: 10.1021/acsami.2c03758.
8. Abhijit Biswas et al. "Growth, Properties, and Applications of Pulsed Laser Deposited Nanolaminate Ti_3AlC_2 Thin Films". In: *Phys. Rev. Applied* 13.1 (2020), p. 044075. DOI: 10.1103/PhysRevApplied.13.044075.
9. Kingshuk Roy et al. "Fe3SnC@ CNF: A 3 D Antiperovskite Intermetallic Carbide System as a New Robust High-Capacity Lithium-Ion Battery Anode". In: *ChemSusChem* 13.1 (2020), pp. 196–204. DOI: 10.1002/cssc.201902508.

Skills

Computational Methods — Density Functional Theory (VASP, Quantum ESPRESSO, SIESTA), Ab Initio Molecular Dynamics (GROMACS), Phonon and Transport Analysis (Phonopy, BoltzTrap2), Quantum Chemistry (PySCF, Gaussian16)

Quantum Simulation — VQE, qEOM, SQD, QPE, Qubit mappings: JW, BK, Parity, Active Space Modeling, Qiskit, Qiskit Nature, PennyLane, IBM Quantum Experience (cloud backends).

Materials AI/ML — Physics-informed descriptors, Neural Networks (PyTorch), Feature Engineering, Model Interpretability, Scikit-learn, PyTorch, Matminer, Pymatgen, XenonPy, M3GNet, CGCNN.

Skills (continued)

Programming & HPC — Python, Bash, Fortran90, LaTeX, Git, Conda, Jupyter, SLURM, Workflow Automation

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

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.

Miscellaneous Experience (continued)

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

Prof. Satadeep Bhattacharjee
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