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 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 Midnapre, 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*, e02076, 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 $lipf_6$, $napf_6$, 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 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.
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 ti_3alc_2 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

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

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