

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*, 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: CuZnSiO_3 outperforms CuSiO_3 and ZnSiO_3 ,” *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 $\text{Cu}_{1-x}\text{Ni}_{x}\text{O}_3$ –y/a–CuFeO antiperovskite as high-performance anode for Li-ion batteries,” *Journal of Physics: Energy*, vol. 6, no. 1, p. 015008, 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 CO_2 reduction to CH_4 using potassium-doped g-C₃N₄,” *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-C₃N₄/NiCr-LDH heterostructure to boost the green ammonia production rate under visible light illumination,” *ACS Applied Materials & Interfaces*, vol. 14, no. 32, pp. 37076–37087, 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. 044075, 2020. DOI: 10.1103/PhysRevApplied.13.044075.
- 9 K. Roy, V. Chavan, **Sk Mujaffar Hossain**, et al., “ $\text{Fe}_3\text{SNC}@\text{CNF}$: 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

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| Technical Programming | ■ Python, Bash, Fortran90, L ^A T _E X, 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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