MD. DIDARUL ISLAM

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EDUCATION

Shahjalal University of Science and Technology, Sylhet April 2024 - October 2025 (Expected)
M.Sc. in Physics (Thesis ongoing) CGPA: 3.55/4

Shahjalal University of Science and Technology, Sylhet January 2019 - March 2024
B.Sc. in Physics CGPA: 3.67/4

RESEARCH INTEREST

- Density Functional Theory
- Material Science
- Condensed Matter Physics
- Computational Physics

TECHNICAL SKILLS

Language	Python
Python Packages	Numpy, Pandas, Matplotlib, DeePMD-kit, Keras, Tensorflow
Software	Quantum Espresso, LAMMPS, Vesta, Xcrysden, Latex, Vim

RESEARCH EXPERIENCE

RESEARCH ASSISTANT Jan 2024 – Present
High Performance Computing Laboratory, Department of Physics, Shahjalal University of Science and Technology (SUST)
Supervisor: Dr. Enamul Haque, Associate Professor, Department of Physics, SUST
Project: Nanoparticle-Induced Signal Enhancement in Biosamples Using the Z-Scan Method.

- Performed DFT and TDDFT simulations to investigate the electronic and optical properties of nanoparticles (iron oxides, copper oxides, aluminum oxides) that were experimentally synthesized via laser ablation in the Nonlinear Optics Laboratory, SUST.
- Processed, optimized, and analyzed data obtained from Z-scan experiments.
- Maintained the GPU node of the High-Performance Computing (HPC) system.

RESEARCH INTERN November 2024 – Present
Supervisor: Dr. Muhammad Omar Faruk, Professor, Department of Physics, SUST.

- Conducted first-principles DFT+U investigations of spinel oxide and double perovskites to study their structural, electronic, optical, and thermoelectric properties.

CONFERENCE PRESENTATIONS

- "Electronic Characterization of FeO using Density Functional Theory with Hubbard Corrections.": **Md. Didarul Islam**, Md. Jahidul Islam, Afroza Akter, Md. Enamul Hoque. National Conference On Physics For The 21st Century, Khulna University, May 2024. (Accepted for oral presentation)
- "Comparative Study of ZnO Nanoparticles: Experimental Evaluation and Density Functional Theory Predictions of Electronic and Optical Properties": **Md. Didarul Islam**, Md. Jahidul Islam, and M.E. Hoque. ICMIME 2024 – International Conference on Mechanical, Industrial, and Materials Engineering, December 2024. (Accepted for full paper submission)

- "First-Principles Calculations and Experimental Investigation of Copper Oxides: Analysis of Electronic Structure and Optical Properties": **Md. Didarul Islam**, Md. Jahidul Islam, M.M Chowdhury and M.E.Hoque. 9th Conference of Bangladesh Crystallographic Association (BCA) 10 – 11 January, 2025, Dhaka. (Accepted for poster presentation)
- "First-Principles Investigation of Structural, Electronic, and Optical Properties of $ZnCr_2O_4$ Using DFT with Hubbard Corrections": **Md. Didarul Islam**, Abdul Wahid Chowdhury, Muhammad Omar Faruk. 8th ICERIE 2025 Conference, April 24–26, 2025, at the SUST Campus, Sylhet. (Accepted for full paper submission)

JOURNAL PUBLICATION IN PROGRESS

- "Structural, Electronic, Optical, and Thermoelectric Properties of Gd_2MnCoO_6 Using DFT with Hubbard Corrections".(Manuscript in preparation)
- "Preparation and Characterization of Iron Oxide Nanoparticles via Laser Ablation Using Nd:YAG Pulsed Laser: Electronic and Nonlinear Optical Properties".(Manuscript in preparation)

PROJECTS

GPU Accelerated Quantum Espresso

- Configured a High-Performance Computing (HPC) node with two Nvidia GTX 1080 Ti GPUs for Quantum Espresso. Link

VC-MD to DeePMD-kit Converter

- Developed a Python package to extract atomic positions, forces, energies, and trajectories from VC-MD simulations run with Quantum Espresso, and convert them into the format required for DeePMD-kit training. Link

TUTORIALS

Tutorial Author – From Quantum Espresso to DeePMD-kit [Link]

- Created a tutorial on installing DeePMD-kit, preparing Quantum ESPRESSO data, training interatomic potentials, and running molecular dynamics in LAMMPS.

HONORS AND AWARDS

- Bronze Medal, University Physics Competition (USA) – 2021, 2022, 2023.
- 20th position in the International Theoretical Physics Competition – 2021.
- Government Scholarships for PSC (2010), JSC (2013), and SSC (2016).

TEACHING EXPERIENCE

- Teaching Eleven Grade and O level students as a home tutor.

EXTRA-CURRICULAR ACTIVITIES

- Seminar and Student Welfare Secretary of the SUST Physics Society.
- General Member of Copernicus Astronomical Memorial (CAM-SUST).

REFERENCES

Dr. Enamul Haque
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Muhammad Omar Faruk
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