Md. Al Mahmud

mdalmahmudanik@gmail.com | mdalmahmud.com | linkedin.com/in/mdalmahmud023

Profile

Fourth-year Materials Science and Engineering undergraduate at the University of Rajshahi with research experience in first-principles computational materials science. Currently investigating fluoride double perovskites using Quantum ESPRESSO and contributing to collaborative WIEN2k electronic-structure calculations. Experienced with Linux-based computational workflows, DFT/DFT+U, scientific data analysis and visualization, with working knowledge of Python.

Education

University of Rajshahi, B.Sc. Engineering in **Materials Science and Engineering** 01/11/2022 – Current

Department of Materials Science and Engineering, Faculty of Engineering

- **Fourth-year undergraduate** | Expected graduation: August 2027
- **CGPA:** 3.77 / 4.00 (cumulative through third year)
- **Relevant Coursework:** Crystallography and Structure of Materials; Electronic Properties of Materials; Optics and Optical Properties of Materials; Materials Thermodynamics and Kinetics; Magnetic and Dielectric Materials; Microscopic Methods in Materials Characterisation; Surface Science and Engineering; Introduction to Nanomaterials and Biomaterials.

Research Experience

Undergraduate Research Project March 2026 – Present

Department of Materials Science and Engineering, University of Rajshahi, Bangladesh
Supervisor: Prof. Dr. Md. Mijanur Rahaman

Current Research – Na_2MgCdF_6

- Conduct first-principles investigation of the fluoride double perovskite Na_2MgCdF_6 using Quantum ESPRESSO with PBEsol and DFT+U.
- Perform convergence testing, variable-cell structural optimization, EOS fitting, band-structure and DOS/PDOS calculations.
- Investigate Hubbard-U and magnetic effects using independently relaxed structures and spin-polarized FM/AFM calculations; the material retains a direct Γ–Γ wide band gap of approximately 4.28–4.73 eV over U = 0–8 eV with essentially zero Cd magnetic moment.
- Perform optical-property calculations including dielectric, refractive, absorption, reflectivity, conductivity and energy-loss responses with systematic numerical convergence testing.
- Use Python, Bash, Linux, OriginPro and VESTA for workflow management, data extraction, post-processing and visualization.

Earlier exploratory study – Na_2CaCdF_6

- Investigated structural, elastic and phonon properties using Quantum ESPRESSO; identified strong cubic-phase phonon instabilities and explored lower-symmetry structures generated from unstable phonon modes.

Research Collaboration

Collaborative Computational Research – $HfNi_2Ga$

- Contribute to a collaborative first-principles investigation of $HfNi_2Ga$ using WIEN2k.
- Performed Ni Hubbard-U screening from U = 2.5–4.5 eV, including spin-polarized band-structure and DOS calculations using TB-mBJ.
- Currently extending the study to combined Hf-U/Ni-U configurations, including Hf U = 6, 8 eV and Ni U = 2 eV.

Projects

Quantum ESPRESSO Workflow GUI March 2026 – Present

Independent Project

- Designed and built an AI-assisted Python/Streamlit GUI for Quantum ESPRESSO computational workflows.
- Supports structure import and 3D visualization, pseudopotential/k-point/calculation configuration, and automatic QE input generation.
- Includes convergence testing, EOS fitting, calculation management, QE output analysis and visualization of band structures and DOS, with structure handling through ASE.

Document Processing Web Application June 2025

CS50x Project

- Developed a Python/Flask web application allowing users to merge and split PDF documents.
- Implemented user registration and authentication using SQLite, together with server-side PDF-processing functionality.

Skills

Computational Materials Science: WIEN2k, Quantum ESPRESSO, DFT and DFT+U, structural optimization and convergence testing, band structures, DOS and PDOS, spin-polarized and magnetic-property calculations, elastic and optical properties, equation-of-state analysis

Data Analysis & Visualization: VESTA, OriginPro, Matplotlib

Scientific Computing: Python (practical scientific use), Bash/Shell, Linux and WSL

Scientific/Development Tools: Atomic Simulation Environment (ASE), Streamlit and Flask, Git and GitHub, NumPy

Materials Characterization Exposure: EDXRF and UV/Visible spectroscopy (training exposure), GC/HPLC (training exposure), corrosion, cathodic protection and NDT (training exposure)

Languages: Bengali (mother tongue), English

Industrial Training

Industrial Engineering Trainee 25/04/2026 – 21/05/2026

Training Institute for Chemical Industries (TICI), Bangladesh

- Completed a four-week Industrial Process Unit Operation & Process Control Technique training programme covering industrial process operations and process control.
- Gained practical exposure to EDXRF, UV/Visible spectroscopy, GC/HPLC, corrosion, cathodic protection and NDT.
- Received training in industrial instrumentation and automation, including PLC, SCADA, PID control, sensors and transmitters.

Certifications

HarvardX CS50AI: Introduction to Artificial Intelligence with Python – 25/08/2025 Certificate

HarvardX CS50x: Introduction to Computer Science – 29/07/2025 Certificate

Open-Source Experience

Unofficial Evolution X Custom ROM Maintainer Sep 2024 – Dec 2025

Xiaomi Mi A2 Lite (daisy) | 8,500+ combined downloads across GitHub and SourceForge

- Compiled and maintained Android custom-ROM builds using Linux and Git/GitHub, including source synchronization, build troubleshooting and public releases.
- Supported the Android 14–15 transition and maintained releases for the device community.