Osman Goni Ridwan

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Education

Ph.D. Candidate, Mechanical Engineering Jan 2022 – Present
University of North Carolina at Charlotte, NC, USA
Research focus: Generative ML systems for crystalline materials — GPA: 4.00/4.00

M.S. in Mechanical Engineering Dec 2025
University of North Carolina at Charlotte, NC, USA
GPA: 4.00/4.00

B.Sc. in Naval Architecture and Marine Engineering Aug 2017 – May 2022
Bangladesh University of Engineering and Technology, Dhaka, Bangladesh
Faculty of Mechanical Engineering — CGPA: 3.45/4.00
Undergraduate thesis: *Numerical Computation of Thermal Performance of Earth Pipe Cooling Systems*, *Proc. 13th Int. Conf. on Marine Technology (MARTEC 2022)*, 2023

Research Interests

- Atomistic and Multi-scale Modeling of Materials
- Structure–Property Relationships and Materials Design
- AI-Accelerated Simulation and Data-Driven Materials Discovery
- Energy, Molecular, Functional Materials

Professional Experience

University of North Carolina at Charlotte NC, USA
Graduate Research Assistant Jan 2022 – Present
Develop generative models for crystal structure prediction (CSP), and build GPU-batched workflows integrating ML interatomic potentials (MLIPs) for large-scale screening and refinement.

SOFTEKO Dhaka, Bangladesh
Team Leader 2022 – 2023
Led a small team delivering Python and Excel–VBA tools, coordinated timelines, and reviewed outputs to ensure quality.

Research Projects

LEGO-xtal: Symmetry-Aware Generative System for Crystal Design
PyTorch, Deep Generative Models, PyXtal, ASE, VASP, HPC

- Developed a symmetry-informed generative model that respects space-group constraints and periodicity for crystal structure generation.
- Expanded from 25 known low-energy sp^2 carbon allotropes to over 1,700 new candidate structures within 0.5 eV/atom of graphite.
- Enabled targeted generation toward local chemical environments using geometry-aware latent representations.

LEGO-xtal-GPU: Differentiable CSP and Latent Optimization
GPU parallelization and batching, CVAE, SO(3) descriptors, differentiable optimization

- Implemented GPU-parallel batched evaluation of structure descriptors and objectives to scale candidate generation and refinement.
- Built a fully differentiable pipeline that backpropagates through representation-space objectives and couples them with latent-space refinement.
- Achieved ∼5× speedup via batching and GPU acceleration, with improved success in meeting target local-environment constraints.

PyXtal-DFTB: High-Throughput Property Screening
ASE, DFTB+, automated workflows

- Built an automated pipeline for elastic-constant computation of organic crystals.

- Enabled mechanical screening of peptide hydrates in collaboration with experimental partners.

ML-Assisted X-ray Absorption and Optical Modeling of Boron Nitride
DFT (VASP), first-principles spectroscopy

- Conducted DFT simulations and collaborated with LLNL on ML-assisted X-ray absorption spectroscopy and optical modeling of boron nitride.

Reciprocal-Space Representations for Structure Matching
Scattering features, geometric embeddings, PyTorch

- Developed 4D scattering-informed representations for structure matching and reconstruction.
- Enabled quantitative comparison between simulation outputs and experimental signals.

xtal-builder: Agentic Crystal Design Assistant
LLM tool-calling, Ollama, LangChain/LangGraph, ASE, PyXtal, MLIP

- Building an agent that orchestrates structure generation, simulation, and refinement.
- Implements log parsing, failure detection, and auto-retry loops on HPC.
- Goal: autonomous crystal design from minimal user input.

Publications

1. **O. G. Ridwan**, S. Pitié, M. S. Raj, D. Dai, G. Frapper, H-F. Xue, Q. Zhu,
AI-Assisted Rapid Crystal Structure Generation Towards a Target Local Environment,
npj Comput. Mater., **12**, 7 (2026). DOI
2. W.-Y. Sun, **O. G. Ridwan**, W. Jeong, S. O. Kucheyev, Q. Zhu, and L.-W. Wan,
Unveiling X-ray Absorption Signatures of Boron Nitride via First-Principles Simulation and Machine Learning,
Next Materials, **9**, 101271 (2025). DOI
3. V. Athiyarath, E. Naranjo, D. Dave, **O. G. Ridwan**, ..., R. V. Ulijn, X. Chen
Context-Adaptive Nanotopology in Peptide Crystals,
ChemRxiv, 2025, *accepted in Matter*
4. **O. G. Ridwan**, H-F Xue, G. Frapper, Q. Zhu,
Crystal Generation using the Fully Differentiable Pipeline and Latent Space Optimization,
arXiv, 2026.

Technical Skills

- **Machine Learning:** PyTorch; generative models (Diffusion, VAE, Transformer); physics-informed ML; Bayesian optimization; representation learning for atomistic systems
- **Agentic ML Systems:** LLM tool-calling with hosted and local models (OpenAI, Ollama); workflow orchestration with LangChain/LangGraph; domain-specific prompt tuning
- **Systems:** Batched data pipelines; large-scale training workflows
- **Computational Tools:** DFT (VASP), LAMMPS, GULP, ASE, PyXtal, MACE, UMA
- **Programming:** Python, C/C++, Bash
- **Data & Visualization:** NumPy, Pandas, Matplotlib, VESTA, OVITO

Professional Memberships

American Chemical Society (ACS); Materials Research Society (MRS)

Conferences & Presentations

1. *Crystal Structure Prediction with Deep Learning Models Using Space Group Symmetry*, Gordon Research Conference, 2024. **Selected as one of five posters** from over 30 submissions for the Spotlight Poster Preview session.
2. *AI-Assisted Rapid Crystal Structure Generation with a Target Local Chemical Environment*, CITRANS Symposium, UNC Charlotte, 2025. **Best Poster Award**.