

Osman Goni Ridwan

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Education

Ph.D. in Mechanical Engineering (3rd year)

Jan 2024 – Present

University of North Carolina at Charlotte, NC, USA

Advisor: Prof. Qiang Zhu — 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 Materials Modeling
- AI generative models for materials structure prediction
- Energy, Molecular and Battery Materials

Research Experience

Graduate Research Assistant

Jan 2022 – Present

University of North Carolina at Charlotte, NC, USA

- Developed **LEGO-xtal**, a symmetry-aware AI framework for crystal structure generation targeting specific local environments, collaborated with UNC Charlotte Computer Science and U-Poitiers (France) Computational Chemistry groups to enable generation of 1,700+ novel sp²-carbon allotropes from only 25 seed structures (**First-authored manuscript under review**)
- Co-developed **PyXtal-DFTB** framework to automate the elastic constants calculation for organic crystals, collaborated with CUNY Experimental Materials group to compute and analyze the mechanical properties of peptide hydrates (**One coauthored manuscript under review**)
- Co-developed materials structure generation tool as part of **PyXtal** using the Crystallographic Symmetry relation, collaborated with LLNL to harness 200 hypothetical boron nitrides for X-ray Absorption Signatures (XAS) analysis (**One coauthored manuscript under review**)
- Developing the AI-powered Crystal Structure Optimization method via latent space learning, collaborated with UNC Charlotte Computer Science team to develop a framework to reach 10x more efficient structure optimization than the ordinary direct-space optimization method (**one first-authored manuscript under preparation, in progress**)
- Developing a physics-informed latent space for materials discovery, deriving crystallographic representations from 4D reciprocal space using Cartesian coordinates and scattering factors for tasks such as crystal structure matching and reconstruction. (**First-authored manuscript in preparation**)

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* [arXiv:2506.08224](https://arxiv.org/abs/2506.08224), 2025, *under review in NPJ Comput. Mater.*
2. W-Y Sun, **O. G. Ridwan**, S. O. Kucheyev, Q. Zhu, and L-W Wan, *Unveiling X-ray Absorption Signatures of Boron Nitride via First-Principles Simulation and Machine Learning*, 2025, *under review in Next Materials*

3. V. Athiyarath, E. Naranjo, D. Dave, **O. G. Ridwan**,, R. V. Ulijn, X. Chen
Context-Adaptive Nanotopology in Peptide Crystals,
[ChemRxiv](#), 2025, *under review in Matter*
4. **O. G. Ridwan**, H-F Xue, Y-X, Chen, H. Cherukuri, Q. Zhu,
Crystal Representation in the Reciprocal Space,
2025, *to submit*
5. **O. G. Ridwan**, H-F Xue, Q. Zhu,
Enhancing Crystal Optimization at the Latent Space,
2025, *under preparation*

Technical Skills

- **Programming:** Python, Bash, MATLAB, Linux HPC job scripting, Git
- **Software:** VESTA, LAMMPS, VASP

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**, ranked first among 26 presentations.