Osman Goni Ridwan

Computational Materials Scientist | Generative AI | Atomistic Simulation

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Research Profile

Ph.D. candidate and computational materials scientist developing symmetry- and physics-informed generative models, atomistic simulations, and high-throughput workflows for crystal structure prediction. Lead developer of open-source scientific software, with two first-author peer-reviewed articles, a 2026 LLNL computational chemistry internship followed by a 2026–2027 virtual Academic Cooperation Participant appointment, and research contributions across DOE, NSF, and ARPA-E programs.

Education

Ph.D. in Mechanical Engineering, University of North Carolina at Charlotte — Jan 2024 – Dec 2027 (expected)
Advisor: Prof. Qiang Zhu | GPA: 4.00/4.00 | Dissertation: *Motif-Guided Generative Modeling for Materials Structure Discovery*

M.S. in Mechanical Engineering, University of North Carolina at Charlotte — Dec 2025
Awarded en route to the Ph.D. | GPA: 4.00/4.00

B.Sc. in Naval Architecture and Marine Engineering, BUET, Bangladesh — Feb 2017 – May 2022
Faculty of Mechanical Engineering | CGPA: 3.45/4.00

Research Expertise

Generative and scientific ML: PyTorch; diffusion and flow-matching models; Transformer and equivariant graph architectures; differentiable, latent-space, and Bayesian optimization; SO(3), reciprocal-space, and scattering representations.
Atomistic simulation: DFT (VASP), DFTB, LAMMPS, GULP; geometry relaxation, elastic constants, molecular dynamics, machine-learning interatomic potentials, and convex-hull stability analysis.
Scientific computing: Python, C/C++, Bash; ASE, PyXtal, NumPy, Pandas, Matplotlib; Slurm, GPU and multi-GPU HPC workflows; Git; VESTA; OVITO.

Research Experience

Lawrence Livermore National Laboratory (LLNL) — Livermore, CA
Academic Cooperation Participant — Sep 2026 – Jun 2027
Graduate Intern, Computational Chemistry and Materials Science — Jun – Aug 2026

- Investigate proton migration pathways and energy barriers in ceramic electrolytes using nudged elastic band (NEB) calculations with VASP and machine-learning interatomic potentials.
- Analyze the relationship between local atomic environments and migration barriers to identify targets for subsequent crystal generation and screening.

University of North Carolina at Charlotte — Charlotte, NC
Graduate Research Assistant, Materials Modeling and Informatics Group — Jan 2024 – Present

- Lead developer of **LEGO-xtal**, a PyTorch-based, symmetry-aware generative framework; expanded 25 seed structures into 1,700+ novel sp^2 carbon allotropes within 0.5 eV/atom of graphite and deployed a public searchable database.
- Designed a fully differentiable, GPU-batched generation and refinement workflow using representation-space gradients and latent-space optimization, achieving approximately 5× faster execution and a 2× higher success rate than the prior CPU workflow.
- Developing **CSPflow**, an end-to-end workflow connecting crystal generation, MLIP screening, convex-hull analysis, and VASP validation for high-throughput magnet discovery under DOE ARPA-E MAGNITO.
- Contributed to **PyXtal** and developed automated DFTB workflows for calculating elastic constants of organic crystals, enabling high-throughput mechanical screening of peptide hydrates with experimental collaborators.
- Developed reciprocal-space crystal representations and PXRD-based structure-determination workflows; curated approximately 200 hypothetical boron nitrides with LLNL collaborators for X-ray absorption analysis.

Open-Source Software and Data

LEGO-xtal: symmetry-aware crystal generation and GPU-based refinement | **CSPflow:** generation-to-DFT screening automation | **PyXtal:** symmetry, DFTB, and screening contributions.

Publications

4 peer-reviewed articles (2 first-author); 4 preprints (1 first-author). Author name in bold.

Peer-reviewed articles

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 Computational Materials***, **12**, 7 (2026). DOI
2. **O. G. Ridwan**, G. Frapper, H. Xue, Q. Zhu, *Crystal Generation using the Fully Differentiable Pipeline and Latent Space Optimization*, ***Machine Learning: Science and Technology***, **7**, 035026 (2026). DOI
3. V. Athiyarath, E. Naranjo, D. Dave, **O. G. Ridwan**, D. A. A. Rodriguez, Q. Zhu, M. Monti, G. Díaz Mirón, D. Banerjee, A. Hassanali, M. C. Neary, E. G. Keeler, S. Zhang, R. V. Ulijn, X. Chen, *Water-Mediated Reconfigurable Topology and Mechanics in Porous Peptide Materials*, ***Matter***, **9**, 102669 (2026). DOI
4. W.-Y. Sun, **O. G. Ridwan**, W. Jeong, S. O. Kucheyev, Q. Zhu, L.-W. Wan, *Unveiling X-ray Absorption Signatures of Boron Nitride via First-Principles Simulation and Machine Learning*, ***Next Materials***, **9**, 101271 (2025). DOI

Preprints

5. **O. G. Ridwan**, H. Xue, Y. Chen, H. Cherukuri, Q. Zhu, *Crystal Representation in the Reciprocal Space*, arXiv:2601.17981 (2026); under revision at *Physica Scripta*.
6. K. Su, **O. G. Ridwan**, H. Xue, Q. Zhu, *Ab-initio Crystal Structure Determination from Powder X-Ray Diffraction*, arXiv:2605.24594 (2026); under review at *PRX Intelligence*.
7. S. Tao, **O. G. Ridwan**, L. Ke, Q. Zhu, *High-throughput Discovery of Magnetic Rare Earth Transition Metal Alloys*, arXiv:2608.25270 (2026); under review at *npj Computational Materials*.
8. M. M. Mukta, **O. G. Ridwan**, R. Perriot, Q. Zhu, *Benchmarking Universal Machine Learning Force Fields for Crystal Structure Prediction of High-Energy Molecular Systems*, arXiv:2609.07477 (2026); under revision at *RSC Advances*.

Conference proceeding: O. G. Ridwan et al., *Numerical Computation of Thermal Performance of Earth Pipe Cooling Systems*, Proc. MARTEC 2022, 2023.

Honors and Presentations

- **Distinguished Research Assistant**, Graduate Student Award, UNC Charlotte, 2026.
- **LLNL Summer Student Symposium**, poster presentation, 2026.
- **Gordon Research Conference Poster Preview**, selected oral presenter in 2024 and 2026
- **Best Poster Award**, CITRANS Symposium, UNC Charlotte, 2025.

Professional Service

Peer reviewer: *npj Computational Materials*; *The Journal of Chemical Physics*; *Crystal Growth & Design*; *Machine Learning: Science and Technology*; *Journal of Physics: Materials*. | **Memberships:** ACS; MRS.