Sadman Sadeed Omee

Email: omee.sadman@gmail.com || **Phone:** +1803-243-3777 || **Website:** www.sadmanomee.com
LinkedIn: linkedin.com/in/sadmanomee || **GitHub:** github.com/sadmanomee || **Google Scholar:** Sadman Sadeed Omee

Research Summary

- **Ph.D. Candidate working on machine learning (ML)** to solve complex problems from the materials science domain, leveraging concepts from core ML areas, such as natural language processing (NLP) and computer vision (CV).
- **Research focus:** Graph Neural Networks (GNNs), AI for Science, Generative AI, Large Language Models (LLMs), Foundation Models, Geometric Deep Learning, and Representation Learning.

Education

University of South Carolina **August 2021 – Present**
Ph.D. in Computer Science | GPA: 3.97/4.00 | **Expected Graduation:** May 2026 Columbia, SC, United States
Dissertation: "Artificial Intelligence-Driven Materials Informatics: From Property Prediction to Crystal Structure Discovery"

University of South Carolina **August 2021 – December 2024**
M.S. in Computer Science (en route to Ph.D.) | GPA: 3.97/4.00 Columbia, SC, United States

Bangladesh University of Engineering and Technology **February 2015 – April 2019**
B.S. in Computer Science and Engineering Dhaka, Bangladesh

Experience

University of South Carolina **January 2022 – Present**
Graduate Research Assistant | *Machine Learning and Evolution Laboratory* Columbia, SC, United States

- **Designed and applied advanced deep learning models**, including graph neural networks (GNNs), large language models (LLMs), and diffusion models, to solve problems from the materials science domain such as crystal structure prediction (CSP), materials property prediction, and generative models for materials.
- **Authored multiple peer-reviewed research publications** in high-impact journals, demonstrating strong research productivity and impact in AI for science.
- **Currently developing a conditional equivariant diffusion model** for 3D crystal polyhedra generation from chemical compositions, targeting fundamental scalability and accuracy bottlenecks in CSP.

KLA Corporation **May 2025 – August 2025**
Summer Intern Ann Arbor, MI, United States

- **Developed a continual transfer learning framework** for predicting semiconductor wafer critical dimensions from spectral data.
- **Improved out-of-distribution (OOD) robustness of ML-based metrology models**, enabling reliable performance under real-world manufacturing distribution shifts
- **Collaborated with cross-functional engineering teams** in a production-oriented research environment.

Lawrence Livermore National Laboratory (LLNL) **May 2024 – August 2024**
Summer Intern Livermore, CA, United States

- **Co-developed a multimodal molecular foundation model** integrating molecular structure, XANES spectra, SMILES representations, and HOMO–LUMO gap data using contrastive learning–based latent space alignment.
- **Implemented modality-specific encoders**, including graph neural networks for molecular structures and deep neural network architectures for spectral and string-based modalities, to enable unified cross-modal molecular representations.
- **Participated in weekly research seminars** with LLNL scientists focused on advanced machine learning models for materials and molecular science, high-performance computing (HPC), and related computational science fields.

Skills

- **Deep Learning:** PyTorch, TensorFlow, Scikit-Learn, PyTorch Lightning
- **Graph & Geometric ML:** GNN, Equivariant Neural Networks, PyTorch Geometric
- **Generative AI & Foundation Models:** Diffusion Models, Transformers, LLMs, VAEs, Contrastive Learning
- **AI for Science:** Pymatgen, ASE, Matminer, RDKit, Atom3D
- **Computer Vision (CV) & Natural Language Processing (NLP):** CNN, OpenCV, Hugging Face, NLTK, spaCy
- **Programming Languages:** Python, C, C++, Java
- **Systems & Tooling:** Docker, Git, AWS, Bash, SLURM

Selected Publications

1. **Omee, S. S.**, Wei, L., Dey, S., & Hu, J. (2025). Polymorphism crystal structure prediction with adaptive space group diversity control. ***Advanced Science***.
   - Devised **ParetoCSP2**, a deep neural network interatomic potential-based algorithm for crystal polymorph prediction that incorporates an adaptive space group diversity control, achieving up to 8.6× performance improvement and faster convergence.
2. **Omee, S. S.**, Louis, S. Y., Fu, N., Wei, L., Dey, S., Dong, R., Li, Q., & Hu, J. (2022). Scalable deeper graph neural networks for high-performance materials property prediction. ***Patterns***.
   - Developed **DeeperGATGNN**, a global-attention-based GNN for materials property prediction that can leverage long-range atomic information, achieving improved performance and scalability (> 50 graph convolution layers) over existing models.
3. **Omee, S. S.**, Fu, N., Dong, R., Hu, M., & Hu, J. (2024). Structure-based out-of-distribution (OOD) materials property prediction: a benchmark study. ***npj Computational Materials***.
   - Developed a **comprehensive benchmark** for out-of-distribution (OOD) materials property prediction, revealing a significant performance gap for current GNNs in predicting properties of novel exceptional materials.
4. **Omee, S. S.**, Wei, L., Hu, M., & Hu, J. (2024). Crystal structure prediction using neural network potential and age-fitness pareto genetic algorithm. ***Journal of Materials Informatics***.
   - Developed **ParetoCSP**, a novel algorithm for crystal structure prediction that integrates a genotypic age-fitness criterion enhanced multi-objective genetic algorithm with a deep neural network inter-atomic potential.
5. Li, Q., Fu, N., **Omee, S. S.**, & Hu, J. (2024). MD-HIT: Machine learning for material property prediction with dataset redundancy control. ***npj Computational Materials***.
   - Proposed **MD-HIT**, a redundancy reduction algorithm for materials datasets, to mitigate overestimated ML performance in property prediction by controlling dataset redundancy, leading to more realistic model evaluation.
6. Fu, N., Wei, L., Song, Y., Li, Q., Xin, R., **Omee, S. S.**, Dong. R., & Hu, J. (2023). Material transformers: Deep learning language models for generative materials design. ***Machine Learning: Science and Technology***.
   - Trained seven transformer **large language models (LLMs)** for generative materials composition design, achieving high chemical validity, novelty, and tunability, demonstrating their potential for discovering new materials.
7. Louis, S. Y., Siriwardane, E. M. D., Joshi, R. P., **Omee, S. S.**, Kumar, N., & Hu, J. (2022.). Accurate prediction of voltage of battery electrode materials using attention-based graph neural networks. ***ACS Applied Materials & Interfaces***.
   - Formulated two **attention-based GNNs** in collaboration with Pacific Northwest National Laboratory (PNNL) that predict battery electrode voltages by leveraging chemical compositions and 3D spatial information.

Research Metrics

• **Citations:** 512 • **h-index:** 12 • **i10-index:** 12 (Last updated: January 6, 2026)

Selected Academic Projects

- **Foundation Model for In-Context Learning:** Developed a structure-aware in-context learning **foundation model** framework for materials property prediction, with ongoing publication work. (PyTorch, PyTorch Geometric, TabPFN)
- **Facet:** Developed an efficient **E(3)-equivariant GNN** that accelerates the training of foundation models for interatomic potentials by over an order of magnitude while maintaining comparable performance. (PyTorch, PyTorch Geometric)
- **FedMat:** Developed a full pipeline for **federated learning** for the out-of-distribution materials property prediction problem using graph neural networks. (FedChem, GNNs, PyTorch, PyTorch Geometric)
- **DeepXRD:** Developed a **convolutional neural network (CNN)** for the challenging task of XRD spectra prediction of crystals given their chemical compositions. (CNN, PyTorch, Pymatgen)
- **Election Information Quality Analysis:** Analyzed the quality of official information available for elections in 2024 across 12 US states based on multiple criteria using **NLP techniques**. (NLTK, Transformers, LLMs)

Services and Memberships

- **Reviewing Services:** More than 35 peer reviewing services for several prestigious journals including *Advanced Science*, *PLOS ONE*, *npj Computational Materials*, *The Innovation*, *Pattern Recognition*, *Neural Networks*, and *Heliyon*.
- **Mentoring Services:** Mentoring undergraduate students in AI/ML research through Bangladeshi Student Research Initiative (**BSRI**, website: `https://sites.google.com/view/bsri-bd/team`).
- **Notable Memberships:** 1. Institute of Electrical and Electronics Engineers (**IEEE**): 2025 – Present & 2. American Association for the Advancement of Science (**AAAS**): 2025 – Present.