Sadman Sadeed Omee

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Research Interests

AI for Science (Materials Science, Molecular Science & Computational Chemistry), Graph Neural Networks (GNNs), Generative AI, Large Language Models (LLMs), Foundation Models, Physics-Informed AI.

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**
Bachelor of Science 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

- Conducting research on deep learning techniques, such as graph neural networks, transformers, and diffusion models to solve materials informatics problems, such as crystal structure prediction (CSP), materials property prediction, generative and physics-informed models for materials.
- Currently developing a generative diffusion model for conditional generation of 3D crystal polyhedra (building blocks of crystals) from chemical compositions. Successful prediction of the polyhedra of a crystal can lead to accurate prediction of the full crystal structure and provide an efficient solution to the CSP problem.

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

- Developed an unsupervised continual transfer learning framework to predict critical dimensions of semiconductor wafers from out-of-distribution spectral data.
- Contributed to AI-driven metrology methods to enhance accuracy and efficiency in semiconductor manufacturing.

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

- Engaged in hands-on research with LLNL scientists to develop advanced ML models in materials and molecular science, high-performance computing (HPC), and related computational science fields.
- Collaborated on a project for developing a multimodal foundation model for molecules using a contrastive learning based latent space alignment approach.

Notable Research Publications

1. **Omee, S. S.**, Wei, L., Dey, S., & Hu, J. (2025). Polymorphism crystal structure prediction with adaptive space group diversity control. *Advanced Science*.
   - Developed ParetoCSP2, an algorithm for crystal polymorph prediction that incorporates an adaptive space group diversity control mechanism into a multi-objective genetic framework guided by a neural network potential, significantly improving polymorph prediction accuracy, crystal structure diversity, and convergence speed over existing methods.
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 by using differentiable group normalization and residual skip-connections, achieving improved performance and scalability (> 50 graph convolution layers) over existing state-of-the-art 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., **Omee, S. S.**, & Hu, J. (2025). Physical encoding improves OOD performance in deep learning materials property prediction. *Computational Materials Science*.
   - Evaluated four atomic encoding methods for materials property prediction and show that physical atomic encoding significantly improves out-of-distribution generalization, especially for models trained on small datasets.
7. 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 and benchmarked seven transformer language models for generative materials composition design, achieving high chemical validity, novelty, and tunability, demonstrating their potential for discovering new materials.
8. 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 that predict battery electrode voltages by leveraging chemical compositions and 3D spatial information, demonstrating strong transferability across different metal-ion batteries.

Notable Academic Projects

- **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, such as LLMs. (NLTK, Transformers, LLMs)
- **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)
- **Human Activity Recognition:** Developed a spiking neural network (SNN) for the the problem of automatically recognizing and understanding the activities performed by a person from sensor data. (Tensorflow, SNN, Scikit-Learn)
- **Messenger and File Transmitter:** Developed a message and file transmission system implemented using socket programming and the Go-Back-N protocol. (Java)
- **Computer Graphics:** Implemented a interactive camera, a bubble collision dynamics, a curve trajectory from points, a conversion of rasterization image from description, and a ray-tracing of simple shapes using OpenGL. (C++, OpenGL)

Technical Skills

- **Programming Languages:** Python, C, C++, Java
- **Machine Learning & Deep Learning:** PyTorch, TensorFlow, PyTorch Geometric, Scikit-learn, PyTorch Lightning
- **Computational Materials Science:** Pymatgen, ASE, Matminer
- **Computational Chemistry:** RDKit, Atom3D
- **Natural Language Processing (NLP) :** Hugging Face, NLTK, spaCy, Gensim
- **Computer Vision (CV):** OpenCV, Pillow
- **Cloud & DevOps:** AWS, Docker, Git
- **Databases:** MySQL, MongoDB
- **Scientific Tools:** LaTeX, Anaconda, Bash, SLURM

Services and Memberships

- **Reviewing Services:** More than 25 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.