Sadman Sadeed Omee

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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 like graph neural networks (GNNs), transformers, and diffusion models to solve materials informatics problems, such as crystal structure prediction, materials property prediction, and generative models for materials.
- Currently developing a diffusion model-based crystal structure prediction (CSP) model for conditional generation of both crystal lattice parameters and 3D atom coordinates from chemical compositions.

University of South Carolina **August 2021 – December 2021, August 2023 – Present**
Graduate Teaching Assistant | Course: CSCE102 (General Applications Programming) Columbia, SC, United States

- Teaching HTML, CSS, and JavaScript to three lecture groups of total of 75 students, and a lab group of total 25 students.

Lawrence Livermore National Laboratory **May 2024 – August 2024**
Summer Research Intern Livermore, CA, United States

- Collaborated on a project for developing a multimodal foundation model for molecules. Specifics of the work cannot be provided due to the lab's confidentiality policies (ongoing as a collaborator).

Notable Publications

1. **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.
2. **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*, 10(1), 144.
   – 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.
3. **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, achieving a 2.5x improvement over existing models in predicting optimal crystal structures across diverse benchmarks.
4. Dong, R., Zhao, Y., Song, Y., Fu, N., **Omee, S. S.**, Dey, S., Li, Q., Wei, L., & Hu, J. (2022). DeepXRD: A deep learning model for predicting XRD spectrum from material composition. *ACS Applied Materials & Interfaces*.
   – Developed DeepXRD, a CNN for the challenging task of XRD spectra prediction of crystals given their chemical compositions.
5. 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.

Relevant Skills

Programming languages: Python, C, C++, Java
Machine learning frameworks: PyTorch, Tensorflow, PyTorch Lightning, Scikit-learn.
Machine learning libraries: PyTorch Geometric (PyG), Deep Graph Library (DGL), Hugging Face libraries (transformers, diffusers, etc.), Wandb, Pandas, NumPy, SciPy, Ray Tune, Pymatgen, ASE, Matminer, RDKit.
Other skills: LaTeX, Git, JavaScript, HTML, CSS, React, Java Spring Boot, Hibernate, MySQL.

Education

University of South Carolina **August 2021 – Present**
Ph.D. in Computer Science Columbia, SC, United States
Cumulative GPA: 3.965/4.00

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