SADMAN SADEED OMEE

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EXPERIENCE

Lawrence Livermore National Laboratory   **May 2024 – August 2024**
Summer Research Intern   Livermore, CA, United States
- Worked on a molecular foundation model project.

University of South Carolina   **January 2022 – Current**
Graduate Research Assistant | Machine Learning and Evolution Laboratory   Columbia, SC, United States
- **Research topic:** We use deep learning techniques to solve materials informatics problems (e.g., crystal structure prediction, materials property prediction, generative models for material) in our lab. My work on crystal structure prediction is similar to the protein structure prediction problem solved by AlphaFold2. I have also developed a state-of-the art global attention-based Graph Neural Network architecture for the materials property prediction problem.
- **Concept / skills usage:** I mostly use Graph Neural Networks (GNNs) for my research. I have also used Convolutional Neural Networks, Transformers, Diffusion Models and other Generative Models for my different research projects. I am fluent in using PyTorch and PyTorch Geometric.

University of South Carolina   **August 2021 – December 2021,   August 2023 – Current**
Graduate Teaching Assistant | Course: CSCE102 (General Applications Programming)   Columbia, SC, United States
- Taught HTML, CSS, and JavaScript to a total of 72 students, and two lab group of total 50 students.

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*.
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.
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*.
4. Varivoda, D., Dong, R., **Omee, S. S.**, & Hu, J. (2023). Materials property prediction with uncertainty quantification: A benchmark study. *Applied Physics Reviews*.
5. 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*.
6. Hu, J., Stefanov, S., Song, Y., **Omee, S. S.**, Louis, S. Y., Siriwardane, E. M., Zhao, Y., & Wei, L. (2022). MaterialsAtlas.org: A materials informatics web app platform for materials discovery and survey of state-of-the-art. *npj Computational Materials*.
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*.
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*.
9. Li, Q., Dong, R., Fu, N., **Omee, S. S.**, Wei, L., & Hu, J. (2023). Global mapping of structures and properties of crystal materials. *Journal of Chemical Information and Modeling*.

RELEVANT SKILLS

Programming languages: Python, C, C++, Java, JavaScript.
Machine learning (ML) / deep learning (DL) frameworks: PyTorch, Tensorflow, PyTorch Lightning, Keras, Scikit-learn.
ML / DL libraries: PyTorch Geometric (PyG), Deep Graph Library (DGL), Transformers (Hugging Face), PyTorch-Ignite, Pandas, NumPy, SciPy, Pymatgen, ASE, Matminer, RDKit.
Other skills: LaTeX, Git, Matplotlib, HTML, CSS, Java Spring Boot, MySQL.

EDUCATION

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