Postdoctoral Position

Machine Learning Foundation Models and Generative AI for Materials Discovery
University of Minnesota, Minneapolis, MN, USA

One or more positions are available starting January 2025 for computational researchers at the postdoc or research scientist levels for projects related to the development of machine learning (ML) based foundation models and generative AI for materials discovery. These projects build upon and integrate with the OpenKIM and ColabFit frameworks pioneered at the University of Minnesota (UMN) in close collaboration with NYU. OpenKIM is a core NSF cyberinfrastructure for archiving and testing interatomic potentials (IPs) used in atomistic simulations of materials, and development of uncertainty quantification (UQ) methods for providing confidence bounds on IP predictions. ColabFit is a repository of curated first principles data for training advanced data-driven machine learning IPs (MLIPs). The work will involve:

- Development of the FERMat foundation model for materials and chemistry. FERMat is an ML encoder trained on very large amounts of heterogeneous and multimodal data for both one-shot prediction of material properties, and for fine tuning to specific applications.
- Development of the Open Materials Generation (OMG) generative AI framework. OMG is based on an innovative stochastic interpolants approach for guided materials discovery, and is currently the field leader in performance.
- Applications of these tools in different domains including simulation and discovery of superconductors, shape-memory materials for biomedical applications, high-entropy alloys for aerospace applications, advanced nonlinear optical materials for sensing, and others.

Required Qualifications:

- PhD in materials/physical sciences, applied mathematics, computer science, or engineering
- Expertise in UQ and/or ML and associated tools (e.g. PyTorch, TensorFlow, GPUs, CUDA)
- Knowledge and expertise in computational science and software development (e.g. Python, C/C++, shell scripting, DevOps, Conda, virtual machines)

Desired Qualifications:

- Expertise in classical atomistic simulations and/or first principles calculations
- Expertise in state-of-the art ML tools in the physical sciences
- Experience in performing collaborative research
- Excellent interpersonal, and oral and written communication skills

The position is based in Minneapolis, MN, USA with option to spend time at NYU in New York, NY as part of this collaborative effort.

To Apply:

Applications will be considered on an ongoing basis until the positions are filled. The positions are available as of January 2025, initially for up to 2 years with possibility of extension. Interested individuals are encouraged to contact Professor Ellad Tadmor (tadmor@umn.edu). Please provide the following:

- Cover letter describing how your background fits the above needs and requirements, and why you are interested in this project
- CV or Resume detailing your background and skills
- Names and contact information for three references familiar with your work

The University of Minnesota is an EEO/AA employer and educator.