Postdocs/Research Scientists Needed for Project on Data-Driven Interatomic Potentials

University of Minnesota, September 2020

Dept. of Aerospace Engineering and Mechanics
Dept. of Chemical Engineering and Materials Science

Several positions are available for postdoctoral fellows or research scientists for the ColabFit project, a collaborative infrastructure for the development of state-of-the-art data-driven interatomic potentials (DDIPs) with applications to 2D materials science.

The ColabFit project aims to create a computational framework that enables researchers to rapidly develop and deploy DDIPs for complex material systems by connecting existing cyberinfrastructure resources of first principles and experimental data with a variety of fitting frameworks. Building on an interoperable standard for machine learning models, researchers using ColabFit will be able to archive their DDIPs and training sets to the Open Knowledgebase of Interatomic Models (OpenKIM) project, and retrieve existing ones to continue their collaborative development within a supported fitting framework of their choosing. Integration with OpenKIM will ensure that any DDIP created with ColabFit can be immediately used in multiple major simulation packages. ColabFit will be tested on a target application of DDIP development for phase transformations in 2D transition metal dichalcogenides. For more information on ColabFit, see https://colabfit.org/

This is an exciting project in a cutting-edge area of molecular simulation with unusually high networking opportunities as it involves a large international consortium of leaders in DDIP development and first principles modeling, and competitive salaries based on experience. Remote employment may be an option.

Candidates must have strong programming skills at both the system and application levels. Prior experience in the development and support of software systems written in multiple scientific programming languages is required, as well as excellent written and oral communication skills. Additional experience in one or more following areas is highly desirable:

- Molecular simulation in physics, chemistry or materials science using first principles methods (e.g. density functional theory) or classical molecular dynamics.
- Machine learning research and development including emerging standards such as ONNX.
- Experience with online databases of first principles or experimental data

Applications will be considered on an ongoing basis until all positions are filled. Positions are available as of October 2020, initially for up to 2 years. 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 what additional special skills you would bring to the ColabFit project.
- CV or Resume.
- Names and contact information for three references familiar with your work.

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