ColabFit Seeking Computational Research Scientists

University of Minnesota, Twin Cities, February 2021

Two positions are available for computational 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. 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.

Two positions are offered with different desired skills sets (required skills are indicated by a *):

Position 1: Machine Learning Specialist	Position 2: First Principles Materials Specialist
• *Experience developing ML methods • *Contribution to Open Source efforts • *Familiarity with ML libraries and standards (e.g. TensorFlow, PyTorch, ONNX, etc.) • *Expertise with C/C++, Python, shell scripting • Familiarity with Fortran • Familiarity with DevOps tools (Git, continuous integration, unit testing, etc.) • Familiarity with high-performance computing • Familiarity with molecular simulation	• *Experience performing electronic structure calculations (e.g. DFT) • *Experience with classical molecular simulations of materials (e.g. LAMMPS) • *Experience with automating workflows • *Experience with online first principles repositories and standards (e.g. AFLOW, NOMAD, OPTIMADE, etc.) • Background in electronic structure method development • Familiarity with 2D material systems (e.g. graphene, MoS_2) • Familiarity with theory and simulation of phase transformations

General requirements for both positions:

- Ability/willingness to work in a fast-paced team development environment
- Excellent written and oral communication skills
- The positions are in Minneapolis, MN, USA.

Applications will be considered on an ongoing basis until all positions are filled. Positions are available as of February 2021, initially for up to 2 years. Interested individuals are encouraged to contact Professor Ellad Tadmor (tadmor@umn.edu). Please provide the following:

- Cover letter specifying which position you are applying for, describing how your background fits the above needs and requirements, and why you are interested in contributing to the ColabFit project.
- CV or Resume.
- Names and contact information for three references familiar with your work.

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