COLUMBIA | ENGINEERING
The Fu Foundation School of Engineering and Applied Science

Computational Postdoctoral Position:

Atomistic Modeling of Interfaces in Energy Materials with Machine Learning Potentials

The Columbia Center for Computational Electrochemistry (CCCE) at Columbia University in the City of New York has an immediate opening for a computational materials postdoctoral researcher for a project related to the modeling of electrochemical energy storage and conversion materials.

The postdoc will work with Dr. Nongnuch Artrith (Department of Chemical Engineering) on a project involving the atomistic modeling of surfaces and interfaces with density-functional theory (DFT) and interatomic potentials to understand and predict the properties electrochemical devices such as Li-ion batteries. In particular, machine learning-based techniques will be used extensively in this project, including the development of machine-learning potentials [1–5] with our open-source Atomic Energy Network (ænet) package.

The postdoc will interact closely with collaborators within the CCCE and the Columbia Electrochemical Energy Center (CEEC). The CCCE partners with Schrödinger, Inc. in New York City.

Applicants should have:

- Background knowledge in first-principles electronic structure theory and
- Experience in scientific programming.

Additional experience in one or more of the following areas will be considered an asset:

- Experience with periodic DFT calculations, ideally for surfaces and/or interfaces;
- Materials for electrochemical energy storage/conversion;
- Application of machine learning to materials science; and
- Automated (high-throughput) calculations.

We ask those interested to send their CV and a list of references to
Nong Artrith (na2782@columbia.edu).

Postdoctoral appointments are on a one-year basis, with a maximum term of three years, subject to available funding and performance evaluation.

Columbia University is one of the world's most important centers of research and at the same time a distinctive and distinguished learning environment for students in many scholarly and professional fields.

We value diversity in our work environment. Candidates of all genders, ages, races, ethnicities, sexual orientations, and disability statuses are encouraged to apply

[1] N. Artrith and A. Urban, *Comput. Mater. Sci.* **114** (2016) 135-150.
[2] N. Artrith, A. Urban, and G. Ceder, *Phys. Rev. B* **96** (2017) 014112.
[3] N. Artrith, *J. Phys. Energy* **1** (2019) 032002.
[4] A. M. Cooper, J. Kästner, A. Urban, and N. Artrith, *npj Comput. Mater.* **6** (2020) 54.
[5] T. Morawietz and N. Artrith, *J. Comput. Aided Mol. Des.* (2020) in press, https://doi.org/10.1007/s10822-020-00346-6