

Computational Postdoctoral Position:  
**Atomistic Modeling of Interfaces in Energy Materials  
with Machine Learning and Computational Spectroscopy**

The Department of Chemical Engineering 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 (Columbia University) and Dr. Deyu Lu (Center for Functional Nanomaterials at Brookhaven National Laboratory, BNL).

The project will involve the atomistic modeling of surfaces and interfaces with density-functional theory (DFT) and computational core-level spectroscopy to understand and predict interface properties. In particular, machine learning-based techniques will be used extensively in this project, including the development of machine-learning potentials [1,2,3] and machine-learning tools for the interpretation of electron energy loss spectroscopy (EELS) or X-ray absorption spectroscopy (XAS) measurements [4, 5]. The postdoc will engage closely with the experimental team of the collaboration led by Dr. Feng Wang (Sustainable Energy Technologies, BNL).

This project is funded by the Department of Energy and is a close collaboration with Dr. Alexander Urban (Columbia University) and Dr. Shinjae Yoo (Computational Science Initiative, BNL).

**Applicants should have:**

- Background knowledge in first-principles electronic structure theory, and
- Experience with periodic DFT calculations, especially for surfaces and/or interfaces.

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

- Materials for electrochemical energy storage/conversion;
- Computational spectroscopy on EELS or XAS;
- 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](mailto:na2782@columbia.edu)) and Deyu Lu ([dlu@bnl.gov](mailto:dlu@bnl.gov)).

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. Women and individuals from other minority groups 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] M.R. Carbone, S. Yoo, M. Topsakal, D. Lu, *Phys. Rev. Mater.* **3** (2019) 033604.

[5] D. Yan, et al., *Nano Lett.* **19** (2019) 3457-3463.