Postdoctoral Positions: Computational Design and Understanding of Energy Materials

The group of Professor Gerbrand Ceder at the Department of Materials Science and Engineering at UC Berkeley and Lawrence Berkeley National Laboratory has postdoctoral positions available. The Ceder group is involved in the development of materials and synthesis theory as well as the design of materials, from *ab initio* computation to experimental synthesis and characterization to machine learning. Applications include energy capture, conversion, storage, and synthesis prediction. Our theory and modeling work is done in close collaboration with our experimental group for synthesis and characterization of novel materials, leading to many opportunities for cross-fertilization. We give individuals the opportunity to collaborate on multiple internal and external projects, as well as supervise graduate students. Many of our alumni have gone on to leading positions in academia and in the private sector. More information about our research group can be found at http://ceder.berkeley.edu.

We particularly value innovation and a passion to bridge fundamental scientific inquiry and high-impact applications. Our group offers candidates the opportunity to work in a highly interdisciplinary and dynamic environment. There are no citizenship restrictions. Starting dates are negotiable. We ask those interested to send their curriculum vitae and references to ceder-hr-comp@lbl.gov.

1. Studying of Materials Synthesis with NLP and Machine Learning Techniques

The successful candidate will employ and extend Machine Learning and Natural Language Processing techniques to train computer models for understand materials synthesis papers, and apply these models to discover, deliver and verify new insightful knowledge on materials synthesis theory. The ultimate goal of this project is to construct a comprehensive theory that may predict and guide experimental designs in materials synthesis. The position requires:

- Basic level of understanding in machine learning.
- Basic understanding of thermodynamics, phase diagrams, common materials synthesis procedures, etc.
- Adequate experience in computer programming and software development, preferably in Python.
- Team working skills.

Experience in the following areas is a plus:

- Background in physics, chemistry related fields.
- Knowledge in Natural Language Processing.
- Database administration.
- Basic knowledge in website technologies (HTMLs etc.)

- Github.
- Familiarity with one deep learning software framework (tensorflow, keras, pytorch).

2. Scientific Data and Text Mining with Machine Learning Techniques

The successful candidate will employ and extend existing data mining and machine learning tools to identify materials with desired properties and will develop novel machine-learning approaches for the discovery of composition-structure-property relationships. This project will involve generating and handling large data sets, such as those in the Materials Project (http://www.materialsproject.com), or other internally generated datasets. The position requires:
- Excellent scientific development skills, preferably in the Python programming language,
- Good understanding of thermodynamics and phase diagrams, and
- Some experience with machine-learning and data-mining/text-mining techniques.

Experience in atomistic simulations, preferably based on density-functional theory, is a plus.

3. Computational Understanding and Discovery of Novel Battery Materials

The successful candidate will work in close collaboration with experimental colleagues by predicting novel materials, providing synthesis guidelines, and/or understanding experimental observations. The position requires:
- A strong background in solid state physics,
- Excellent practical knowledge of density-functional theory, and
- Good knowledge of thermodynamics and statistical mechanics.

Scientific programming skills and experience with electrochemical energy storage are a plus.

4. Theory and Modeling to Predict Materials Properties, Phase stability, and Synthesis

The candidate will work on the development of novel methods for the prediction of materials properties and phase stability. We are particularly interested in the prediction of phase stability and metastability. The position requires:
- Good practical knowledge of density-functional theory,
- Excellent knowledge of thermodynamics, statistical mechanics, and kinetics of materials, and
- Working knowledge of crystallography.

Experience in the modeling of surfaces and interfaces is a plus.