University of California Berkeley

# Postdoctoral Positions: Computational Materials Science

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 theory and design of materials, from *ab initio* computation to experimental synthesis and characterization. Applications include energy capture, conversion, and storage. 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@lists.lbl.gov.

## 1. High-throughput computing and materials design with the Materials Project

The successful candidate will employ work with the Materials Project to design and implement methods for high-throughput property prediction and materials design, including finite temperature phase stability and defect calculations. The candidate will have the opportunity to work with a team focussed on novel materials design and machine learning of materials properties. The position requires:

- Excellent scientific development skills, preferably in the Python programming language,
- Background in ab-initio DFT methods
- Good understanding of thermodynamics and phase diagrams, and
- Some experience with machine-learning.

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

## 2. 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.

## 3. 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.