

## **Postdoctoral Opportunity in Computational Materials Science and Machine Learning at Los Alamos National Laboratory**

Staff in both the Physics and Chemistry of Materials Group (T-1) in the Theoretical Division, the Materials Science in Radiation and Dynamics Extremes Group (MST-8) in the Materials Science and Technology Division, and the Finishing Manufacturing Science Group (Sigma-2) in Sigma Division of Los Alamos National Laboratory are seeking multiple candidates for postdoctoral appointment in computational materials science research. The positions are in support of several research projects that address problems in radiation damage and corrosion of materials, defect evolution in complex oxides, and the development of long time scale methodologies and simulation codes. Areas of particular interest are:

- Computational methods for simulating long time scale atomistic dynamics (accelerated molecular dynamics and related methods)
- Applications of long time scale methods for simulating defect kinetics in complex oxide ceramics
- Data mining and machine learning approaches for materials discovery using both electronic structure and experimental input
- Density functional theory studies of fundamental defect properties in metallic alloys and oxide ceramics
- Development of high performance scientific software

The ideal candidate would have expertise in multiple areas.

In addition, depending on his/her expertise, the candidate may contribute to a broad range of research projects including scintillator discovery and characterization, materials under extremes of radiation and corrosion, the simulation of nuclear fuels, and the development of advanced methods for treating long time scale problems. The initial appointment is for two years, with a possible third year extension depending on performance and funding availability.

Candidates may also be nominated for a Director's Fellowship and outstanding candidates may be considered for the prestigious Darleane Christian Hoffman, Richard P. Feynman, J. Robert Oppenheimer, or Frederick Reines Fellowships. Applicants with US citizenship will also be considered for the Metropolis Postdoctoral Fellowship in Computational Physics. For these fellowships, the research scope can be broadened to include any topic of mutual interest.

For general information to the Postdoc Program go to <http://www.lanl.gov/careers/career-options/postdoctoral-research/index.php>.

### **Minimum Job Requirements:**

- Demonstrated ability to carry out independent and collaborative research in computational materials science at the atomistic scale.

- Solid understanding of fundamental defect properties in materials.
- Significant experience in running high performance simulation tools for modeling these systems.
- Demonstrated ability to communicate both technically and interpersonally both orally and in writing.

**Desired Skills:**

- Familiarity with multiple scales of simulating materials (e.g. density functional theory, molecular dynamics, kinetic Monte Carlo, accelerated molecular dynamics).
- Experience with writing code and implementing algorithms into high performance parallel codes.

**Education:**

- A Ph.D. in physics, materials science or very closely related discipline, earned within the last five years.

**Notes to Applicants:**

- In addition to applying online, interested candidates should send their inquiries, cover letter, CV including a list of peer-reviewed publications and invited talks, and the names and contact information of three references to Blas Uberuaga (blas@lanl.gov)
- The cover letter should address the minimum job requirements and desired skills of this position, with specific examples from your academic and research experience.
- To receive full consideration, please ensure that your application package provides all of the information requested above.
- Evaluation of applications will commence immediately and continue until the position is filled.

**Additional Details:**

No Clearance Required: Position does not require a security clearance. Selected candidates will be subject to drug testing and other pre-employment background checks.

New-Employment Drug Test: The Laboratory requires successful applicants to complete a new-employment drug test and maintains a substance abuse policy that includes random drug testing.