

Job Title: Postdoctoral Appointee – Atomistic and Multi-scale Simulation of Materials

Job ID: 636004

Location: Livermore, California

Full/Part Time: Full

Regular/Temporary: Temporary

Sandia National Laboratories is the nation's premier science and engineering lab for national security and technology innovation. We are a world-class team of scientists, engineers, technologists, postdocs, and visiting researchers—all focused on cutting-edge technology, ranging from homeland defense, global security, biotechnology, and environmental preservation to energy and combustion research, computer security, and nuclear defense. To learn more, visit <http://ca.sandia.gov/casite/>.

#### DEPARTMENT DESCRIPTION:

Sandia/California's Thermal/Fluid Science and Engineering Department is a multidisciplinary group of engineers and technologists who specialize in fluid mechanics and heat and mass transfer. The work mix in the group spans theory and scientific computing to mechanical design and applied experimentation. The group plays three primary roles in science-based engineering at Sandia: (1) developing new computational methods and tools to describe fluid mechanics and heat transfer; (2) performing computational analysis to predict the design performance of engineered systems; and (3) designing, building, and testing prototype systems. Recent activities within the group include hydrogen storage and safety technology, combustion and heat transfer modeling, and material process modeling. Our department is part of the Transportation Energy Center.

The Mechanics of Materials Department performs experimental and analytical studies to understand the mechanical behavior of materials. Our experimental work covers the entire discovery-characterization-validation spectrum. Motivated by observations, we develop models to simulate material responses under various loading and environmental conditions. Our models and simulations vary from atomic to continuum scales corresponding to the requirement of Sandia applications. Accuracy of the models for specific applications is validated by experimental data. Numerical methodologies are developed to allow implementation of the material models for high performance computing simulations.

#### JOB DESCRIPTION:

Multiple postdoctoral positions are available for scientists or engineers with experience and interest in studying structural, physical, and mechanical behavior of materials at the atomic scale using computational mechanics and material science methods. Current projects involve using atomistic and meso-scale simulation methods to study topics such as the mechanical behavior of defects in solid materials, and charge and energy transport in ionic fluids. Research is also needed in the development of new approaches for atomistic-to-continuum coupling and multi-scale simulation, and for the implementation of molecular and multi-scale simulation algorithms for use in efficient, high-performance computing. Persons with experience in techniques such as inter-atomic potential development, molecular statics and dynamics, atomistic-to-continuum coupling, and multi-scale modeling are needed to expand Sandia's capabilities to model and analyze materials and phenomena with characteristics at the nano- and micro-scale.

#### QUALIFICATIONS:

Applicants for this position should have recently received a PhD degree (conferred within the past five years) in physics, mechanical engineering (with a specialty in fluid or solid mechanics), materials science, mechanics of materials, computational mechanics or a related field. Expertise or experience in using molecular simulation methods and codes is essential, as is knowledge about the physics and mechanics of solid or fluid states of matter. Also required is proficiency in developing C++ computer programs. Experience with the molecular simulation code LAMMPS is desirable, as is knowledge of scripting languages such as Perl or Python. The candidate must demonstrate strong writing and communication skills, the ability to function in a team environment with other researchers, and past experience at publishing in technical journals.

#### ABOUT SANDIA

Located in Livermore, Sandia/California enjoys close proximity to San Francisco, Silicon Valley, several world-class educational institutions, and diverse cultural and year-round recreational opportunities. Sandia provides employees with a comprehensive benefits package that includes medical, dental, vision, and a 401(k) savings plan. Our culture values work-life balance; we offer programs such as flexible work schedules with alternate Fridays off, on-site fitness facilities, three weeks of vacation, and more.

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