

## Multiple postdoctoral positions in computational materials science

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Three postdoctoral positions in computational materials science are available in Professor Izabela Szlufarska's research lab in the Department of Materials Science and Engineering at the University of Wisconsin – Madison. Prof. Szlufarska's group is focused on development and application of state-of-the-art theoretical and multiscale simulation methods, combined with advanced materials characterization to discover fundamental materials behavior and to develop new advanced materials for future technologies. Our alumni find jobs ranging from faculty positions at R1 Universities to leading materials science and/or data science industries. Members of the group are exposed to a broad range of applications of computational tools and are encouraged to collaborate with each other and to identify new research opportunities beyond their core projects.

The first position is in the field of nano-tribology. It involves multiscale simulations of friction and adhesion to enable fundamental discoveries related to mechanochemical coupling at interfaces and to develop models of interface evolution under applied stress over multiple time scales and length scales. The work involves primarily atomistic simulations (DFT and classical) as well as development of kinetic Monte Carlo type models. It is a collaborative project with experimental teams at multiple other Universities.

The second position is focused on high-temperature ceramics for nuclear energy applications. It involves multi-scale modeling of radiation-induced defects in ceramics, including compositionally complex materials, as well as understanding of the interactions between defects and interfaces. This work involves a close collaboration with other researchers in Prof. Szlufarska's group who carry out experimental studies on the same materials systems.

The third position is focused on modeling of properties of molten salts for nuclear reactor applications. This project involves development of new machine learning potentials based on DFT calculations. These potentials will be then used to determine thermokinetic properties of the salts, with the ultimate goal of guiding the design of salt chemistries for reactor conditions.

A PhD in materials science, physics, or a related field is required, as well as familiarity with atomistic simulations of materials.

### **Additional information**

The appointments are initially for one year with the expectation of being extended if the work is going well. Interested applicants should send (1) CV in PDF format, (2) a brief cover letter describing suitability for the position, and (3) contact information for three references to Prof. Izabela Szlufarska at szlufarska@wisc.edu. Review of applicants will begin immediately and will continue until the positions are filled.