Multiple Postdoctoral Positions with Dane Morgan at University of Wisconsin (UW) – Madison

We invite applications for the following three postdoctoral position at the University of Wisconsin – Madison with Prof. Dane Morgan in the Department of Materials Science and Engineering:

Position 1: Discovery of Ultrahigh Vacancy Oxide Nanostructures for Defect Induced Ferromagnetism. This work will understand the stabilization mechanisms of massive cation vacancy concentrations in quasi twodimensional (2D) transition metal oxides, and thus to reveal how to induce strong ferromagnetism in nonferromagnetic oxides by dimension confinement and point defect engineering. The work builds on our recent discovery of ultrahigh vacancy ZnO magnetic nanosheets (<u>10.1021/acs.nanolett.9b02581</u>) and will be in close collaboration with experimental work lead by Prof. Xudong Wang (UW-Madison). The impact of this work will be transformative knowledge on nanoscale defects stabilization and ferromagnetism coupling effects in 2Dconfined oxide material systems, bringing a new pathway for creating strong room temperature ferromagnetism in a broad range of functional oxide materials. Results may offer many new multifunction coupling phenomena in applications such as spintronics, memories, quantum computing building blocks, and energy conversion.

Position 2: Development of Machine Learning Potentials with Applications to Molten Salts. This work is focused on the development of machine learning potentials to allow efficient treatment of many element systems with application to understanding thermophysical properties of impure molten salts of relevance for molten salt nuclear reactor applications. The work will use existing, and develop new, machine learning potential approaches to integrate active learning, on-the-fly learning, uncertainty quantification, and methods to treat many element systems. The work is in close collaboration with Prof. Izabela Szlufarska (UW-Madison). The impact of this work will be new approaches to machine learning potential forms, fitting, and uncertainty quantification for many element systems, and development of a database of important thermophysical properties of advanced nuclear salts.

Position 3: Modeling of Reactor Pressure Vessel (RPV) Mechanical Properties for Extended Life: This work is focused on the development of physics and data-centric models for hardening and ductile to brittle temperature shifts of irradiated steels, with a focus on behavior of RPV steels under light water reactor life extension conditions to 80 or 100 years. The work will apply *ab initio*-based thermodynamic and kinetic modeling to explore the sink behavior of nanoscale precipitates and machine learning to understand and predict hardening trends. The work is done in close collaboration with Prof. Robert Odette (UC Santa Barbara) and Dr. Mikhail Sokolov (Oak Ridge National Lab), with strong integration of experiment, modeling, and unique databases. The impact of this work will be new understanding of precipitate sink behavior, an unprecedented database for reactor materials properties, and guidance for light water reactor life extension and properties of irradiated materials.

Additional information: A PhD in materials science, nuclear engineering, or a related field is required. Familiarity with molecular modeling and/or machine learning and data science tools and a strong programming background are preferred, but capable and enthusiastic applicants with varied backgrounds will be considered. The appointment is initially for one year with the expectation of this being extended if the work is going well. Interested applicants should send (1) a CV in PDF format, (2) a brief cover letter describing which positions (more than one is fine) are of interest and suitability for the position, and (3) contact information for three references to Dr. Ryan Jacobs at uwcmghire21@gmail.com. Review of applicants will begin immediately and will continue until the positions are filled.

Professor Dane Morgan and the Computational Materials Group (CMG) (http://matmodel.engr.wisc.edu/): CMG is a joint effort of Izabela Szlufarska and Dane Morgan in the Department of Materials Science and Engineering at UW Madison. We are a highly active group leveraging simulation, machine learning and experiment and work in areas including nuclear materials, amorphous alloys, nanomechanics, nano-bio interfaces, fuel cells, batteries, semiconductors, and geophysics.