

Postdoctoral Research Associate in Modeling Radiation Effects

The Department of Mechanical and Materials Engineering (MME) at Queen's University, Canada, invites applications for two full-time Postdoctoral Research Associate positions to join the Canada Excellence Research Chair (CERC) program in Impact of Radiation in Energy and Advanced Technologies, a federal funded \$8M project led by Prof. Yanwen Zhang. Interested applicants should contact Prof. Zhang directly at yanwen.zhang@queensu.ca with a cover letter, CV, and names of two referees.

Project Opportunity

Nuclear energy provides over half of Ontario's electricity and close to 13% of Canada's total electricity demand, making it the country's second-largest source of non-emitting electricity. As the demand for clean energy grows, improving the performance and durability of nuclear materials is critical. However, conventional alloy development and traditional materials science approaches remain insufficient for addressing the challenges posed by extreme reactor environments. Fundamental mechanisms governing materials performance under irradiation are not fully understood, limiting the design of next-generation materials for safer, longer-lasting reactors.

The RE-MAT (Radiation Effects in Materials and Advanced Technologies) team within the CERC program adopts a multidisciplinary approach combining experimental and computational methods. Focused on concentrated solid-solution alloys, conventional dilute alloys, and complex ceramic materials, this research aims to develop radiation-resistant materials with enhanced structural stability and deformation tolerance under high temperature, stress, and radiation environments. Collaborative efforts with academic institutions, national laboratories, and industry partners seek to accelerate materials innovation for nuclear energy systems, contributing to Canada's low-carbon future.

This project focuses on understanding radiation effects in complex materials, including high-entropy materials (HEMs). The chemical complexity, driven by local elemental variation, enables a wide range of tunable bonding environments that are not achievable in conventional materials. Under extreme conditions, such as high temperature, pressure, or irradiation, these materials can be driven from thermal equilibrium into far-from-equilibrium states. Substitutional disorder in HEMs significantly influences defect dynamics and energy dissipation mechanisms, presenting unique challenges in predicting their behavior under irradiation. A mechanistic understanding requires detailed knowledge of elemental distribution, associated electronic structures, lattice distortion, and the resulting scattering and energy transfer processes. Harnessing this chemical disorder to control physical properties, optimize energy transport, and improve irradiation tolerance is essential for the development of advanced nuclear materials and other energy technologies. Gaining such insights will enable the design of complex materials with tailored functionalities and enhanced performance, opening new directions in materials science research.

Role Description:

The successful candidates will work closely with the RE-MAT team to investigate how tunable bonding environments and energy deposition from energetic particles influence the structure and properties of complex materials. This research aims to elucidate fundamental mechanisms governing defect generation, migration, and evolution under irradiation. Multi-scale modeling methods will be used, including density functional theory (DFT), *ab initio* molecular dynamics (AIMD), classical molecular dynamics (MD), two-temperature MD (2T-MD), and kinetic Monte Carlo (KMC). The work will focus on both nuclear and electronic energy deposition mechanisms, explicitly accounting for electron-phonon coupling and ionization effects, which are increasingly recognized as critical in modeling damage formation beyond traditional displacement damages alone. Collaboration with experimental teams will ensure validation of simulation

predictions and refinement of modeling approaches, with particular emphasis on how chemical disorder and multi-elemental interactions affect defect dynamics. The goal is to provide mechanistic understanding of phenomena, such as defect clustering, radiation-induced segregation, ionization-induced defect annihilation, and amorphization, bridging fundamental science with applied materials development.

Duties/Responsibilities:

- Conduct atomistic and mesoscale simulations of defect generation and radiation-induced damage in complex materials.
- Density functional theory (DFT) modeling bonding characteristics to elucidate the intrinsic nature and strength of bonds between atoms.
- High-throughput DFT calculations & *ab initio* Modeling to identify stable defects and compositions.
- Advancing modeling techniques to understand short-range disorder, defect formation, and evolution of various radiation-induced damage structures in HEMs.
- Work with other team members to maintain a high level of scientific productivity. Present and report research results and publish scientific results in peer-reviewed journals in a timely manner.
- Ensure compliance with health, safety, and quality requirements.

QUALIFICATIONS:

- PhD in Materials Science and Engineering or a closely related field with several years of relevant modeling experience; must have completed all degree requirements before starting the appointment and be within 4 years of receiving their Doctorate.
- In-depth knowledge and a minimum of three years of demonstrated experience in modeling radiation effects in metal alloys or ceramics.
- Experience in advanced modeling and data analysis techniques of complex metal alloys and/or ceramics performance under extreme conditions. For example, proficiency in DFT, AIMD, on-the-fly machine-learning, classical MD, and 2T-MD to achieve detailed insights into material structures at the electronic and atomic level, including bonding characteristics, partial charge transfer and electron redistribution, and potential transient ionization in scenarios far from equilibrium.
- Strong record of productive and creative research demonstrated by publications, both as a lead author and a contributor, in peer-reviewed journals and presentations at scientific conferences.
- Excellent organizational, planning, and time management skills, with adaptability and flexibility. Able to anticipate deadlines, prioritize activities and tasks, and independently set priorities to accomplish multiple tasks within required timeframes.
- Capable of innovative, independent research with the ability to work collaboratively in a team environment and interact effectively with a broad range of colleagues, both within and outside the Nuclear Materials Group and MME.
- Motivated and safety-conscious, with excellent interpersonal, written, and oral communication skills in English for engaging with an international scientific audience.

Application Process

Please submit a cover letter, CV (including full publication list), and contact information for two referees to Prof. Yanwen Zhang at yanwen.zhang@queensu.ca. Applications will be reviewed on a rolling basis until the positions are filled.