**POSITION SUMMARY**

**QUEEN’S UNIVERSITY – Postdoctoral Researcher *modeling***

We are looking for an enthusiastic candidate for postdoctoral position(s) on modeling defect formation and dynamics in complex alloys and ceramics. This position will be part of the recently $8M funded *Impact of Radiation in Energy and Advanced Technologies* CANADA EXCELLENCE RESEARCH CHAIRS (CERC) program.

This project focuses on radiation effects in high-entropy materials (HEMs). The composition complexity in HEMs gives rise to local chemical disorder and a diverse range of tunable bonding environments not typically possible in conventional materials. Extreme conditions, such as high temperature, current, pressure, and radiation environments, can push materials from thermal equilibrium to far-from-equilibrium states. Substitutional disorders in HEMs are expected to modify defect dynamics and energy dissipation processes, posing unique challenges in predicting their performance. To reveal the atomic and/or electronic structure responsible for differences in material properties, it is crucial to effectively describe elemental distribution, the accompanying electronic structures, and lattice distortion, as well as the corresponding scattering mechanisms and energy transfer processes. Understanding how chemical disorder can be harnessed to tailor physical properties, enhance or control energy transport, and improve irradiation tolerance is key for advanced technological applications. This knowledge of chemical disorder and elemental substitution will enable the design of complex materials with specific functionalities and improved performance, opening numerous exciting research directions in materials science.

The successful candidates will work closely with the CERC, Prof. Yanwen Zhang to conduct research activities. The activities also include collaboration with other experimentalists and theorists in the Nuclear Materials Group. Working with the PI and a multi-disciplinary team of graduate students, Post-Doctoral Fellows, and senior researchers, the incumbent will have significant opportunities for joint experiment-modeling-theory efforts and publications. This position is part of the Nuclear Materials Group within the Department of Mechanical and Materials Engineering (MME) at Queen’s University.

**Duties/Responsibilities:**

* Conduct studies of defects, defect processes, and radiation effects in complex materials in a radiation environment.
* Density functional theory (DFT) modeling of bonding characteristics to elucidate the intrinsic nature and strength of bonds between atoms.
* High–throughput DFT calculations & *ab initio* Modeling to identify stable compositions and defects.
* Advancing modeling techniques to understand short-range disorder, defect formation, and evolution of various radiation-induced damage structures in HEMs.
* Responsible for presenting and reporting research results and publishing scientific results in peer-reviewed journals in a timely manner.
* Self-motivated and working with other team members to maintain a high level of scientific productivity.
* Ensure compliance with environment, safety, health and quality program requirements.
* Maintain strong commitment to the implementation and perpetuation of values and ethics.

**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, *ab initio* molecular dynamics, on-the-fly machine-learning, classical molecular dynamics (MD), and two–temperature 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 limited 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.