

## **DESCRIPTION FOR THE GENERAL PUBLIC**

The acute toxicity and radioactivity of actinide materials complicate experimental studies of the “soup” of nuclear waste produced in nuclear reactors. This motivates research into computational methods for predicting the chemical reactivity and molecular properties of actinide-containing compounds. Unfortunately, the computational resources required by conventional quantum chemistry methods grow exponentially with the size of the system, an effect known as the curse of dimension. Since the actinide-containing molecules of importance to nuclear waste separation and reprocessing contain a very large number of electrons, typically hundreds or thousands of electrons, quantum chemistry has to develop innovative new approaches that break the curse of dimension. One such family of approaches exploits a neat and compact parameterization scheme of the electronic wavefunction. Specifically, the density matrix renormalization group algorithm represents a cheap and reliable quantum-mechanical approach that can be used to describe a large number of electrons, typically encountered in actinide atoms and molecules. To reliably model actinide chemistry, the effects of the fast movement of electrons (special relativity) have to be properly accounted for in computational studies. This can be achieved by solving the relativistic (four-component) Dirac equation instead of the Schrödinger equation, which usually forms the central equation for lighter elements. In the proposed research project, the relativistic DMRG algorithm will be used to model the fundamental structure and properties of actinide atoms and small actinide clusters across the actinide series as well as some model actinide oxide complexes formed by cation-cation interactions encountered in the soup of nuclear waste. The DMRG calculations will represent the first systematic, atomistic, and quantitative computational study for understanding actinides and their building blocks formed during nuclear waste reprocessing and will yield new insights into the physical properties of actinide species, the nature of the bonding and the reactivity of actinide-containing compounds, and how to control the formation of actinide clusters like cation-cation interactions. This will provide the essential information that is needed to efficiently model large scale actinide materials that can be used to separate Uranium and Plutonium from the other components in the “soup” of nuclear waste.