
# Computational Molecular Modeling for Nuclear Waste Management and Other Radiochemical Applications

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## Abstract

Safe and sustainable management of nuclear energy poses major scientific and engineering challenges, one of which is the necessity, to make the environmental impacts of the long-term nuclear waste storage as small as possible. This requires significant improvements in our understanding of the behaviour of radionuclides and their retention mechanisms in geological formations of nuclear waste repositories over the ranges of time and distance spanning many orders of magnitude. Detailed molecular scale knowledge of the complex chemical and physical processes controlling the interaction of radionuclides with clay and cementitious materials is crucial for building better predictive models of their adsorption and mobility in natural and engineered barriers of the nuclear waste repositories. The presence of natural organic matter (NOM) in clayey formations and its complexation with metal ions in aqueous solutions has significant effect on the transport properties of the radionuclides.

In this presentation, we will overview our current efforts to apply computational molecular modeling techniques to address these problems on the fundamental molecular level. We use classical molecular dynamics (MD) simulations for detailed quantitative studies of the structural, energetic and dynamic aspects of interactions between radionuclides, organic matter and clay particles. Structural and thermodynamic parameters are obtained by studying different processes such as hydration, adsorption, complexation, and intercalation. The complexation mechanisms of organic molecules with aqueous metal ions will then be presented using the free energy calculations. Metal cations can strongly associate with negatively charged functional groups of organic molecules and with negatively charged clay surfaces. This allows us to predict that cationic bridging could be the most probable mechanism responsible for the controlling effects of organics on the behaviour of radionuclides in clays and other repository materials. Our most recent results demonstrating how the nature of the adsorbed cations affects the structural and dynamic properties of the mineral-water interface and also the effect of disordered substitution in on the adsorption and swelling behaviour of clay minerals will then be discussed briefly.