

Abstract Submitted
for the TSS14 Meeting of
The American Physical Society

Atomistic Modeling of Uranium (IV) Ion Interaction with Water

AUSTIN MCDONALD, RAYMOND ATTA-FYNN, Department of Physics, The University of Texas at Arlington — A fundamental understanding of the interaction of toxic heavy metal ions with the biosphere, particularly water, is important for their remediation from the environment. Predicting the behavior of such ions in water requires a detailed atomic and molecular scale understanding of the ion-water interaction. In this talk, we will describe the process for modeling the interaction of the U^{4+} ion with water using static first principles and classical molecular dynamics methods. The hydrations shell structure of U^{4+} and other properties such as the radial distribution function, solvent angular tilts, and ion diffusion will be discussed and compared to available experimental and theoretical data.

Raymond Atta-Fynn
Department of Physics, The University of Texas at Arlington

Date submitted: 26 Feb 2014

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