On the solvation of actinide ions

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Simulation of the universal ions in water solution is a standardized tool commonly used today. The route to simulation of actinide ions is normally tough because the evaluation of the simulation parameters are normally not given empirically and standard Hartree-Fock calculations are not accurate enough. We use multiconfigurational quantum chemical calculations when deriving the parameters for actinide ion-water potential[1]. The parameters are then simulated using classical molecular dynamics. A case study of the Cm3+ ion will be presented on the poster. Results from the simulations will be also be discussed, e.g. the radial distribution functions and the coordination number.

[1] D. Hagberg, G. Karlstrom, B.O. Roos and L. Gagliardi The coordination of uranyl in water: a combined quantum chemical and molecular simulation study J. Am. Chem. Soc. 127, 14250-14256 (2005)