

Heavy Element Solution Chemistry – A Sojourn Through Ideal and Non-Ideal Solutions and Their Interfaces

Aurora E. Clark^a

^a Department of Chemistry, Washington State University
auclark@wsu.edu

Heavy elements, including those actinides and lanthanides, often exist as highly charged ions that induce extended polarization across multiple solvation shells and organizational structure in solution.[1,2] Their metal-ligand complexes are also prone to supramolecular self-assembly facilitated by long-range electrostatic interactions with solvent or background electrolyte participation.[3] Tackling the solution chemistry of *f*-elements requires an in-depth understanding of electronic structure and hierarchical interactions they impose upon their surroundings. This work will discuss different strategies for performing condensed phase simulations of actinides and lanthanides in solution environments that systematically approach realistic conditions associated with purification and synthesis. Such work spans both *ab-initio* and classical molecular dynamics simulations and underpinning methods (e.g. the development of new polarizable potentials for An(III)). Further, we discuss the practical impacts of hierarchical interactions associated with actinides in realistic solutions, and how this challenges traditional computations that rely on well-understood energy landscapes and narrow ensemble distributions of solution phase environments.

References

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