Machine-learned approaches to study the dynamic fluctuations local structure of actinides in molten salts

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The chemical properties of the 4f and 5f elements have long captured our attention, due to both experimental and computational challenges surrounding their studies. The study of heavy elements under realistic conditions requires the use of sophisticated methods and extended models. Computer advances in modern algorithms and data science have opened new avenues to better understand the chemical structure and speciation, reactivity prediction of chemical properties. In my presentation, I will review recent contributions in the study of heavy elements in condensed phase. The development of pseudopotentials and companion basis sets for the entire actinide series represents a reliable computational tool for *ab initio* molecular dynamics (AIMD) studies of these elements [1]. When supplemented with machine-learned potentials [2, 3, 4], it allows us to extend simulation times and extract descriptors that can serve as structural fingerprints of actinides in a molten salt matrix.

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