

Structural and Transport Properties of Actinide-Containing Molten Salts: Machine Learning-based Studies

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Actinide-containing molten salts are a critical part of next generation nuclear reactors. Yet, studying their fundamental properties is highly challenging for both experiment and modeling. In this talk, I will present our recent efforts in understanding these materials at the atomistic level by using statistical mechanics and machine learning. First, I will discuss our development of pseudopotentials and basis sets for the actinide series [1,2] that allow for large scale ab initio molecular dynamics (AIMD) simulations. Next, I will talk about our AIMD studies and machine learning -based analyses of the coordination structure of single actinide ions in host molten salts [3]. Finally, I will present how we used machine learning interatomic potential molecular dynamics and graph theory to discover the breakdown of entropy-scaling laws of the diffusion of actinide ions and learn about their clustering [4,5].

Keywords: Machine learning interatomic potentials, molecular dynamics, molten salts, graph theory

References

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