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Force Field Optimization for Molten Salts TALMAGE PORTER, DENNIS DELLA CORTE, TODD MILLECAM, Brigham Young University — With the inclusion of Molten Salt Reactors (MSRs) in the selection of Generation IV Nuclear Reactors (Gen IV - a selection of nuclear reactor designs to be researched for commercial applications), molten salts have come into focus. The primary use of molten salts is as coolant for MSRs. In-lab testing of various salt mixtures has proven to be difficult with issues including safety hazards and time constraints. Due to these complications, simulation techniques, like molecular dynamics (MD), are a viable option for testing. Atomic level simulations are a well-researched field primarily due to its heavy use in biophysical and material science research, but the necessary forcefields for molten salts are still lacking in quality. Here, we will discuss current shortcomings in available molten salt forcefields and approaches that will lead to better parametrization. We will also present how improved MD can be used to derive relevant thermodynamical properties, necessary for MSR design regulatory approval.

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