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Molten Salt Eutectics from Atomistic Alchemical Simulations SAIVENKATARAMAN JAYARAMAN, AIDAN THOMPSON, Advanced Device Technologies department, Sandia National Laboratories, Albuquerque, NM, O. ANATOLE VON LILIENFELD, Leadership Computing Facility, Argonne National Laboratory, Argonne, IL — Molten salt mixtures are gaining importance in solar thermal power applications. Unfortunately, their phase diagrams cannot be easily computed from first principles calculations. The eutectic mixture composition and temperature are located using the liquid mixture free energy and the pure component solid-liquid free energy differences. The liquid mixture free energy is obtained using thermodynamic integration of alchemical transformations of one atom to another. Numerical results for binary and ternary mixtures of alkali nitrates agree well with experimental measurements [1]. Some results involving mixtures of monovalent and divalent cations will also be presented.

[1] Jayaraman, Thompson, and von Lilienfeld, PRE, 84, 030201 (2011).

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