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Eutectics and Phase Diagrams of Molten Salts from Molecular Dynamics simulations SAIVENKATARAMAN JAYARAMAN, ANATOLE VON LILIENFELD, AIDAN THOMPSON, Sandia National Laboratories — The use of alkali nitrate salt mixtures as heat transfer fluids in solar thermal power plants is limited by their relatively high melting point. Certain compositions of quaternary and higher dimensional mixtures of alkali and alkaline earth nitrates and nitrites have low melting points. However, the high dimensionality of the search space makes it difficult to find lowest melting compositions. Molecular simulations offer an efficient way to screen for promising mixtures. A molecular dynamics scheme general enough to identify eutectics of any HTF candidate mixture will be presented. The eutectic mixture and temperature are located as the tangent point between free energies of mixing for the liquid and a linear plane connecting the pure solid-liquid free energy differences. The free energy of mixing of the liquid phase is obtained using thermodynamic integration over “alchemical” transmutations sampled with molecular dynamics, in which particle identities are swapped gradually. Numerical results for binary and ternary mixtures of alkali nitrates agree well with experimental measurements.

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