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**Molecular Simulations of Liquid/Vapor Phase Equilibria for Single Component and Binary Mixtures of Nanoparticles** MARK HORSCH, PIETER IN'T VELD, JERMEY LECHMAN, GARY GREST, Sandia National Labs
— Self-assembly of nano and colloidal particles into ordered structures is an important technological challenge for the design of future materials and devices. One promising self-assembly technique is the evaporation of nanoparticles suspended in droplets. However, it is difficult to experimentally observe the self-assembly process in the evaporating droplet. Computer simulation provides an avenue with which to address and directly observe the self-assembly of model nano and colloidal particles within the droplet provided an efficient model can be developed. Here we present the liquid-vapor phase envelopes for model particles as a function of particle size. We compare the liquid/vapor phase envelopes and the computational efficiency for several different models including composite particles comprised of Lennard-Jones (LJ) atoms and particles interacting via integrated LJ potentials. Results for binary mixtures of nanoparticles in a solvent of LJ atoms will also be presented. These studies provide a framework for the size range of particles that can be addressed by each model. Sandia is a multiprogram laboratory operated by Sandia Corp., a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under Contract DE-AC04-94AL85000.

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