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Phase Separation in Charge-Stabilized Colloidal Suspensions: A Simulation Study¹ BEN LU, ALAN R. DENTON, Department of Physics, North Dakota State University — A variety of experiments^{2,3} suggest that deionized suspensions of highly charged colloids may exhibit an unusual fluid phase separation. Here we report results of Gibbs ensemble Monte Carlo simulations of a model system consisting of charged colloidal macroions and microions (dissociated counterions and salt ions) dispersed in water. As input to the simulations, we use effective electrostatic interactions – a screened-Coulomb macroion-macroion pair potential and a one-body volume energy – predicted by mean-field linear response theory⁴. The volume energy – a natural byproduct of integrating out from the partition function the microion degrees of freedom – plays a crucial role in the acceptance probabilities for trial volume changes and particle transfers in the Gibbs ensemble. We present the bulk fluid phase diagram, which exhibits vapor-liquid coexistence at low salt concentrations ($c_s < 1$ mM), and compare with theoretical predictions.

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