Use of the Trappe Model to Predict P-V-T Data at Extreme Conditions

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The thermophysics of materials at extreme pressure and temperature conditions is essential for our understanding of many planetary and detonation processes. There remain significant gaps in our knowledge of the behavior of materials at high density and high temperature, due in part to the limitations and dangers of performing experiments at the necessary extreme conditions. Through the use of equations of state and particle-based simulation methods, the range of pressures and temperatures that can be studied is significantly extended. However, to improve the reliability of these calculations, accurate and quantitative models are required. We present an assessment of the united-atom and explicit-hydrogen versions of the TraPPE (Transferable Potentials for Phase Equilibria) force field for several important molecules at extreme conditions. The TraPPE models, despite being parameterized to the vapor-liquid coexistence curve (i.e. relatively mild conditions), perform remarkably well in the high pressure/high temperature regime. For comparison, we use a single-site exp?6 representation with parameters also determined from the vapor-liquid coexistence curve. Configurational-bias Monte Carlo simulations in the canonical and isobaric-isothermal ensembles are carried out for methane, methanol, oxygen, and ammonia. Results obtained for these multi-site and single-site potentials are compared to experimental data and equation of state predictions.