Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Three dimensional phase behaviour of core-softened potentials
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Interest in core-softened pair potentials originates in the work of Stell and Hemmer which proposed that such models may produce a liquid-liquid phase transition in a single component system. In this work we concentrate of the 'shoulder' form of core-softened potential, constructed as a superposition of the Lennard-Jones potential and an outer Gaussian minimum. This potential has been subject to much study in two dimensions, in which various liquid anomalies have been reported. The behaviour of these models in three dimensions is unclear, with previous studies limited to small or meta-stable regions of the phase diagram. We have mapped the full stable phase diagram in three dimensions for a family of core softened potentials as a function of the outer well depth, using a variety of computational techniques. In the solid, we note a replacement of fcc structure by simple hexagonal with increasing outer well depth, with further phase transitions at high pressure. Trends in melting temperature and the location of the critical point are also explored. We then search for anomalies over the full thermodynamically stable liquid, paying particular attention to the region close to the melting temperature.

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Date submitted: 06 Dec 2004 Electronic form version 1.4