Title: Phase diagram mapping of soft shoulder systems
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Abstract:

Monodisperse spheres interacting via `hard core/soft shoulder' (HCSS) pair potentials (e.g., hard spheres with an additional repulsive step interaction) exhibit extremely rich phase behavior, comprising a diverse array of two- and three-dimensional liquid crystal phases and a wide variety of complex crystal structures [M. A. Glaser et al., EPL 78 (2007) 46004], including relatively open crystal structures such as the 2D honeycomb lattice [E. A. Jagla, J. Chem. Phys. 110, 451 (1999)] and the 3D diamond lattice. The complex phase behavior of this class of systems derives from competition between an underlying `soft shoulder' clustering instability [W. Klein et al., Physica A 205, 738 (1994)] and excluded volume constraints. Previously we have mapped out the zero temperature phase diagram for the 2D and 3D systems. We generalize these results to continuous HCSS models (soft sphere with generalized exponential steps) and observe qualitatively similar results. In addition, dynamical matrix calculations for the continuous model confirms the stability of several of these interesting phases. We present a method of extending the phase diagram into finite temperature based on a tournament model as well as preliminary results. Work supported by NSF MRSEC Grant DMR-0213918 and GAANN Fellowship P200A030179.