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Directing self-assembly by tailoring pair potentials of soft shoulder systems ZACH SMITH, PAUL BEALE, NOEL CLARK, MATT GLASER, Dept. of Physics, University of Colorado, Boulder — 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, including a diverse array of two- and three-dimensional liquid crystal phases and a wide variety of complex crystal structures [M. A. Glaser et al., cond-mat/0609570], including relatively open crystal structures such as the 2D honeycomb lattice [E. A. Jagla, J. Chem. Phys. 110, 451 (1999)]. 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. We show that it is possible to derive soft shoulder potentials to promote self-assembly of specific target structures using only geometrical information. We have applied this approach to the self-assembly of a stable 3D diamond lattice in systems of particles with isotropic pair interactions, demonstrating that anisotropic, directional bonding is not a necessary requirement for formation of the diamond lattice. This approach, which exploits soft shoulder clustering behavior, is a powerful tool for the directed design of a variety of unusual and complex self-assembled systems. Work supported by NSF MRSEC Grant DMR-0213918 and GAANN Fellowship P200A030179.

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