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Reentrant and Isostructural Transitions in the Cluster-Crystal Forming GEM-4 KAI ZHANG, PATRICK CHARBONNEAU, Duke University, BIANCA MLADEK, University of Cambridge — Systems governed by soft, bounded, purely repulsive interactions show two possible equilibrium behaviors under compression: reentrant melting, as in the Gaussian core model (GCM), or clustering, as in the penetrable sphere model (PSM). The generalized exponential model of power 4 (GEM-4), which is the intermedia of the GCM and PSM with a simple isotropic pair interaction $u(r) \sim e^{-r^4}$, is thought to belong to the second family and was indeed found to form clusters at sufficiently high densities at high temperatures. Here, we present the low-temperature behavior of GEM-4 through Monte Carlo simulations using a specially developed free energy integration scheme. We find the phase behavior to be hybrid between the GCM and the PSM limits, showing a surprisingly rich phase behavior in spite of the simplicity of the interaction form. For instance, S- shaped doubly reentrant phase sequences and evidence of a cascade of critical isostructural transitions between crystals of different average lattice site occupancy are observed. The possible annihilation of lattice sites and accompanying clustering moreover leads to an unusual softening upon compression, which suggest that these materials may have interesting mechanical properties. We discuss possible experimental realizations and challenges of this class of materials.

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