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An [N]PT Ensemble for Studying the Intricate Thermodynamics of Cluster Crystals KAI ZHANG, PATRICK CHARBONNEAU, Duke University — Exotic soft matter systems such as certain dendrimers can overlap with only a finite energy penalty. Systems governed by steep, bounded repulsive interactions, such as the penetrable sphere model (PSM), indeed form cluster crystals with multiple particles per lattice site under compression. Standard simulation approaches that keep NVT, NPT, or μVT constant cannot directly equilibrate cluster crystals, because either N or lattice constant is not free to relax. It is tempting to allow all fields to fluctuate by keeping "μPT" constant, but basic thermodynamics indicates that infinite fluctuations then result. We avoid this caveat by using a $[N]PT$ ensemble, in which P and T are fixed but N is allowed to fluctuate within bounds $[N_{\min}, N_{\max}]$ under a conjugate field analogous to μ. The approach provides the equilibrium properties of neighboring state points through histogram reweighing. We solve the phase diagram of the PSM, and confirm that the FCC crystal lattice occupancy linearly increases with ρ at high T. At low T the occupancy plateaus at integer values, but the transitions remain continuous and the crystal does not phase separate. We also examine the critical behavior of another related model.

Kai Zhang
Duke University

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