

Abstract Submitted
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Enthalpy versus Entropy: the Thermodynamic Origin of Hard Particle Ordering¹ MITCHELL ANTHAMATTEN, SHAW CHEN, JANE OU, JEFFREY WEINFELD, University of Rochester, DEPARTMENT OF CHEMICAL ENGINEERING TEAM — The topic of hard particle ordering transitions is important in the development of molecular to mesoscale materials with potential applications in biomedicine, catalysis, optoelectronics, and renewable energy. The first step toward deterministic materials design rests on understanding the thermodynamic nature of ordering transitions involving two phases in equilibrium. We apply classical thermodynamics to show that (i) first-order, hard particle ordering transitions are forbidden at constant volume; and that (ii) hard-particle ordering is driven by a loss in enthalpy through volume reduction that outweighs a concomitant entropy loss upon ordering. The traditional approach considers minimization of Helmholtz energy, at constant volume, whereas the current study exclusively focuses on equilibrium phase transitions and, therefore, targets minimization of Gibbs energy at constant pressure. The Gibbs energy platform offers physically intuitive interpretations consistent with existing computation and experiments. The prevalent idea of entropy-driven ordering at constant V is restricted to transitions from non-equilibrium initial states that have yet to be properly defined for quantification.

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