A More Direct Approach to Finding Phase Transitions in Realistic Alloy Models[1] DEREK W. OSTROM, Brigham Young University, LANCE J. NELSON, Brigham Young University - Idaho, CONRAD W. ROSENBROCK, GUS L.W. HART, Brigham Young University — Cluster expansions provide fast Hamiltonians, allowing for thermodynamic Monte Carlo searches for phase transitions. Monte Carlo simulations often converge slowly and require tuning. A simpler approach may be to use Wang-Landau sampling and compute the transition temperature directly from the partition function. The Wang-Landau algorithm has been successfully demonstrated for toy alloy models. We compare Wang-Landau sampling with thermodynamic Monte Carlo simulations for realistic cluster expansion models with many terms.

Derek W. Ostrom
Brigham Young University

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