Abstract Submitted
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Rapid and Accurate Estimates of Alloy Phase Diagrams for Design and Assessment[1] TECK TAN, DUANE JOHNSON, University of Illinois, Urbana-Champaign — Based on first-principles cluster expansion (CE), we obtain rapid but accurate assessments of alloy T vs c phase diagrams from a mean-field theory that conserves sum rules over pair correlations. Such conserving mean-field theories are less complicated than the popular cluster variation method, and better reproduce the Monte Carlo (MC) phase boundaries and T_c for the nearest-neighbor Ising model [1]. The free-energy f(T,c) is a simple analytic expression and its value at fixed T or c is obtained by solving a set of n non-linear coupled equations, where n is determined by the number of sublattices in the groundstate structure and the range of pair correlations included. While MC is "exact," conserving mean-field theories are 10 to 10^3 faster, allowing for rapid phase diagram construction, dramatically saving computation time. We have generalized the method to account for multibody interactions to enable phase diagram calculations via first-principles CE, and its accuracy is showed vis-à-vis exact MC for several alloy systems. The method is included in our Thermodynamic ToolKit (TTK), available for general use in 2009.
[1] V. I. Tokar, Comput. Mater. Sci. **8** (1997), p.8

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