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Optimal Cluster Expansions: Predicting Alloy Thermodynamics with Desired Accuracy[1] NIKOLAI ZARKEVICH, DUANE D. JOHNSON, University of Illinois at Urbana-Champaign — We show how to achieve a desired accuracy in first-principles prediction of alloy thermodynamics using an optimal cluster expansion [1], and discuss reliability of error estimates. We illustrate the scaling of computational complexity versus accuracy, and demonstrate that with controlled accuracy a reliably predicted phase-transition temperature converges to the experimental value. We also show there is a simple and rapid means to estimate transition temperatures using the optimal cluster expansion. [1] N.A. Zarkevich and D.D. Johnson, Phys. Rev. Lett. **92**, 255702 (2004).

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