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Computational Toolkit for First-Principles Multicomponent Alloy Thermodynamics[1] TECK TAN, NIKOLAI ZARKEVICH, D.D. JOHNSON, Materials Science and Engineering, University of Ilinois Urbana-Champaign — A "toolkit" for the simulation of alloy thermodynamics has been developed by integrating first-principles, electronic-structure calculations and the cluster expansion (CE) with Monte Carlo (MC) methods. This Thermal Toolkit (TTK) is aimed at producing reliable thermodynamics of alloys with limited input from the user. Given an alloy, TTK first generates a comprehensive set of structures, automatically submits an electronic-structure calculation to determine the structural energies, stores the structure and its energy in a database,[2] then constructs the CE via the structural inversion method that conforms to a set of mathematical conditions to produce an optimal truncated cluster expansion.[3] Using this optimal CE, a MC code (included in TTK) can be used to calculate thermodynamic properties, such as structural phase diagram (T vs c). We present here example application and functionality of TTK on binary and ternary alloy.

[1]We acknowledge funding from NSF ITR grant DMR-03-25939 and DOE grant DE-FG02-03ER46026.
[2]The "Structural Database" http://data.mse.uiuc.edu
[3]Nikolai Zarkevich and D.D. Johnson, Phys. Rev. Letts 92, 255702 (2004)

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