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**Rapid First-Principles Design Estimates of Alloy Order-Disorder Temperatures**<sup>1</sup> TECK L. TAN, NIKOLAI ZARKEVICH, D.D. JOHNSON, Materials Science & Engineering, UIUC — From DFT calculations, we propose a rapid, mean-field estimate for order-disorder temperatures  $T_c$  and phase diagrams via cluster expansion Hamiltonians  $H = \sum_i V_i \phi_i$ , where  $V_i$  and  $\phi_i$  are, respectively, the  $i$ -th cluster interaction and correlation function. We discuss when the estimate is valid and confirm its accuracy via Monte Carlo simulation. As the cost of Monte Carlo (MC) increases with number and size of clusters, such rapid estimates are desirable both for design and to limit the T and composition range needed for MC. We show two broad classes of systems as determined by  $V_i$  in which  $T_c$  is given accurately by (i)  $\Delta H_{d-o}/\Delta S_{d-o}$  or (ii)  $\Phi\Delta H_{d-o}$ , where  $\Delta H_{d-o}$  and  $\Delta S_{d-o}$  are the enthalpy and entropy differences between fully disordered and ordered phases, respectively, and  $\Phi$  is a lattice-topology dependent constant. With no finite-T intermediate phases, phase boundaries are found analytically by  $T_c(x - x_s) = \eta^2(x - x_s)T_c(x_s)$ , where  $\eta$  ( $0 \leq \eta \leq 1$ ) is the long-range order parameter and  $(x - x_s)$  is deviation from stoichiometry,  $x_s$ , found rapidly by CE ground-state analysis, and  $T_c(x_s)$  is from (i) or (ii). We exemplify results for several alloys in each class.

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