Relaxation and the Robustness of Cluster Expansions[1] ANDREW NGUYEN, GUS HART, Brigham Young Univ - Provo — Cluster expansion (CE) has been used extensively to predict stable structures of metal alloys. Cluster expansions model alloys on a fixed lattice as a purely configuration problem. CE models are built from data taken from first-principles calculations. In these first-principles calculations, individual atoms move away from the ideal lattice position. A perennial question in the CE community is how accurate the expansion is when these relaxations are allowed - formally, the formalism of CE breaks down when the underlying lattice is not preserved. We compare fits using relaxed and unrelaxed training sets in an attempt to quantify the effects of relaxation on the robustness of CE predictions.

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