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The Robustness of Cluster Expansion: Assessing the Role of Relaxation[1] ANDREW H. NGUYEN, CONRAD W. ROSENBROCK, GUS L. W. HART, Brigham Young Univ - Provo — Cluster expansion (CE) has been used widely in combination with first-principles calculations to predict stable structures of metal alloys. CE treats alloys as a purely configuration problem, i.e., a problem in the distribution of the alloying elements on a fixed lattice. CE models are usually built from data taken from "relaxed" first-principles calculations where the individual atoms assume positions that minimize the total energy. A perennial question in the cluster expansion community is how the accuracy of the CE is affected by relaxations—technically, the formalism of CE breaks down when the underlying lattice is not preserved—but practitioners often argue that there is a one-to-one correspondence between relaxed and unrelaxed structures so that the formalism holds. We quantify the effect of relaxation on the robustness of cluster expansions by comparing CE fits for relaxed and unrelaxed data sets. Our results give a heuristic for when CE models can be trusted.

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