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Chasing Exotic Binary Alloy Compounds: The Necessary Synergy of Cluster Expansion and High-Throughput Methods[1] STEFANO CURTAROLO, Duke University and Weizmann Institute of Science, GUS L. W. HART, Brigham Young University, Provo, UT, USA, OHAD LEVY, NCRN, Negev, Israel — Predicting the stable crystal structures of alloys from their components is a major challenge of current materials research. Ab initio methods explore the phase stability landscape of binary alloys by calculating the formation enthalpies of a large number of structures, and identifying the minima at various component concentrations. Major methods of this type are cluster expansion (CE) and high-throughput ab initio calculations (HT). The CE explores structures on specific types of lattices while the HT method explores experimentally-known structures representing all crystal systems. The CE may find derivative superstructures missed by the HT but is not applicable off-lattice. Combining and reciprocally informing both methods resolve their respective drawbacks. We demonstrate this in a several technologically important Hf, Rh alloy systems. These results emphasize the complementary strengths of the CE and HT methods and the need for using both in searching for new stable compounds in metallic systems.

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