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Genetic-Algorithm first-principles prediction of novel ground state[1] ALEX ZUNGER[2], VOLKER BLUM[2,3] — Binary $A_{1-x}B_x$ alloys can exist in any of the 2^N possible configurations on a lattice of N points; finding the true ground-state thus requires mapping the LDA total-energies on an Ising-like Hamiltonian with generally numerous pair and many-body interactions. Finding which many-body interactions best reproduce the LDA energies is tedious, and often involves subjectives choices. Here we use artificial (but objective) intelligence to make such choice. We combine DFT calculated total energies of $O(50)$ configurations for each binary alloy in the Nb, Ta, Mo, W system with a "Mixed Basis Cluster Expansion" whose interaction types are chosen by a *genetic algorithm* search.[1] We thus derive the energy for *any* bcc configuration (in practice, $\sim 3,000,000$ structures). This (Ising-like) functional is then searched for 2^N configurations to find $T = 0$ ground state structures, and to compute (via Monte Carlo) finite T thermodynamics and short- range order. We find rather surprising ground state – very different from those suspected by the approach of "rounding up the usual suspects"
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