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Using genetic algorithms to find from first-principles the minimum-energy crystal structure starting from random cell vectors and random atomic positions.[1] G. TRIMARCHI, M. D'AVEZAC, ALEX ZUNGER, NREL, Golden CO 80401 — We address the global space-group optimization problem in binary metallic A_qB_{1-q} alloys using an evolutionary algorithm. A set of crystal structures with randomly-selected lattice vectors and atomic positions is evolved, replacing the highest energy structures with new ones generated through mating or mutation, as well as ab-initio structural relaxation to the nearest local minimum. This was applied to a few compounds whose lattice-type is difficult to guess because the constituent solids A and B have different lattice types (e.g., A is fcc and B is bcc): (i) compounds with the crystal lattice of either A or B constituents, i.e., $CdPt_3$, $AlSc_3$, Al_3Sc; (ii) compounds with a crystal lattice different than that of either constituents, i.e., AlSc and CuPd; (iii) compounds whose crystal lattice is not even of a Bravais type, e.g., $PdTi_3$. The optimization scheme retrieved the lowest energy structures within about 100 total-energy evaluations. Not all independent GA sequences end up giving the same final structure; we select the lowest energy structure from all sequences. Using a model calculation, we will discuss how many independent GA sequences are needed to find the lowest energy structure with given confidence.

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