

Abstract Submitted
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Determination of the ground state structures of binary alloys via global space group optimization (GSGO) with no restrictions on composition: Al-Sc.¹ GIANCARLO TRIMARCHI, ARTHUR J. FREEMAN, Northwestern U., ALEX ZUNGER, NREL, Golden, CO 80401 — Here, we extend the GSGO evolutionary algorithm scheme to survey crystal structures of binary A-B systems *without* constraint on the A_pB_q composition. At each generation of the randomly started evolutionary sequences, the formation energy convex hull for the actual population is determined. The search proceeds by replacing the structures farthest away from the convex hull with new ones produced via mating and mutation with no constraints on composition. As a test of this new procedure, we searched the ground state compounds of the Al-Sc alloy whose lattice types are not easily inferred from that of the Al and Sc constituents, respectively fcc and hcp solids. Repeated, independent evolutionary sequences with six and eight atoms in the supercell were performed yielding as ground states respectively B8₂, B2, and C15, and D0₁₉, B2, and L1₀, as known from experiment and previous *ab-initio* studies. This yields a synthesis of the final convex hull.

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