Abstract Submitted
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The global space-group optimization approach to crystal structure prediction[1] GIANCARLO TRIMARCHI, ALEX ZUNGER, National Renewable Energy Lab., Golden, CO 80401 — We present the global space-group optimization (GSGO) approach to the prediction of both the lattice structure and the atomic configuration of a crystalline solid. The GSGO method is based on an evolutionary algorithm within which a population of crystal structures is evolved substituting the highest total-energy structures with new ones. The search is performed directly on the atomic positions and the unit-cell vectors, after a similarity transformation is applied to bring structures of different unit-cell shapes to a common basis. Following this transformation, we can define a crossover operation that treats on the same footing structures with different unit-cell shapes. Newly generated structures are fully relaxed to the closest local total-energy minimum. Starting from random unit-cell vectors and atomic positions, and using the VASP code, the GSGO procedure found for Si, GaAs, SiC the correct lattice structure and configuration. In the case of Au_8Pd_4, the search retrieved the correct underlying lattice type (fcc), but energetically closely spaced (~ 2 meV/atom) alloy configurations were not resolved. The GSGO approach opens the way to predicting unsuspected structures, using, in the cases noted above, an order of ≤ 100 total-energy *ab initio* calculations.

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