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Finding the minimum-energy atomic configuration in large multi-atom structures: Genetic Algorithm versus the Virtual-Atom Approach[1]
MAYEUL D'AVEZAC, ALEX ZUNGER, National Renewable Energy Lab — In many problems in molecular and solid state structures one needs to determine the energy-minimizing decoration of sites by different atom-types (i. e. *configuration*). The sheer size of this configurational space can be horrendous even if the underlying lattice-type is known. The ab-initio total-energy surface for different (relaxed) configurations can often be parameterized by a spin-like Hamiltonian (*Cluster-Expansion*) with discrete spin -variables denoting the type of atom occupying each site. We compare two search strategies for the energy-minimizing configuration: (i) A discrete-variable genetic-algorithm approach(S. V. Dudiy and A. Zunger, PRL **97**, 046401 (2006)) and (ii) a continuous-variable approach (M. Wang et al, J. Am. Chem. Soc. **128**, 3228 (2006)) where the discrete-spin functional is mapped onto a continuous-spin functional (*virtual atoms*) and the search is guided by local gradients with respect to each spin. We compare their efficiency at locating the ground-state configurations of fcc Au-Pd Alloy in terms of number of calls to the functional. We show that a GA approach with diversity-enhancing constraints and reciprocal-space mating easily outperforms the VA approach.

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