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The search for minimum-energy atomic configurations on a lattice: Lamarckian twist on Darwinian Evolution[1] MAYEUL D'AVEZAC, ALEX ZUNGER, National Renewable Energy Lab — We examine how two different mechanisms proposed historically for biological evolution compare for the determination of crystal structures from random initial lattice-configurations. The Darwinian theory of evolution contends that the genetic makeup inherited at birth is the one passed on to offsprings. Lamarck surmised additionally that offspring can inherit acquired traits. In the case of lattice-configurations, such improvements consist in A$\leftrightarrow$B transmutations of atomic sites as guided by "Virtual Atom" energy-gradients(M. d'Avezac and Alex Zunger, J. Phys.: Cond. Matt. **19**, 402201 (2007)). This hybrid evolution is shown to provide an efficient solution to a generalized Ising Hamiltonian, illustrated by finding the ground-states of face-centered cubic $Au_{1-x}Pd_x$ using a cluster-expansion functional fitted to first-principles total-energies. For example, finding all minimum-energy structures of a 32-atom supercell with 95 % confidence requires evaluating $750,000$ configurations using local improvements only, $150,000$ using a reciprocal-space genetic algorithm only, and $14,000$ using the hybrid approach. We consider applying the lamarckian search to further functionals.

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