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Traveling the configurational space of binary alloys[1] G. TRIMARCHI, S. V. BARABASH, A. ZUNGER, National Renewable Energy Lab., Golden CO 80401 — Binary $A_{1-x}B_x$ alloys can exist in any of the 2^N possible configurations on a periodic lattice of N sites. In many areas of the alloy theory one needs to search all lattice configuration. Such a problem arises, for example, when the $T = 0$ ground state configurations are sought, or in problems of materials design, where it is desirable to scan all the configurations to find the configuration σ^* that has specific property. This task is complicated by (i) the huge computational demand for large N and (ii) by the possibility that the $P(\sigma)$ is sensitive to the cell shape. In this talk we present a new computational approach for defining and searching the configurational space, that is based on (i) the exhaustive *enumeration* of the "Inequivalent Cell Shapes", and, for a given cell shape on (ii) the *sampling* of the related "Same-Shape-Structures" via a Genetic Algorithm. We apply this procedure to few ground state problems in semiconductor and metal alloys: For $(AC)_x(BC)_{1-x}$ tetrahedral semiconductor alloys we predict the lattice configurations of minimum bond-bending and bond-stretching strain both in free-floating bulk and under the epitaxial strain. We show that the chalcopyrite structure remains a ground state even under epitaxy. For Au-Pd alloy modelled with the mixed basis cluster expansion Hamiltonian, we determine the ground state structures and compare the convex hull to the one found previously by the direct enumeration approach.

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Giancarlo Trimarchi
National Renewable Energy Lab., Golden CO 80401

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