

Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Where are Nature's missing structures¹ GUS L.W. HART, Brigham Young University — Our society's environmental and economic progress depends on the development of high-performance materials such as lightweight alloys, high-energy-density battery materials, recyclable motor vehicle and building components, and energy-efficient lighting. Meeting these needs requires us to understand the central role of crystal structure in a material's properties. Despite more than 50 years of progress in first-principles calculations, it is still impossible in most materials to infer ground-state properties purely from a knowledge of their atomic components—a situation described as 'scandalous' in the well-known essay by Maddox. Many methods attempt to predict crystal structures and compound stability, but here I take a different tack—to infer the existence of structures on the basis of combinatorics and geometric simplicity. The method identifies 'least random' structures, for which the energy is an extremum (maximum or minimum). Although the key to the generic nature of the approach is energy minimization, the extrema are found in a chemistry-independent way.

¹Supported by NSF DMR-0650406.

Gus Hart
Brigham Young University

Date submitted: 12 Dec 2007

Electronic form version 1.4