

Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Predicting new structures in B-cation ordering perovskites

MATTHEW LORDS, Brigham Young university — Material properties are intimately tied to crystal structure. Many materials, alloys in particular, share a common, underlying motif, such as an fcc, bcc, or hcp parent lattice but have different chemical orderings on the lattice. For example, the well-known structure in the Cu-Au system, L1₀, has an underlying fcc lattice where each (001) plane contain only Cu or Au. The planes are stacked so that the Cu and Au layers alternate. Among the countably infinite possibilities for such chemical orderings, why does nature choose only the few it does? Are others possible or likely? We answer this question generally and give an example of the perovskite structure, important in ferroelectrics, catalysts, and superconductors. We show which structures are possible combinatorially and which might actually be observed in real materials.

Matthew Lords
Brigham Young university

Date submitted: 21 Nov 2008

Electronic form version 1.4