Abstract Submitted
for the 4CF09 Meeting of
The American Physical Society

**Ordered Magnesium-Lithium alloys** RICHARD TAYLOR, Brigham Young University, STEFANO CURTAROLO, Duke University, GUS HART, Brigham Young University — Emerging technologies increasingly depend on the production of ultra-lightweight materials. Magnesium-lithium (MgLi) alloys are the lightest metallic alloys, having densities near that of plastics, and are strong enough to be used in a variety of high- performance applications. Although considerable work has been done on the MgLi system, little is known regarding potential ordered phases. An analysis of the system with first-principles methods revealed an unexpected wealth of stable zero- temperature phases. Of particular practical interest are configurations containing more than 13 atomic percent lithium, as they will be more ductile due to partial or complete formation on a cubic lattice. The analysis was extended to finite temperature using a Monte Carlo algorithm on large lattices with periodic boundary conditions. Discontinuities in specific heat measurements revealed order-disorder transition temperatures in the range 200-400K. Given the comparatively low melting point of Li ($\sim$450K), kinetics at these temperatures may be sufficient to permit spontaneous partial ordering for Li rich alloys.

Richard Taylor
Brigham Young University

Date submitted: 28 Sep 2009 Electronic form version 1.4