

Abstract Submitted
for the 4CF10 Meeting of
The American Physical Society

The experimental search for new predicted binary-alloy structures K.C. ERB, LAUREN RICHEY, Brigham Young University, CANDACE LANG, University of Cape Town, BRANTON CAMPBELL, GUS HART, Brigham Young University — Predicting new ordered phases in metallic alloys is a productive line of inquiry because configurational ordering in an alloy can dramatically alter their useful material properties. One is able to infer the existence of an ordered phase in an alloy using first-principles calculated formation enthalpies.¹ Using this approach, we have been able to identify stable (i.e. lowest energy) orderings in a variety of binary metallic alloys. Many of these phases have been observed experimentally in the past, though others have not. In pursuit of several of the missing structures, we have characterized potential orderings in PtCd, PtPd and PtMo alloys using synchrotron x-ray powder diffraction and symmetry-analysis tools.²

¹G. L. W. Hart, “Where are Nature’s missing structures?,” *Nature Materials* 6 941-945 2007

²B. J. Campbell, H. T. Stokes, D. E. Tanner, and D. M. Hatch, “ISODISPLACE: a web-based tool for exploring structural distortions,” *J. Appl. Cryst.* 39, 607-614 (2006)

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Date submitted: 13 Sep 2010

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