

Abstract Submitted
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The Experimental Search for New Predicted Binary-alloy Structures K.C. ERB, LAUREN RICHEY, BRANTON CAMPBELL, GUS HART, CANDACE LANG, DEPARTMENT OF PHYSICS & ASTRONOMY, BRIGHAM YOUNG UNIVERSITY COLLABORATION, CENTRE FOR MATERIALS ENGINEERING, DEPT. OF MECHANICAL ENGINEERING, U. OF CAPE TOWN COLLABORATION — 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 Pt-based alloys, many of which have never before been observed experimentally. After preparing alloys of the desired composition, we performed synchrotron x-ray powder diffraction experiments to prove or disprove the expected orderings.

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

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