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Alternative alloys for catalysts and platinum jewelry? New structures in Pt-Hf and Pt-Mo ERIN GILMARTIN, JACQUELINE CORBITT, GUS HART, Brigham Young University — The only known intermetallic structure with an 8:1 stoichiometry is that of Pt₈Ti. It is intriguing that an ordered phase would occur at such low concentrations of the minority atom, but this structure occurs in about a dozen binary intermetallic systems. The formation of an ordered phase in an alloy can significantly enhance the performance of the material, particularly the hardness. We have taken a broad look at possible systems where this phase forms. Using first-principles, we calculated the stability of this structure relative to experimentally known phases for more than 80 Pt/Pd binary systems. We find the Pt₈Ti structure is a possible ground state in more than 20 cases. Our experimental collaborators have verified our prediction in Pt-Mo and observed order-hardening in Pt-Hf. We discuss the discovery of new ground states that are likely to be verified experimentally and their impact on materials for Pt- and Pd-based catalysts and jewelry.

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