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First Principles Predictions of Unsuspected Ordered Structures in Au-Pd fcc Alloys[1] SERGEY V. BARABASH, VOLKER BLUM, ALEX ZUNGER, National Renewable Energy Lab, Golden, CO 80401, STEFAN MÜLLER, Universität Erlangen-Nürnberg — Experimentally, the phase diagram of Au-Pd shows only a disordered solid solution, but even though $\Delta H < 0$, no ordered bulk phases have yet been detected. To find what are the ordered structures at lower temperatures, we perform a mixed-basis cluster expansion of $T = 0$ and finite T properties of Au-Pd fcc alloys. Starting from *ab- initio* data, and using genetic algorithm to select most relevant figures, we build a cluster expansion able to predict total energies of arbitrary lattice configuration with precision comparable to that of ab-initio calculations themselves. We predict many unusual low-temperature ground state structures for bulk Au-Pd alloys. In particular, at $x = 0.5$, we predict Kanamori's structure "40" (common in zincblende semiconductors yet extremely rare in metallic alloys). At both $x = 0.25$ and $x = 0.75$, we find tendencies for forming $L1_2$-based superstructures, however the energetic competition between such structures is different at the two compositions, which imposes specific requirements on the properties of the cluster expansion Hamiltonian. Having met those requirements, we are able to further predict novel ground state structures in the Au-rich region of the phase diagram. The stability of those compounds at finite temperatures, their ordering temperatures, the short-range order and the properties of the random alloy are analyzed.

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Sergey V. Barabash
National Renewable Energy Lab

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