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High-precision mixed-space cluster expansion for Cu-rich Cu-Pd alloys: Explaining the "$L1_2$"*phase*[1] S. BÄRTHLEIN, S. MÜLLER, Universität Erlangen-Nürnberg, Germany, G.L.W. HART, Northern Arizona University, Flagstaff, Arizona 86011-6010, A. ZUNGER, National Renewable Energy Lab, Golden, Colorado 80401 — A remarkable feature of Cu-Pd alloys is the existence of long-periodic superlattices (LPS) on the Cu-rich side of the phase diagram. Whereas earlier studies did not include necessary information about the diversity of important, but until then inaccessible formation enthalpies, we are able by combining DFT calculations with a mixed-space cluster expansion, genetic algorithms [1] and Monte Carlo to predict the phase stability from millions of possible candidates. Effective interactions were constructed, enabling us to predict the ground state line in order to determine the stable configurations a $T = 0$K. As a matter of special interest, we investigate the so-called "$L1_2$" phase, which emerges as a domain-mixture between the LPS3 and a newly discovered low-temperature phase at $x_{Pd} = 0.125$. Examination of the system's short-range order reveals a continuous transition from the domain-mixture to the disordered solid solution. Hence a natural explanation for the existence of this off-stoichiometry phase can be given. [1] G.L.W. Hart et al., Nat. Mater. **4**, 391 (2005)

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