Abstract Submitted
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The hierarchy of 1D-, 2D- and 3D-dimensional LPS in Cu-Pd and Ag-Pd: A first-principles study[1] S. BÄRTHLEIN, E. WINNING, 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 — Throughout many decades the marvelous variety of so-called long-periodic superlattices (LPS) - being constructed from stacks of $L1_2$ with a certain period M after which an anti-phase boundary is introduced - has been a matter of interest for binary compounds consisting of Pd and noble metals such like Cu, Ag and Au. Whereas $Au_{0.75}Pd_{0.75}$ puts forth the $D0_{23}$ (i.e. $M = 2$) structure as ground state [1], $Cu_{0.75}Pd_{0.75}$ and $Ag_{0.75}Pd_{0.75}$ exhibit LPS3 (i.e. $M = 3$) as $T = 0$K ground state. Moreover, the formation enthalpies for a whole class of superlattices are almost degenerated. In order to control the energetical hierarchies of *all* LPS in question the usual 1D-LPS configuration space must be overcome. We therefore demonstrate how for each system a set of suitable interactions can be constructed by first principles means. Questions concerning a complete description and exhaustive predictive power will be asked and answered by a mixed-space cluster expansion that allows us to handle 1D-LPS with average M, 2D- and 3D-LPS with arbitrary integer M and to predict their energies in order to investigate their abilities to serve as ground state candidates. [1] S. Barabash et al., submitted to Phys. Rev. B

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