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First-Principles Cluster Expansions for Predicting Missing-row Surface Reconstructions WEI CHEN, CHRIS WOLVERTON, Northwestern University, Dept. of Materials Science and Engineering, DAVID SCHMIDT, WILLIAM SCHNEIDER, University of Notre Dame, Dept of Chemical and Biomolecular Engineering, Dept. of Chemistry and Biochemistry — It is well-known that the (110) surfaces of late 5d transition metals (e.g. Au, Pt) undergo a (1×2) missing-row reconstruction, while clean surfaces of 3d and 4d metals (e.g. Cu, Ag) do not. Here, we report the use of a cluster expansion (CE) approach to study this particular class of "missing-row" surface reconstructions of some transition metals. We have used first-principles density functional calculations along with a CE to study the (110) surface of late transition metals by considering the reconstructed surface as a 2D binary system of metal atoms and vacancies. Without any experimental input or intuition-based "guessing", the CE results demonstrate the (1×2) missing-row structure is the T=0K ground state for the (110) surface of Au and Pt, but not for Cu and Ag. The finite temperature properties of the missing-row surfaces were also studied by a CE+Monte Carlo approach, and we find a (1x2) to (1x1) transition temperature in good agreement with experimental results.

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