

Abstract Submitted
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Ordered and disordered surface alloys in Au-Pt(111) and their effect on oxygen adsorption¹ WEI CHEN, C. WOLVERTON, Northwestern University, DAVID SCHMIDT, WILLIAM SCHNEIDER, University of Notre Dame — Bimetallic surface alloys are considered a promising type of catalyst for improved activity and selectivity. Understanding surface structure and its effect on catalytic performances plays a critical role in designing catalysts from surface alloys. We have studied the surface structure and ordering of AuPt(111) using a first-principles cluster expansion based method. Even though the Au-Pt system is phase-separating in the bulk, we find a series of thermodynamically stable, laterally ordered striped structures of AuPt(111) surfaces. The formation of such ordered structures is the result of a competition between the strain relaxations from stripes and the unfavorable Au-Pt bonds at stripe interfaces. We have also investigated the oxygen adsorption on these structures. The oxygen binding energy is found to be highly correlated with the type of nearest neighbor surface atoms of oxygen.

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