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Atomistic Mechanism of Surface Oxide Formation on Pt(111)

ZHENGZHENG CHEN, CHAO WU, Department of Chemical and Biomolecular Engineering, University of Notre Dame, WILLIAM SCHNEIDER, Department of Chemical and Biomolecular Engineering, Department of Chemistry and Biochemistry, University of Notre Dame — A detailed understanding of the interaction of oxygen with Pt surfaces is essential for understanding its catalytic activity and deactivation in oxidizing environments. Here we analyze the transition between metallic and oxidized Pt surfaces. Using first-principles calculations, we characterize the chain-like oxide reconstruction on the Pt(111) surface associated with O coverage $>50\%$. We describe the sensitivity of the reconstruction energy to the occupancy of adjacent fcc and hcp sites and present a phenomenological model that relates the reconstruction to the balance between elastic strain energy and screening of O-O repulsions. Core level shift calculations indicate the reconstruction generates two O states with different binding energies and reactivity. Finally, we analyze the thermodynamic stability and equilibrium states of the reconstruction a cluster expansion model. The results are important in developing models of oxidation catalysis on Pt (111) surface.

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