

CO+O₂ Reaction on Pt(110) at High Pressure

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The catalytic properties of transition metals have been the subject of many both experimentally and theoretically studies. Adsorption and reaction on low index surfaces and on the defected surfaces having e.g. steps and kinks have been studied intensively. Recently attention has also turned toward transition metal oxides [1].

The interaction between CO and O₂ on Pt(110) under high pressure has been addressed in a recent scanning tunneling microscopy (STM) experiment by Hendriksen and Frenken [2] in which they observe a higher CO oxidation rate under O-rich conditions coinciding with a roughening of the surface which the authors interpret as a thin surface oxide layer.

In this paper we present a density functional theory investigation of the structure and reactivity of the Pt(110) surface under O-rich and CO-rich conditions, respectively.

The O-rich condition is modeled by a two monolayer (ML) reconstructed (2×1)-O chemisorption structure while the CO-rich condition is modeled by a one ML unreconstructed (2×1)-p1g1-CO structure. Coadsorption of CO under O-rich conditions is stable by -0.41 eV with an adsorption barrier of 0.50 eV. Oxidation of CO by a neighboring oxygen is relatively easy having a reaction barrier of 0.31 eV. The CO covered surface is both very dense (leaving no room for O₂ dissociation) and stable (creating a vacancy has a heat of formation of 1.32 eV), making the overall reaction barrier of creating a vacancy followed by O₂ adsorption, dissociation, and oxidation high.

Various structures of the oxidized Pt surface are being discussed.

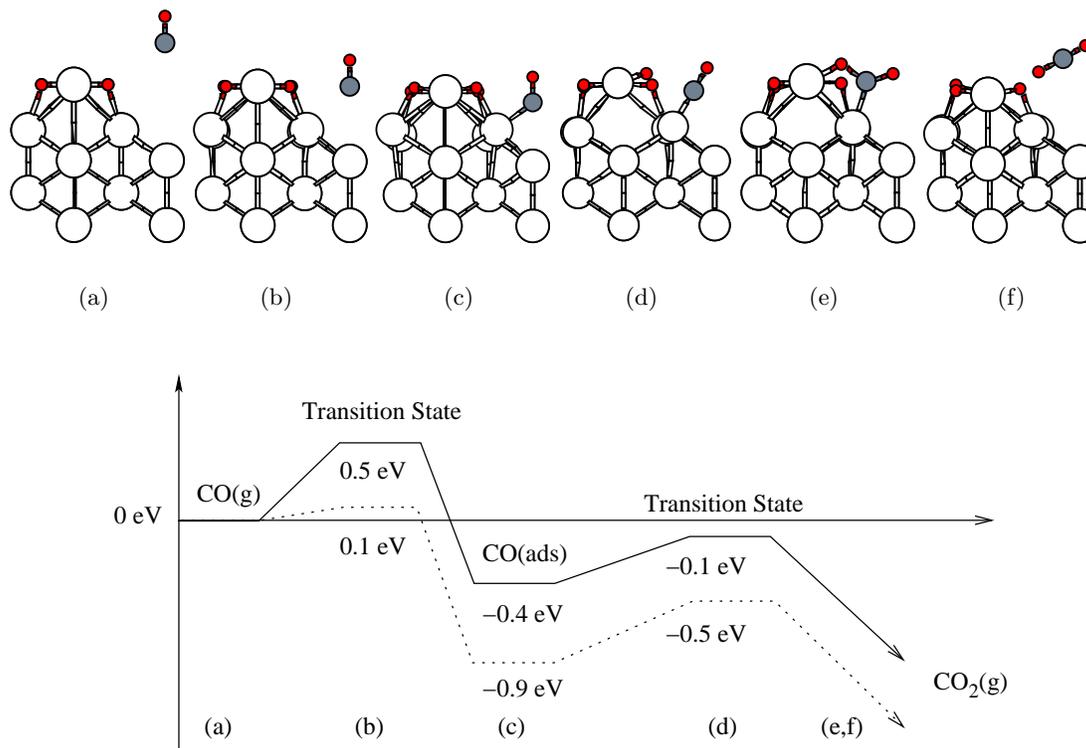


Figure 1: (Upper panel) Small cartoon of the CO adsorption and oxidation on the 2 ML oxygen precovered surface. From left to right: (a) CO in gas phase, (b) transition state of CO adsorption, (c) CO adsorbed at the trough bridge site, (d) the transition state of CO oxidation, (e) the (very weakly bound) O-CO complex, (f) CO₂ in gas phase. (Lower panel) Energy diagram showing RPBE (solid line) and PW91 (dashed line) potential energies for CO adsorption and oxidation. (a-f) correspond to the figures in the upper panel.

References

- [1] H. Over, Y. D. Kim, A. P. Seitsonen, S. Wendt, E. Lundgren, M. Schmid, P. Varga, A. Morgante, and G. Ertl, "Atomic-Scale Structure and Catalytic Reactivity of the RuO₂(110) Surface," *Science* **287** (2000), no. 5457, 1474–1476.
- [2] B. Hendriksen and J. Frenken, "CO Oxidation on Pt(110): Scanning Tunneling Microscopy Inside a High-Pressure Flow Reactor," *Phys. Rev. Lett.* **89** (2002) 046101–1.