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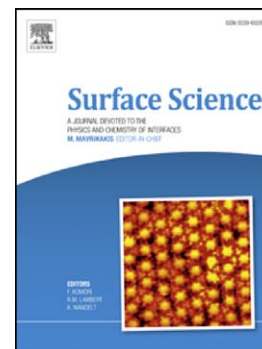
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# CO Oxidation on Ag(111): the Catalytic Role of H<sub>2</sub>O

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## ABSTRACT

The reaction mechanism for the oxidation of CO on Ag(111) in the presence of trace amounts of water is investigated via density-functional-theory calculations. A four-step cycle for the reaction is proposed: (1)  $\text{H}_2\text{O} + \text{O}_2 \rightarrow \text{HO} + \text{HO}_2$ ; (2)  $\text{HO}_2 + \text{CO} \rightarrow \text{OH} + \text{CO}_2$ ; (3)  $\text{CO} + \text{OH} \rightarrow \text{cis-OCOH}$ ; (4)  $\text{cis-OCOH} + \text{OH} \rightarrow \text{CO}_2 + \text{H}_2\text{O}$ . In the mechanism, water is found to directly participate in the reaction as a catalyst, in addition to the previously proposed role of stabilizing the weakly adsorbed oxygen molecules on Ag(111). Moreover,  $\text{HO}_2$  is an important reaction intermediate, which is produced by transferring a hydrogen atom from water to an oxygen molecule. Because the overall reaction barrier is as low as 0.20 eV, the mechanism is expected to be operative at low temperatures.

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