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CO Oxidation on Ag(111): the Catalytic Role of H_2O

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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) $H_2O + O_2 \rightarrow HO + HO_2$; (2) $HO_2 + CO \rightarrow OH + CO_2$; (3) $CO + OH \rightarrow$ *cis*-OCOH; (4) *cis*-OCOH + $OH \rightarrow CO_2 + H_2O$. 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, 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.