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Effect of adsorbed water molecules on reaction profile of CO oxidation catalyzed by Au_5 nanoclusters

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CO oxidation is an important reaction from the perspective of environment remediation techniques. The improvised, better end-of-pipe solution are desired to reduce the impact of anthropogenic activities on the environment. CO oxidation can take place at the surface of gold nanoparticles even at low temperatures, thereby providing solution to cold-emission problem. In this study, we explore the effect of water in adsorbed state on the reaction profile of CO oxidation catalysed by gold nanoclusters. It has been found that the main effect of water adsorbed onto gold nanoclusters is to reduce the barrier for carbonate formation. The carbonate formation is reported to negatively impact the catalytic properties of gold nanocluster. Here, we also report an alternative pathway through which the carbonate decomposition can be accomplished leading to the regeneration of the catalyst surface. This Eley – Rideal pathway involves reaction between CO and nanocluster-carbonate adduct. No effect of adsorbed water on energetics of carbonate decomposition at the surface of gold nanocluster has been observed.

Keywords: CO oxidation, Gold nanoclusters, Reaction profile, DFT, Catalysis