Catalytic CO oxidation over Au nanoparticles supported on CeO2 nanocrystals: Effect of the Au-CeO2 interface

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Superior catalytic performance of gold nanoparticles (NPs) in low temperature CO oxidation have attracted attention. Catalytic function of gold-catalyzed CO oxidation can be further developed by controlling the properties of the oxide support materials. Here, a combinatorial approach of experimental and theoretical analyses was applied to demonstrate the effect of supporting oxide materials and the corresponding CO oxidation activity of supported Au NPs. 3 nm size of Au NPs were synthesized on the CeO2 nanocrystals (NCs), cubes and octahedra. CeO2 NCs terminated by (100) for cubes and (111) for octahedra, which are served as model of Au/CeO2 (100) and Au/CeO2 (111) via density functional theory (DFT) calculations. The experimental turnover frequency (TOF) of Au/CeO2 cubes was 4 times higher than Au/CeO2 octahedra in CO oxidation. The DFT calculation showed that the O-C-O intermediate was spontaneously formed at the Au-CeO2 (100) interface, accelerating CO oxidation via the Mars-van Krevelen mechanism. The combined approach of experimental and theoretical studies provides a deep insight into the catalytic function of Au-CeO2 interface toward CO oxidation.