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Water Enhanced Catalysis of CO Oxidation on Free and Supported Gold Nanoclusters ANGELO BONGIORNO, UZI LANDMAN, Georgia Institute of Technology — The enhancement by water molecules of the catalytic activity of gas-phase and supported gold nanoclusters toward CO oxidation is investigated with first-principles calculations. Coadsorption of water and oxygen molecules leads to formation of a complex well-bound to the gold cluster, even on a defect-free MgO(100) support. Formation of the complex involves partial proton-sharing between the adsorbates, that in certain configurations results in proton transfer leading to the appearance of a hydroperoxyl-like complex. The O-O bond is activated, leading to a weakened peroxo or superoxo-like state, and consequently the reaction with carbon oxide to form carbon dioxide occurs with a small activation barrier of about 0.5 eV. A complete catalytic cycle of the water-enhanced CO oxidation is discussed.

Angelo Bongiorno
Georgia Institute of Technology

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