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Control and manipulation of Au nanocatalysis: effects of metal oxide support thickness and composition BOKWON YOON, School of Physics, Georgia Institute of Technology, CHRIS HARDING, VAHIDEH HABIBPOUR, SEBASTIAN KUNZ, ADRIAN NAM-SU FARNBACHER, UELI HEIZ, Lehrstuhl fur Physikalische Chemie, Technische Universitat Munchen, Germany, UZI LANDMAN, School of Physics, Georgia Institute of Technology — Control and tunability of the catalytic oxidation of CO by gold clusters deposited on MgO surfaces grown on molybdenum, Mo(100), to various thicknesses, are explored through temperature programmed reaction measurements on mass selected 20-atom gold clusters and via first-principles density-functional theory calculations. Dependencies of the catalytic activities and microscopic reaction mechanisms on the thickness and stoichiometry of the MgO films, and on the dimensionalities and structures of the adsorbed gold clusters are demonstrated and elucidated. Langmuir-Hinshelwood mechanisms and reaction barriers corresponding to observed low and high temperature CO oxidation reactions are calculated and analyzed. Along with the oxidation reactions on stoichiometric ultra thin MgO films we also study reactions catalyzed by Au_{20} nanoclusters adsorbed on relatively thick defect-poor MgO films supported on Mo, and on defect-rich thick MgO surfaces containing oxygen vacancy defects.

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