CO adsorption onto gold nanoparticles supported on thin film substrates

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William McKee1, chadm_@yahoo.com, Mattew Patterson2, Dali Huang3, Li Liu3, Richard Kurtz2, Phillip Sprunger2, Ye Xu1

1 Department of Chemical Engineering, Louisiana State University, Baton Rouge, Louisiana, United States; 2 Department of Physics and Astronomy and CAMD, Louisiana State University, Baton Rouge, Louisiana, United States; 3 Department of Chemistry, Texas AM University, College Station, Texas, United States

Abstract: Au nanoparticles supported on transition metal oxide surfaces exhibit remarkable catalytic properties, especially for low-temperature selective oxidation and hydrogenation reactions. However, the precise role of Au is still unclear even for simple reactions such as CO oxidation because of the potential involvement of the support material and reaction environment. We show that an inert monolayer hexagonal boron nitride (BN) film supported on Rh(111), which exhibits a periodic long-range pore-wire superstructure, provides an array of identical trappings sites for the self-assembly of size controlled monodisperse Au nanoparticles. The resulting arrays of densely packed Au nanoparticles remain confined to the pore regions even at multi-layer Au coverages and on annealing to room temperature. The chemisorption of CO onto these particles under varying conditions is examined, using a variety of complimentary experimental and theoretical techniques, as an early probe of their catalytic properties. Significant charge transfer from the support to the Au nanoparticles is evident, and the negative charge density is shown to localized at periphery Au sites which are also highly active toward CO chemisorption, causing the C-O stretching frequency to dramatically red-shift. The Au/BN/Rh(111) system represents an attractive model system for examining Au nanocatalysis in the isolated Au limit.