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Support-induced Catalytic Activity of Gold Nanocluster CHUN ZHANG, BOKWON YOON, UZI LANDMAN, School of Physics, Georgia Institute of Technology — The catalytic activity of gold nanoclusters supported on metal-oxide surfaces is a topic of active research efforts. Recently, a dimensionality crossover of gold clusters, adsorbed on a metal-supported thin film of MgO(100), has been predicted[1]. We present here a first- principles study of the catalytic activity of a planer Au_{20} cluster on two- layer MgO(100) film supported by a Mo surface. Both Langmuir-Hinshelwood (LH) and Eley–Rideal (ER) mechanisms of CO oxidation are investigated. The barrier of the LH mechanism is found to be 0.15 eV. For the ER mechanism, the barrier depends on the direction of approach of the CO molecule to the preadsorbed oxygen molecule, varying between a vanishing barrier height and 0.2 eV. Charge transfer from the Mo surface to the cluster supported on the thin MgO(100) film plays a key role in the catalyzed CO oxidation process.

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