Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

CO oxidation reaction on Au clusters supported on the $TiO_2(110)$ surface DAVIDE RICCI, ANGELO BONGIORNO, UZI LANDMAN, Georgia Institute of Technology, School of Physics, ANKE WOERZ, MATTHIAS ARENZ, UELI HEIZ, Technical University of Munich, Lehrstuhl fuer Phyzsikalische Chemie — We have studied by means of density functional theory (DFT) plane waves calculations, the CO oxidation reaction on Au_8 clusters adsorbed on both the stoichiometric and reduced rutile $TiO_2(110)$ surfaces. O_2 molecules bind at the interface between the $TiO_2(110)$ surface and the gold particle, where they become partially charged through the population of the anti-bonding molecular orbital, resulting in the extension of the O-O bond length to values of peroxo-like states. When CO is co-adsorbed on the gold-particles, the Langmuir-Hinshelwood and the Elay-Rideal mechanisms are possible for the oxidation reaction. Both the catalytic cycles have been considered and the theoretical results have been compared with experimental findings obtained on size-selected Au_8 clusters deposited on thin, oxidized and reduced TiO_2 films.

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Date submitted: 01 Dec 2005

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