Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Atomic structure of a Ultrathin TiO_2 film on Mo(112) surface[1]

RUQIAN WU, DEPARTMENT OF PHYSICS AND ASTRONOMY,UCI, CA —

Materials with reduced dimensions attract much interest because their properties are often significantly different from the properties of bulk materials. Additionally, thin oxide films represent model systems well suited for studying structure reactivity relationships on oxides and oxide supported metal particles considered as models for heterogeneous catalysts. Recently, gold clusters on titania/Mo(112) surface are found to be high catalytic activity, attributing to the structural effects. Despite extensive experimental and theoretical studies the detailed atomic structure of TiO_2 films on Mo(112) substrate remain unknown. The geometrical and electronic structures of a ultrathin TiO_2 film expitaxially grown on a Mo(112) substrate have been determined by first principles density-functional theory calculations. The results show that the TiO_2 perfer to the 8×2 surface structure on the Mo(112) surface, which is well agreement with the experiments.

[1]Work was supported by the DOE (grant No: DE-FG02-04ER15611) and ICTS, Chinese Academy of Science.

Ruqian Wu
DEPARTMENT OF PHYSICS AND ASTRONOMY,UCI, CA

Date submitted: 06 Dec 2005 Electronic form version 1.4