Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Electronic structures and adsorption configurations of gold nanoclusters on cerium oxide defect surfaces LU WANG, WAI-NING MEI, Department of Physics, University of Nebraska at Omaha, Omaha, NE 68132, NEIL LAWRENCE, JOSEPH R. BREWER, JAMES WELLS-KINGSBURY, MARCELLA IHRIG, GONGHUA WANG, CHIN LI CHEUNG, Department of Chemistry, University of Nebraska-Lincoln, Lincoln, NE 68588, YUN-LIANG SOO, Department of Physics, National Tsing Hua University, Taiwan — Fluorite-structured cerium oxide (or ceria, CeO_{2-x}, $0 \leq x \leq 0.5$) has been shown to be an important material in catalysis, yet few study has investigated the effect of non-dopant introduced oxygen vacancy defect (OVD). In addition, we found experimentally that when doped with Au nanoclusters, the catalytic ability of ceria enhanced. In this work, we modeled and optimized an (111) fluorite-structured slab model of defective ceria with a chemical formula corresponding to $CeO_{1.5}$. The optimized surface structure of this model was found to contain both surface and sub-surface OVDs, similar to those observed in our HRTEM data for low pressure activated nanoceria. Significantly, the model captures comparable reduction in the average Ce-O bond distance and also atomic coordination numbers observed in our EXAFS data. To explore the roles of Au nanoclusters, we adsorbed flat clusters of 3, 4, 9, 10, and 19 Au atoms on ceria slabs, optimized their configurations, and computed the corresponding electronic structures applying first-principle approach. Consequently, we present the density of states results to elucidate the experimentally observed optical property change and $s-d$ hybridization.

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Date submitted: 06 Dec 2011 Electronic form version 1.4