Joint CQSE and CASTS Seminar

Weekly Seminar
Dec. 28, 2012 (Friday)

TIME Dec. 28, 14:30 ~ 15:30
TITLE First Principles Calculations to Study CO Oxidation on Au nanoparticles and CeO2-based Surfaces
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PLACE Rm716, CCMS & New Physics Building, NTU

Abstract

Low-temperature CO oxidation is needed in many practical processes, such as automotive exhaust purification, preferential CO oxidation, and the production of clean H_2. In order to search highly active and cheaper catalysts for the CO oxidation, we apply theoretical methods to investigate the electronic structures and density of states as well as the detailed mechanisms of the CO oxidation in the M-modified CeO_2 surfaces (M =Fe, Ru, and Mn) and nano-size Au clusters. In this work, we use the spin-polarized density functional theory with the inclusion of on-site Coulomb correction (DFT+U) calculation to study the oxygen vacancy of $Ce_{1-x}M_xO_2$ (M = Fe, Ru, and Mn) and CO adsorption on the M-doped CeO_2 (111) surface and nano-size Au clusters. Substitution of Metal in CeO_2 results in strong structural distortions and smaller oxygen vacancy formation energies compared to undoped CeO_2. It is found that CO adsorbs much strongly on the M-doped surfaces compared to the undoped surface. The vibrational frequency calculations are carried to characterize these species. Our calculations also show that Metal dopant facilitates O-vacancy formation and CO oxidation.

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