Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Effects of co-adsorbed C and K on energetics of CO oxidation on Pd(111)[1] FAISAL MEHMOOD, SERGEY STOLBOV, TALAT S. RAHMAN, Department of Physics, Kansas State University, Manhattan, KS 66506 — In the course of catalytic oxidation of CO, carbon may atomically adsorb on catalyst surface and change (presumably poison) its reactivity. On the other hand, the reactivity of many catalysts is enhanced upon alkali co-adsorption. To gain insight into the nature of these effects, we carried out ab initio electronic structure calculations based on density functional theory with the generalized gradient approximation. The energetics and reaction pathways for CO oxidation on the clean Pd(111) and on Pd(111) co-adsorbed with C or K are calculated. We find that even at coverages as small as 1/12 ML, co-adsorbed C increases the activation energy barrier for the reaction by 20%, while K reduces it by 10%. This clearly shows the role of K as a promoter and C as a poison for this catalytic reaction. To understand the microscopic mechanism of these phenomena, we analyze the effects of the co-adsorbate coverage and the CO — co-adsorbate distance on the activation energy barriers and the local densities of electronic states and valence charge densities calculated for the initial and transition states of the reaction.

[1] We acknowledge financial support from DOE under grant No. DE-FGO3-03ER15445, NSF under grant No. CHE-0205064 and computational resources provided by NSF Cyberinfrastructure and TeraGrid grant No. DMR050039N.

Faisal Mehmood

Date submitted: 30 Nov 2005

Electronic form version 1.4