Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

First principles calculations of the vibrational dynamics of c(2x2)-CO on Ag(001).[1] M. ALCANTARA ORTIGOZA, T.S. RAHMAN, University of Central Florida, R. HEID, K.P. BOHNEN, Forschungszentrum Karlsruhe, Germany — The reaction pathway of CO oxidation on Ag surfaces is still a subject of debate because of the complicated chemistry of O and the possibility that contaminants stabilize CO. Indeed, at ∼150 K, the dissociative O_2 adsorption is scarcely triggered while the CO adsorption on clean Ag(001) is hardly stable. The nature of the CO adsorption is thus by itself a matter of discussion and the characteristic energy losses for exciting the phonon modes introduced by the adsorbed species have an uncertain assignment. We present an *ab initio* study of the structure and phonon dispersion of a c(2x2), atop, CO overlayer on Ag(001). Comparison with a similar study of c(2x2) CO on Cu(001) indicates that CO chemisorbs on Ag(001) despite the low binding energy. The frequency of the C-O stretch mode at the Γ-point is in excellent agreement with HREELS measurements and is reduced on Ag(001) almost as much as on Cu(001). The weak Ag-CO bond is reflected in the low frequency of the rest of the CO modes. Yet, in the Ag-CO stretch, the Ag surface atoms are strongly coupled, as in the case of CO on Cu(001). Likewise, the CO frustrated translation mode couples to the substrate in the vicinity of the Γ-point but, unlike that on Cu(001), the CO frustrated rotation mode on Ag(001) couples to the substrate inside the surface Brillouin zone.

[1] Work supported in part by NSF under grant CHE-0548632.

Talat Rahman
University of Central Florida

Date submitted: 28 Dec 2007

Electronic form version 1.4