

Abstract Submitted  
for the MAR06 Meeting of  
The American Physical Society

**Effect of the substrate-adsorbate coupling on the dispersion of phonons of CO on Cu(001).**<sup>1</sup> TALAT S. RAHMAN, Kansas State University, KLAUS PETER BOHNEN, Forschungszentrum Karlsruhe, MARISOL ALCANTARA ORTIGOZA, Kansas State University — In order to understand the effect of the substrate on the dynamics of the adsorbate we have carried out first principle calculations of the dispersion of phonons of the c(2x2) CO overlayer on Cu(001) based on the Density Functional Theory, using ultrasoft pseudopotentials and the PBE-GGA approximation for the exchange-correlation energy. Comparing with frozen-substrate calculation, at the gamma point, we found that the frequencies of the C-O stretch mode,  $\nu_1$ , and the adsorbate-substrate stretch mode,  $\nu_2$ , are almost independent of the substrate. However, while  $\nu_2$  is dispersionless,  $\nu_1$  presents a 10 meV dispersion at the M-point. The frustrated translation and frustrated rotation modes present a dispersion of less than 5 meV, nevertheless having the frustrated translation mode such a low energy a  $\sim 1$  meV dispersion is rather considerable. Moreover, Helium atom scattering studies of this mode found that it splits into two branches everywhere other than the  $\Gamma$  point; they attributed one branch to the frustrated translation mode of a perfect c(2x2) CO overlayer, and the other one to defects in the same. Here we show that the splitting is an intrinsic feature of the perfect c(2x2) CO overlayer.

<sup>1</sup>DOE under grant No. DE-FG03-ER15445 and NSF under grant No. CHE-0205064

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Date submitted: 22 Dec 2005

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