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Dissociative versus molecular chemisorption of oxygen on Cu(110)

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Abstract. Recent experimental studies have led to much confusion regarding the low-temperature structure of oxygen chemisorption on Cu(110) with both atomic and molecular models being proposed. Restricted Hartree–Fock total energy calculations on a Cu_{12} cluster are presented, which strongly support the atomic viewpoint.

The low-temperature structure of oxygen on Cu(110) has been the subject of two recent experimental studies that yielded conflicting results. Prabhakaran and co-workers [1, 2] find bands in their EELS signal at 610, 660, and 880 cm^{-1} which they ascribe to an O–O stretching mode and hence they conclude that adsorption is molecular. On the other hand Mundenar and co-workers [3, 4] using EELS and UPS find no evidence of molecular adsorption and only find a Cu–O stretch mode centred on 49 meV and hence claim that only atomic oxygen is present on the surface.

We calculate the total energies for both atomic and molecular chemisorption in all high-symmetry sites on a Cu_{12} cluster within a restricted Hartree–Fock framework using the GAMESS molecular orbital package† and Gaussian basis sets due to Huzinaga [5]. No evidence for molecular chemisorption has been found with the O–O axis either parallel to or perpendicular to the Cu surface. Atomic oxygen is found to be most stable while occupying a long bridge site forming Cu–O bonds of $\simeq 1.8$ Å with both the first- and second-layer Cu atoms. The vibrational mode corresponding to vertical displacements of the oxygen atom about this position with the Cu atoms held invariant is found to have an energy of 52.9meV, in agreement with Mundenar's experimental value of 49 meV.

References

[1] Prabhakaran K, Sen P and Rao C N R 1986 *Surf. Sci.* **177** L971
[2] Prabhakaran K and Rao C N R 1988 *Surf. Sci.* **198** L307
[3] Mundenar J M, Baddorf A P, Plummer E W, Sneddon L G, Didio R A and Zehner D M 1987 *Surf. Sci.* **188** 15
[4] Mundenar J M, Plummer E W, Sneddon L G, Baddorf A P, Zehner D M and Gruzalski G R 1988 *Surf. Sci.* **198** L309
[5] Huzinaga S 1984 *Gaussian Basis Sets for Molecular Calculations* (Amsterdam: Elsevier)

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