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Adsorption of atomic oxygen on the Si(100) surface

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Abstract. Previous studies on the oxidation of Si(100) have neglected the effects of surface reconstruction. Using total energy methods within a restricted Hartree–Fock framework we explicitly include the effects of reconstruction on the adsorption of atomic oxygen on this surface. A new low-coverage 2×1 structure has been found in which the Si surface–sub-surface bonds are tilted by about 12° with respect to the surface normal. This structure reverts to a 1×1 as the oxygen coverage increases in agreement with experimental predictions.

Previous theoretical work [1, 2] has shown that atomic oxygen is adsorbed at the bridge sites of the Si(100) surface, but has ignored the effects of surface reconstruction. The aim of the present paper is to report on the results of calculations employing the GAMESS SCF molecular orbitals package[‡] in which the reconstruction of the Si(100) surface into a pattern of 2×1 dimers is explicitly taken into account. In agreement with experimental predictions [3], atomic oxygen is found to be adsorbed at the dimer bridge sites with each atom breaking an Si–Si dimer bond to form a new Si–O–Si bonding configuration. Evidence of both a physisorbed and a chemisorbed state has been found with the lower-energy chemisorbed configuration corresponding to the surface–sub-surface Si–Si bonds being tilted by approximately 12° inward with respect to the surface normal. Each oxygen atom is found to lie essentially in the surface plane. The vibrational frequency corresponding to normal displacement of the oxygen from this ideal position is in excellent agreement with the experimental value of 370 cm^{-1} . All of the results have been shown to be consistent with respect to both cluster size and choice of basis set.

We also show that in the high-coverage case the dimer and non-dimer bridge sites become equivalent, which gives rise to a 1×1 pattern as observed experimentally. The vibrational frequency referred to above is found to increase with increasing exposure, in agreement with experiment.

References

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