

Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Characterization of hydroxyls on Si(001)-2×1:H₂O using O 1s core-level spectroscopies and core-excited state DFT calculations
STEPHANE CARNIATO, Universite Pierre et Marie Curie, SYLVIE RANGAN, University of Texas at Dallas, JEAN-JACQUES GALLET, FRANCOIS ROCHET, GEORGES DUFOUR, FABRICE BOURNEL, Universite Pierre et Marie Curie, ALBERTO VERDINI, LUCA FLOREANO, TASC-INFN National Laboratory — The Si(001)-2×1 surface exposed to water molecules at room temperature has been chosen to single out the electron structure of the hydroxyl Si-OH, a surface species playing an important role in many technologically relevant processes. We confront here original core-electron spectroscopy DFT calculations to O 1s XPS (X-ray Photoelectron Spectroscopy) and NEXAFS (Near Edge Absorption Fine Structure) data. On various Si-OH environments (unpaired and paired hydroxyls), the impact of hydrogen bond on the calculated core-ionized and/or neutral core-excited states is examined, and compared to the limit case of the water dimer. The theoretical approach enables to label the main experimental NEXAFS transitions and to interpret their polarization-dependent dichroism. As water dissociation on the surface can go beyond the formation of hydroxyls, the DFT electron structure of bridging oxygens (Si-O-Si) is calculated. It is predicted that the XPS line associated to the latter species is shifted by 0.5-1.0 eV to lower binding energy with respect to hydroxyls.

Sylvie Rangan
University of Texas at Dallas

Date submitted: 27 Nov 2007

Electronic form version 1.4