

## The electronic structure and reactivity of tri-coordinated silicon atoms on water-covered Si(001) surface : time-resolved XPS and STM studies

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**Grand Amphithéâtre SOLEIL**

This work focuses on the study of the electronic properties of isolated silicon dangling bonds left on the Si(001)-2x1 surface after its saturation by water at room temperature. These tri-coordinated defects Si-SiH/Si-SiOH are similar to the Si-SiH defects produced by H stimulated desorption (under a STM tip) on H-terminated Si(001)-2x1. The latter have recently attracted much attention due to their possible use as qubits, or as starting points of radical reactions. The tri-coordinated Si defects on (H,OH)-Si(001)-2x1 have also much in common with the Pb1 defects of the Si(001)/SiO<sub>2</sub>, a key issue in microelectronics. Isolated dangling bonds on (H,OH)-Si(001)-2x1, whose areal density is ~0.01 ML, are amphoteric (donor and acceptor). Their charge state (+,0,-) can be controlled by the substrate doping, that ranged between degenerate p-doped to degenerate n-doped. Due to the presence of charged defects at the surface, band bends in the semiconductor. This band bending can be easily measured by synchrotron radiation photoemission spectroscopy of the Si 2p core-level, in surface sensitive conditions. This in turn can be translated into a surface charge density using the classical semiconductor physics models. The novelty of the present work lies in the fact that a global spectroscopic technique like synchrotron radiation photoemission is combined with a local probe like STM that gives access to the density of surface defects. The exploration of the time aspects is also a characteristic feature of our work. We observed how the electronic band scheme changes during a chemical reaction in *real-time* with photoemission (at a pace of tens of seconds).

Using photoemission in combination with STM, the following topics were tackled: the real-time study of water adsorption on Si(001), as a function of pressure and doping; the electronic characterization of the water-saturated surface; the reactivity of the water-reacted surface towards  $\pi$ -bonded molecules (styrene, benzaldehyde).

We also monitored how the band bending changes after a *fs* laser pump excitation, with *time-resolved* surface photovoltage experiments, down to a time-scale limited by the synchrotron pulse duration, ~50 ps, comparing the (H,OH)-Si(001) surface to the thermally oxidized Si(001). We explored, for the two surfaces, the variation of surface photovoltage with laser fluence, and found substantially the same characteristics, for a given doping level. The return to equilibrium, involves a characteristic time in the 0.1  $\mu$ s to 10  $\mu$ s range, depending on the surface termination and bulk doping. For the thermally oxidized surface, we have examined the fast processes leading to the establishment of the surface photovoltage, and found two rise-times, one faster than the synchrotron time resolution (<50 ps) and one of the order of a few ns.

### Jury de thèse

Mme Wendy FLAVELL	Rapporteur
M. Guy HOLLINGER	Rapporteur
M. Andrew MAYNE	Examineur
M. Christophe PETIT	Examineur
M. François ROCHET	Directeur de Thèse
M. Fausto SIROTTI	Co-Directeur de Thèse
M. Ahmed NAITABDI	Invité
M. Mathieu SILLY	Invité



**Vous êtes cordialement invités au pot qui suivra**



Formalités d'entrée : accès libre dans l'amphi du Pavillon d'Accueil. Si la manifestation a lieu dans le Grand Amphi Soleil du Bâtiment Central, merci de vous munir d'une pièce d'identité (à échanger à l'accueil contre un badge d'accès).

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