

Surface transfer doping: F4-TCNQ on 2-methylpropene chemisorbed Si(100)

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Introduction

We investigated the adsorption states of F4-TCNQ on the 2-methylpropene (= 2MP) chemisorbed Si(100) surface using high-resolution X-ray photoelectron spectroscopy (HR-XPS) and X-ray absorption spectroscopy (XAS) as well as He-I ultraviolet photoelectron spectroscopy (UPS).

Since the valence band maximum of the 2MP saturated Si(100) surface is located at 4.62 eV below the vacuum level and the electron affinity of F4-TCNQ is 5.24 eV, a spontaneous charge transfer from the substrate to F4-TCNQ is expected. With increasing the coverage of F4-TCNQ, the workfunction change was monotonically increased and saturated at ~1.5 eV. At sub-monolayer coverage of F4-TCNQ on the 2MP saturated Si(100) surface, we found that an occupied LUMO peak at 1.5 eV and a relaxed HOMO peak at 2.7 eV below E_F by UPS [1]. The UPS results indicate that a charge transfer occurs and F4-TCNQ becomes an anion-like state. We have obtained more detailed information about the electronic states of F4-TCNQ and the chemically modified Si substrate using HR-XPS and XAS at Photon Factory BL13A.

Experimental

HR-XPS and XAS measurements were carried out at Photon Factory BL13A using a SPECS Phoibos100 electron analyzer and a homemade micro-channel electron detector, respectively. Gaseous 2-methylpropene (2MP) was adsorbed onto the clean Si(100)c(4x2) surface at 100 K up to saturation. F4-TCNQ was evaporated on thus prepared Si(100) surface at 200 K using a homemade miniature K-cell [2]. The coverage of F4-TCNQ was estimated from C 1s XPS. The core-level spectra of N 1s, C 1s and Si 2p were measured with photon energy (h ν) of 500 eV. In addition, HR-XPS spectra of Si 2p were measured with h ν = 150 eV.

Results and discussion

Figure 1 shows a series of Si 2p HR-XPS spectra as a function of F4-TCNQ coverage on the 2MP saturated Si(100) surface. At a clean Si(100) surface (Fig. 1a), distinct peaks are observed at 99.2, 99.7 and 100.3 eV as well as shoulders at 100.0 and 100.6 eV. According to the previous studies [3], the 99.2 eV peak is assigned to the $2p_{3/2}$ of the up-dimer Si on the clean Si(100) surface, and the 99.7 eV peak is assigned mainly to the $2p_{3/2}$ of bulk Si and the down-dimer Si. The shoulders at 100.0 and 100.6 eV are assigned to the $2p_{3/2}$ and $2p_{2/1}$ of subsurface Si species, respectively. Note that small peaks above 101 eV are due to dissociative adsorption of water from the background.

Upon the adsorption of 2MP (Fig. 1b), only two broad peaks are observed at 99.7 and 100.3 eV indicating that most of the dangling bonds are reacted with 2MP. With increasing the coverage of F4-TCNQ on the 2MP saturated Si(100) surface, the intensity of Si 2p peaks is decreased, because the surface is covered with F4-TCNQ. In addition, the Si 2p spectra were gradually shifted to lower binding energy with increasing the amount of F4-TCNQ. At 0.634 ML of F4-TCNQ where the second layer F4-TCNQ develops, the shift is 0.18 eV. These phenomena are interpreted to indicate that a band bending occurs in the Si substrate as a result of p-type surface transfer doping [4] by the charge transfer from the Si substrate to adsorbed F4-TCNQ species.

References

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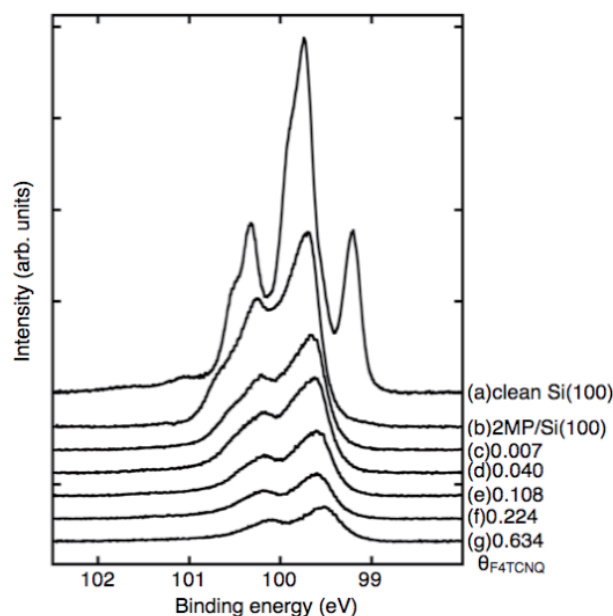


Fig. 1 Si 2p HR-XPS spectra as a function of F4-TCNQ coverage. h ν = 150 eV. 60° off normal emission.

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