

## VIII-M Nanoscale Characterization of Heterogeneous Catalyst Surfaces

Heterogeneous catalysis occurs on a surface of a solid catalyst. Active centers for heterogeneous catalysis commonly consist of clusters of several surface atoms, and thus a long-range order of surface atoms is not normally required. Therefore, when using precious metals as catalysts, nanometer-scale superfine particles are commonly employed in order to increase its surface area and to decrease the amount of catalysts. This introduces difficulties in characterizing the catalyst surfaces and their active centers, because characterization techniques of solid surfaces at nanometer-scale are not well established. Here we mainly used scanning probe microscopes, in conjunction with other surface characterization techniques, to characterize catalytically active centers as well as the nature of catalyst-support interactions.

### VIII-M-1 Determination of Extra-Framework Cation Positions and Their Occupancies on Heulandite(010) by Atomic Force Microscopy

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Atomic images of a cleaved heulandite(010) surface were obtained under an aqueous condition by atomic force microscopy (AFM). In addition to the framework oxygen atoms on the (010) plane, extra-framework cations on the surface were also imaged. An AFM imaging simulation was performed using published X-ray diffraction data to assist the assignment of the AFM-observed framework and extra-framework atoms. By comparing it with the observed AFM images, local variations of position and occupancy of individual cations were determined.

### VIII-M-2 Molecular Orbital Interpretation of Thymine/Graphite NC-AFM Images

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Recent non-contact atomic force microscopy (nc-AFM) images of a deoxyribonucleic acid (DNA) base thymine (2,4-dioxy-5-methylpyrimidine), vacuum-deposited on a highly-oriented pyrolytic graphite (HOPG) surface, are interpreted by means of theoretical adsorption simulations, and the molecular geometry and the energetics of the adsorption system are estimated. The lowest-energy dimer configuration was found to be the one in which the respective hydrogen on number 1 nitrogen and oxygen on number 6 carbon of two thymine molecules make a hydrogen bond to each other. A surface unit cell structure was reproduced. Adsorption energy for the thymine pair on HOPG is rather small, amounting to only *ca.* 1 kcal/mol, with small variations depending on the molecular orientation with respect to the substrate surface. A possibility of having a mirrored adsorption configuration in adjacent domains is also suggested.

### VIII-M-3 Partial Reduction of Si(IV) in SiO<sub>2</sub> Thin Film by Deposited Metal Particles—An XPS Study

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Metal-support interactions in the systems of dispersed metals supported on thin film silica surfaces were examined by X-ray photoelectron spectroscopy. Four metal-silica systems, Pt-, Pd-, Ag- and Au-SiO<sub>2</sub>, all indicated the formation of partially reduced Si(IV) species by the metal deposition. The extent of the reduction varied little with the kind and the amount of deposited metal species. On the other hand, the amount of this newly formed Si(IV- $\delta$ ) indicated a strong metal species dependence.

### VIII-M-4 Apparent Local Structural Change Caused by Ultraviolet Light on a TiO<sub>2</sub> Surface Observed by Scanning Tunneling Microscopy

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An apparent local surface structural change at nanoscale was observed by scanning tunneling microscopy on a TiO<sub>2</sub> surface upon irradiation with ultraviolet (UV) light. This phenomenon was reversible with UV light irradiation, and was interpreted to be due to the local accumulation of photoexcited states. This is the first real-space observation of inhomogeneous local charge distribution under UV light irradiation at nanoscale on a semiconductive photocatalyst surface, which may help identify the photocatalytic active sites and elucidate their reaction mechanisms.

### VIII-M-5 Various Phases on Natural Stilbite (010) Surface Observed by Atomic Force Microscopy under Aqueous Conditions

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Various phases on a natural stilbite (010) surface were observed by atomic force microscopy (AFM) under aqueous conditions. In a wide-area observation, oriented protrusions observed on the surface differed from the “sheaflike” structure which has been found in stilbite in an aqueous NaOH solution. Narrow-area observations showed surfaces consisting of an island structure, or a structure of alternating ridges and trenches. The latter is similar to the one reported previously under ambient conditions. The atomically resolved AFM image of the stilbite confirms that its surface is in good agreement with the known crystallographic parameters of the bulk-terminated (010) surface. Defects such as dislocations and grain boundaries at the atomic level were also observed.