

IV-O Photoelectron Spectroscopy of Organic Solids in Vacuum Ultraviolet Region

The works of ultraviolet photoelectron spectroscopy (UPS) with synchrotron radiation light source (UVSOR-UPS) of advanced organic materials have been proceeded to find their quantitative electronic structures and also to analyze their structures of assemblies.

IV-O-1 Angle-Resolved Photoemission Measurements of ω -(n-pyrrolyl)alkanethiol Self-Assembled Monolayers Using *in-situ* Sample Preparation Apparatus

HASEGAWA, Shinji; HORIGOME, Toshio; YAKUSHI, Kyuya; INOKUCHI, Hiroo; OKUDAIRA-KAMIYA, Koji¹; UENO, Nobuo¹; SEKI, Kazuhiko²; WILLICUT, J. Robert³; McCARLEY, L. Robin³; MORIKAWA, Eizi⁴; SAILE, Volker⁴
(¹Chiba Univ.; ²RCMS, Nagoya Univ.; ³Louisiana State Univ.; ⁴Louisiana State Univ. CAMD)

[*J. Electron Spectrosc. Relat. Phenom.* in press]

An *in-situ* sample preparation apparatus was developed for measuring intrinsic angle-resolved ultraviolet photoemission spectra (ARUPS) from ω -(n-pyrrolyl)alkanethiol self-assembled monolayers (pyrrolyl-SAMs) on an Ag surface. The apparatus enables the preparation of the SAMs directly from the thiol solution and the measurement of ARUPS without exposing the sample to air. The spectral features of the SAMs were analyzed with the aid of *ab-initio* molecular orbital calculations. It was observed that the ARUPS features associated with the π bands originating from the substituent pyrrole are distinct from the features associated with the alkyl chain.

IV-O-2 Photoemission Spectra of LiNiO₂ Catalyst for Oxidative Coupling of Methane

MIYAZAKI, Takafumi¹; AOKI, Masaru; TAKAYASU, Osamu¹
(¹Toyama Univ.)

[*Jpn. J. Appl. Phys.* **38**, 51 (1999)]

Surface-lattice oxygen species of LiNiO₂ with a layered structure were investigated for an oxidative reaction of methane. LiNiO₂ resulted in formation of C₂-hydrocarbons without by-products of carbon dioxide at an initial stage reaction which was an oxidative coupling process by surface lattice oxygen. For understanding of the origin of the catalytic activities, photoemission spectra of Li_xNi_{2-x}O₂ (0 < x ≤ 1) were measured. From comparison of the valence band structures, it was suggested that an anisotropic charge distribution and the layered structure contributed to the formation of active lattice oxygen and the catalytic performance of LiNiO₂, respectively.

IV-O-3 Intramolecular Energy-Band Dispersion in Oriented Thin Films of *n*-CF₃(CF₂)₂₂CF₃ Observed by Angle-Resolved Photoemission with Synchrotron Radiation

MIYAMAE, Takayuki; HASEGAWA, Shinji; YOSHIMURA, Daisuke¹; ISHII, Hisao¹; UENO, Nobuo²; SEKI, Kazuhiko³
(¹Nagoya Univ.; ²Chiba Univ.; ³RCMS, Nagoya Univ.)

[*J. Chem. Phys.* **112**, 3333 (2000)]

Angle-resolved ultraviolet photoelectron spectra were measured for oriented films of perfluorotetracosane, *n*-CF₃(CF₂)₂₂CF₃, as a model compound of poly(tetrafluoroethylene) using synchrotron radiation. The main spectral features showed continuous changes in both peak positions and intensities with photon energy, incident angle, and photoelectron take-off angle. The intramolecular energy-band dispersion of poly(tetrafluoroethylene) was mapped from the photo-energy dependence of the normal emission spectra.