To understand the chemical structure, property and reactions in a two-dimensional molecular aggregate, the keywords of molecular interactions and orientation are focused on, and the fluctuated molecular aggregates are investigated by using originally developed spectroscopic and theoretical techniques. The current major topics are: (1) a new chemical model accounting for bulk properties specific to perfluoroalkyl compounds; (2) analysis of molecular orientation and conformation in a thin film of organic semiconductor polymer; (3) study on a novel surface selection rule for discussing the molecular orientation in a thin film adsorbed on a rough surface.

**KEYWORDS**

- Infrared and Raman Spectroscopy
- Organic Semiconductor
- Surface and Interface Chemistry
- Polymer Electrolyte Membrane
- Perfluoroalkyl Compounds
- Nano Particle and Fibril Analysis

**Selected Publications**


Stratified Dipole-Arrays Model Accounting for Bulk Properties Specific to Perfluoroalkyl Compounds

Perfluoroalkyl compounds are known to exhibit a hydrophobic character on the surface of the material, although the C-F bond has a large dipole, which should make the molecular surface polar and hydrophilic. This inconsistency has long been a chemical matter to be solved. Herein, a stratified dipole-arrays model is proposed: the molecular polar surface can be fully hidden by forming a two-dimensional aggregate of perfluoroalkyl (Rf) groups; this aggregate is spontaneously induced by dipole–dipole interaction arrays owing to the helical structure of the Rf group. In this model, a ‘short’ Rf group should play the role of a single Rf group with a hydrophilic character, whereas a ‘long’ Rf group should spontaneously form a hexagonal aggregate. To examine this model, Rf-containing myristic acids with various Rf lengths have been synthesized and their aggregation properties are analyzed by using the Langmuir monolayer technique aided by precise IR spectroscopic analysis.

Analysis of Molecular Orientation and Conformation of Poly(3-hexylthiophene) Thin Films on Silicon by Infrared p-Polarized Multiple-angle Incidence Resolution Spectrometry

Infrared (IR) p-polarized multiple-angle incidence resolution spectrometry (p-MAIRS) has been employed for the first time to reveal the molecular orientation in two different poly(3-hexylthiophene) (P3HT) thin films having face-on and edge-on orientations. The CH out-of-plane deformation vibration mode (ca. 820 cm⁻¹) of the thiophene ring is found to be highly localized on the ring, which is quite useful for molecular orientation analysis coupled with IR p-MAIRS. On the other hand, the CH stretching vibration region is useful for determining the molecular order, conformation, and folding of the hexyl chain via MAIRS dichroism.