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Division of Multidisciplinary Chemistry
- Molecular Aggregation Analysis -

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Scope of Research

The research at this subdivision is devoted to correlation studies on structures and properties of both natural and artificial molecular aggregates from two main standpoints: photoelectric and dielectric properties. The electronic structure of organic thin films is studied using photoemission and inverse photoemission spectrosocpies in connection with the former, and its results are applied to create novel molecular systems with characteristic electronic functions. The latter is concerned with heterogeneous sturcutres in mocrocapsules, biopolymers, biological membranes and biological cells, and the nonlinearity in their dielectric properties is also studied in relation to molecular motions.

Research Activities (Year 2005)

Presentations

Simulation of Dielectric Relaxation in Biological Cells of Arbitrary Shape (in Japanese), Asami K, The 27th Annual Meeting of the Membrane Society of Japan (Tokyo, Japan), 19 - 20 May.

Frontier Electronic Structures in Organic Semiconductor Thin Films Studied Using Ultraviolet and Inverse Photoemission Spectroscopies, Sato N, Murdey R J, The 3rd Workshop on Advanced Spectroscopy of Organic Materials for Electronic Applications (ASOMEA III) (Vadstena, Sweden), 2 - 5 June.

Frontier Electronic Structure of Fluorinated Copper Phthalocyanine Thin Films Studied Using Ultraviolet and Inverse Photoemission Spectroscopies, Murdey R, Bouvet M, Sato N, The 54th Fujihara Seminar: Organic Semiconductors and Conductors - Half Century and Future Prospects (OSCC50) (Tomakomai, Japan), 31 August - 4 September.

Contribution of Electronic Polarization to Electrostatic Lattice Energy in Organic Molecular Crystals (in Japanese), Tsutsumi J, Kato S, Sato N, The 14th Organic Crystals Symposium (Kyoto, Japan), 30 September - 1 October.

Evaporation of Aluminum Clusters on Organic Semiconductor Thin Films (in Japanese), Yoshida H, Sato N, Bunshi-kozo Sogo Toronkai (Symposium on Molecular Structures and the Related Problems) 2005 (Tokyo, Japan), 27 - 30 September.

Dielectric Dispersion of Lysed Erythrocytes (in Japanese), Asami K, The 43rd Annual Meeting of the Biophysical Society of Japan (Sapporo, Japan), 23 - 25 November.

Grants

Sato N, Development of Novel Electronic Systems Based on Hybridization of Characteristic Molecular Properties and Specific Aggregate Structures, Grant-in-Aid for Scientific Research (2) on Priority Areas of Molecular Conductors, 17 October 2003 - 31 March 2008.

Yoshida H, Controlling Reactivity and Diffusion at

Frontier Electronic Structures in Fluorinated Copper Phthalocyanine Thin Films Studied Using Ultraviolet and Inverse Photoemission Spectroscopies

Copper phthalocyanine [CuPc] and the fluorinated analog [Cu(F_{16}Pc)] are very different materials from the standpoint of their electronic properties. CuPc is a hole transport material, typical of organic semiconductors. In contrast Cu(F_{16}Pc) is one of the few air-stable compounds known to exhibit electron transport, characteristics that make it of considerable interest in the development of molecular electronic devices. In an recent example, an ambipolar transistor has been demonstrated using thin layers of pure, undoped CuPc and Cu(F_{16}Pc) as the p-type and n-type semiconductors, respectively.

We have examined the effect of fluorine substitution on the electronic structure of phthalocyanines, with particular attention paid to the states near the HOMO-LUMO gap. Unoccupied states were directly observed with inverse photoemission spectroscopy (IPES), while the corresponding measurement on occupied states was performed with ultraviolet photoelectron spectroscopy (UPS).

Thin films of CuPc, a partially fluorinated intermediate compound Cu(F_8Pc), and Cu(F_{16}Pc) were prepared by vacuum deposition on clean gold substrates. Spectra were taken in-situ under UHV conditions. As seen in Fig. 1, the results show that while the transport energy gap remains almost constant at about 2 eV, there is a readily apparent, rigid shift of the gap to higher binding energies with increasing fluorine substitution. The charge injection barrier heights stay essentially unchanged, however, as the substrate Fermi level is pinned near the middle of the phthalocyanine HOMO-LUMO gap in all three systems. This work was carried out in collaboration with Prof. Marcel Bouvet at Laboratoire de Chimie Inorganique et Matériaux Moléculaires, CNRS, France.

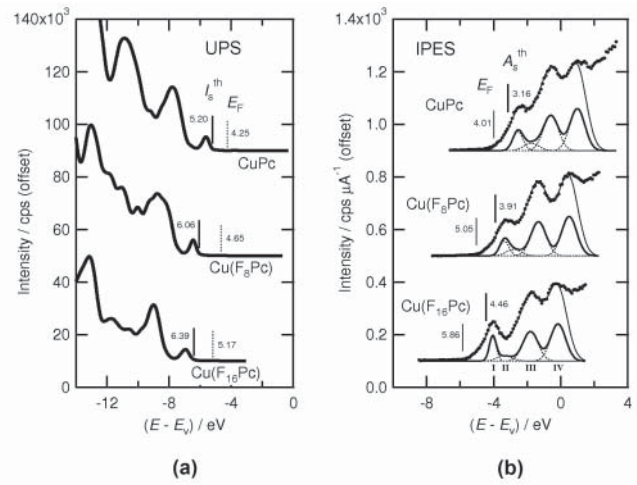

Figure 1. (a) UPS and (b) IPES spectra of 8 nm-thick CuPc, Cu(F_8Pc) and Cu(F_{16}Pc) films on gold substrates. The energy scale is plotted against the vacuum level of the organic film. Gaussian fits are shown for the IPES spectra, compensated for the resolution of the instrument. Determined energy positions are indicated by vertical bars with respective values.

Numerical Simulations of Dielectric Dispersion in Biological Cells of Complex Geometry

Biological cells show dielectric dispersion due to interfacial polarization, i.e., accumulation of charges at the membrane interfaces by the applied electric field. For cells of simple geometry, we have used analytical approaches for analyzing the dielectric dispersion. However, it is difficult to derive analytical formulas for cell models of complex geometry. Hence, a numerical technique based on the three-dimensional finite difference method has been developed to calculate the equivalent complex permittivity of a system including a single cell or periodically arranged cells in a continuous medium. The numerical method successfully simulated dielectric dispersion of cells in cell division, i.e., a spherical cell divides into two spherical cells via a doublet-shaped cell with a narrow cytoplasmic junction. Further, it has uncovered the underlining mechanism of the α-dispersion of osmotically-lysed erythrocytes, which has remained open since its finding in 1957. The α-dispersion is caused by formation of a single hole of several tens nm in radius in the plasma membrane.

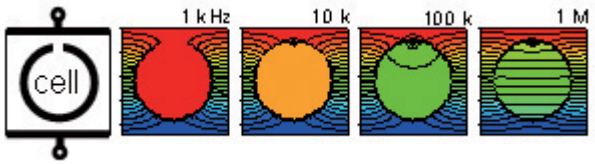

Figure 2. Electrical potential distributions in a cell model with a hole.

Metal-Organic Semiconductor Interfaces through the Deposition of Metal Clusters, Grant-in-Aid for Scientific Research for Young Scientists (B), 19 October 2004 - 31 March 2006.