Division of Multidisciplinary Chemistry
- Molecular Aggregation Analysis -

http://www.kuicr.kyoto-u.ac.jp/labos/is2/scope.html

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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 microcapsules, biopolymers, biological membranes and biological cells.

Research Activities (Year 2008)

Publications

Yoshida H, Sato N: The Crystallographic and Electronic Structures of Three Different Polymorphs of Pentacene, *Phys. Rev. B*, **77**, 235205 (2008).

Asami K: Simulation for the Dielectric Images of Single Biological Cells Obtained using a Scanning Dielectric Microscope, *J. Phys. D: Appl. Phys.*, **41**, 085501 (2008).

Presentations

A Neutral Radical Complex as a "True" Molecular Semiconductor: Lutetium Bisphthalocyanine, Murdey R, Bouvet M, Sato N, 2008 Symposium on Coordination Compounds as Inorganic-Organic Composite Materials (Sanda, Japan), 19 April 2008.

Structures and Electronic Structures of Pentacene Thin Films in Polymorphism, Yoshida H, Sato N, The 14th International Conference on Solid Films and Surface (Dublin, Ireland), 29 June–4 July 2008.

The Evolution of the Energy Band Structure in Polythienoacene; Photoemission Study of Bis(benzo)pentathienoacene as a Function of Film Thickness, Yoshida H, Watazu Y, Sato N, Kawabe E, Yamane H, Kanai K, Seki K, Okamoto T, Yamaguchi S, International Symposium on Molecular Conductors 2008 (Okazaki, Japan), 23–25 July 2008.

Structural Analysis and Energy Band Calculation of Polymorphic Pentacene Thin Films, Yoshida H, Sato N, The 21st IUCr Satellite Meeting "Molecular Crystals Exhibiting Exotic Functions" (Osaka, Japan), 21–22 August 2008.

Single Cell Analysis Using a Scanning Dielectric Microscope, Asami K, The 5th International Conference on Broadband Dielectric Spectroscopy and Its Applications (Lyon, France), 26–29 August 2008.

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.

Asami K, Dielectric Monitoring of Cultured Cells Responding to External Stimuli, Collaboration Research with Sony Corporation (Life Science Laboratory, Material Laboratories), 27 October 2008–31 March 2009.

Yoshida H, The Relation between Electronic Structure and Spin Injection Efficiency at Organic Semiconductor/Metal Interfaces: Towards the Development of Organic Spin Device, Grant-in-Aid for Scientific Research (C), 1 April 2008–31 March 2012.

Topics

Correlation between Crystallographic and Electronic Structures of Three Different Polymorphs of Pentacene

The energy bands of three polymorphs of pentacene, i.e., the thin-film, bulk, and single-crystal phases, were calculated. In the calculation of the thin-film phase, we applied the structural data obtained from our recent studies on the X-ray diffraction analysis using the reciprocal space mapping method. The band structures are essentially two-dimensional as shown in Figure 1, i.e., only small dispersions are found along the c* direction. The energy dispersion of the thin-film phase is examined to be larger and more isotropic than those of the other phases. The energy dispersions of the bands derived from highest occupied molecular orbital (HOMO), HOMO-1, lowest unoccupied molecular orbital (LUMO) and LUMO+1 levels are analyzed by comparing with the corresponding results on the basis of the tight-binding approximation; the dispersions are well described by transfer integrals among only the nearest neighbor molecules. In accordance with this result, a simple model is presented to explain the relation between the crystal structure and the energy dispersion. From the calculated bands, the effective masses are derived to discuss the charge-carrier transport properties in the respective phases. Further, photoemission spectra were measured for the thin-film and bulk phases, to confirm that the observed spectral features of the HOMO-derived bands are interpreted by the calculated density of states.

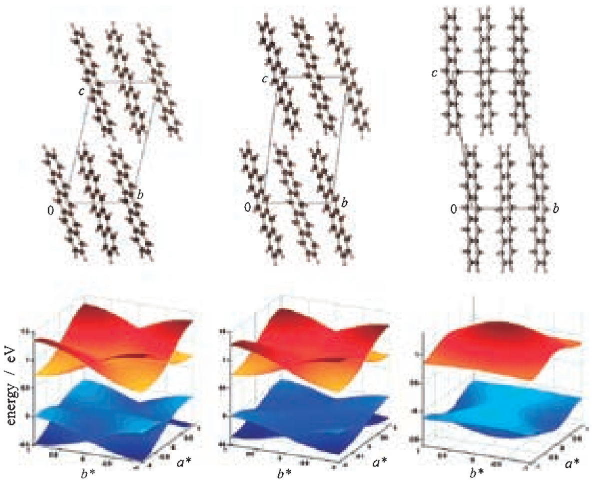

Figure 1. Crystallographic structures and corresponding calculated energy-band structures of pentacene polymorphs: (a) single-crystal phase, (b) bulk phase and (c) thin-film phase.

Dielectric Cytometry of Erythrocytes

Biological cells are polarized in an ac electric field due to charge accumulation at the interfaces between the plasma membrane and the aqueous phases, namely interfacial polarization. The polarization depends on the cell shape as well as the electrical properties of the membrane and the cytoplasm, and therefore the dielectric spectrum of the cell suspension is specific to the cell shape. However, there have been few systematic studies on this issue with erythrocytes, whose shape is susceptible to the metabolic states, the external conditions and diseases. We measured dielectric spectra of four types of erythrocytes as shown in Figure 2 (Hayashi, et al., *Phys. Med. Biol.*, **53**, 2553 (2008)). This figure clearly demonstrates that the spectrum shape or broadening is sensitive to the cell shape and that dielectric spectroscopy is a useful tool for studying the cell shape change. The dielectric spectra of discocytes and echinocytes were respectively simulated with the biconcave-discoid model and the spinous-sphere model using the three-dimensional finite difference method (Katsumoto, et al., *Biophys. J.*, **95**, 3043 (2008)). The agreement between the observed and theoretical spectra was satisfactory for both of discocytes and echinocytes. We also devised an efficient method to estimate the capacitance of the plasma membrane and the conductivity of the cytoplasm on the basis of the numerical simulations.

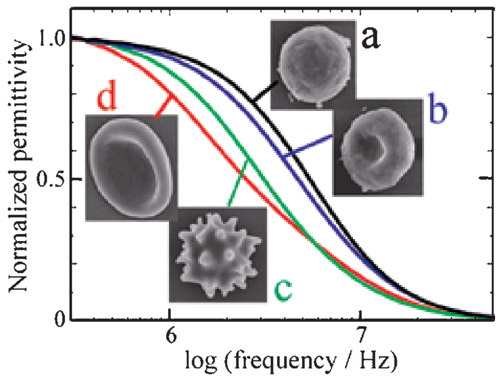

Figure 2. Dielectric spectra of erythrocytes with different shapes. (a) spherocyte, (b) stomatocyte, (c) echinocyte and (d) discocyte.