

MS25 P01

Organic monolayers and lipid-protein nanostructures on solid and liquid surfaces studied by TR-XSW technique. S.I.Zheludeva, N.N.Novikova, N.D.Stepina, E.A.Yurieva, E.Yu.Tereschenko, O.V. Kononov*, *Shubnikov Institute of crystallography RAS, Moscow, Russia.* * *European Synchrotron radiation facility (ESRF), Grenoble, France.*

Keywords: X-ray standing wave, Liquid surfaces, Langmuir-Blodgett films

Model cell membranes can be obtained using the Langmuir-Blodgett method of layer-by-layer deposition of amphiphilic organic molecules on solid substrate. Langmuir molecular layers on the surface of a liquid subphase can be used as a basis for formation of lipid-protein membrane systems in native state under the conditions close to physiological. Investigation of barriers, transport and protective functions of membrane is connected with necessity of ion localization in such molecular systems.

In the present paper it is shown that X-ray standing wave technique at total reflection (TR-XSW) allows to reveal the position of atoms in organic macromolecules and nanostructures of nm range linear dimensions on solid or liquid substrate.

The technique was used to study:

- the molecular mechanisms of the protective effect of bisphosphonate drug xydiphon on biomembrane model on the base of Ca-ATPase damaged by heavy metals (station EKMC 2; BESSY II); [1]

- organic surfactants containing heavy ions and forming well-ordered Langmuir layers on liquid surface: metal-substituted phthalocyanines, polyorganosiloxanes and phospholipids. Quantitative structural information from an individual organic monolayer on a liquid surface was obtained. (station ID10B, ESRF); [2]

- lipid-protein system containing enzyme alkaline phosphatase, formed by Langmuir technique on water subphase. The analysis of angular dependent fluorescence intensities from metal ions that enter into the composition of a protein molecule; from phosphor ions of phospholipids and from trace bivalent metal ions (Ni) that have been incorporated into nanostructure, allowed to localize ions and to propose complicated layered model of molecular self-organization on water surface. (station ID10B, ESRF).

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MS25 P02

Biomolecular hydrogen bonds assessed by neutron inelastic scattering Ahmed Aamouche^a, Mahmoud Ghomi,^b ^a*Matter science department, Faculté Polydisciplinaire, CadiAyyad University, Safi, Morocco.* ^b*BioMoCeTi-CNRS UMR7033, Paris, France.* E-mail: a.aamouche@gmail.com

Keywords: Neutron inelastic scattering spectra, nucleic acid structures, hydrogen bonding.

Neutron inelastic scattering (NIS) is now a powerful tool to analyze molecular vibrations. Since hydrogen atoms have the highest NIS cross-section and are significantly the main constituent of the biological systems NIS spectroscopy is advantageous than other vibrational spectroscopies for hydrogen motions monitoring.

NIS spectra of nucleic acid bases are recorded from polycrystalline samples on time-focused crystal analyzer spectrometer (Rutherford Appleton Laboratory, UK). Harmonic wavenumbers and intensities are predicted via Density Functional Theory (DFT) calculation at B3LYP/6-31G* level. The predicted DFT atomic displacements have been used to simulate first-order NIS spectra. [1]

As X-ray diffraction patterns show an intermolecular H-bond network between NH and C=O groups, we have taken into account explicitly intermolecular effects in our DFT calculation to imitate condensed phase environment. The comparison of the resultant spectra with the experimental ones corrects considerably the assignment particularly for the normal modes involving hydrogen. [2] The determined structural proprieties are of primary importance as H-bonding play a functional role in molecular shape and dynamic throughout bases pairing and stacking.

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[2] Ghomi, M. and al. *J. Mol. Struct.*, 1997, 323.

MS25 P03

Analogy of Polymorphism in Salicylideneaniline and its Ethoxy Derivative. Frédéric Arod^a, Philip Pattison,^{a,b} Kurt J. Schenk,^a and Gervais Chapuis,^a ^a*Laboratoire de Cristallographie, EPFL, Switzerland.* ^b*SNBL-ESRF, Grenoble, France.* E-mail: frederic.rod@epfl.ch

Keywords: photochromism, phase transitions crystal characterization, structure-property relationships in solids.

Organic compounds exhibiting photo- or thermochromicity are of considerable interest owing to their properties and possible applications. The photochromism of salicylideneaniline (SA) was discovered by Senier *et al.* at the beginning of last century, and in 1964, Cohen *et al.* [1] established its polymorphism. We have recently demonstrated its thermochromism in solids [2] by differential scanning calorimetry and also by *in situ* X-ray diffraction.

We report on three polymorphs of SA, two of its ethoxy derivative (ESA) and their inter-relation, in particular, an irreversible phase transition between the β and α_1 forms of SA leading to a less stable α_1 form. We discuss the different packings observed in these polymorphs, with the goal of understanding their structure-property relationships in solids.

The thermal behaviour of the ESA polymorphs is similar to that of the SA phases. The non-planar α -phase undergoes the fusion transition at 88°C, but re-solidifies, in a two-step process, 30°C lower to a likely different form, which however has a similar melting point. The planar β -form transforms into the α -phase at 85°C, then becomes isotropic at 89°C, but does not seem to return to the same form during the solidification at 54°C. One might therefore conjecture that the liquid phase of ESA is not so