O 53 Organische Dünnschichten V

Zeit: Mittwoch 10:45–13:00 Raum: TU EB420

O 53.1 Mi 10:45 TU EB420

Dynamics of colloidal thin films at the nanometer scale using surface XPCS — •Simone Streit[1], Henning Sternemann[1], Virginie Chamard[2], Michael Sprung[1], Christian Gutt[1], Anders Madsen[3], and Metin Tolan[1] — [1]Exp. Physik I, Universität Dortmund, 44221 Dortmund — [2]LTPCM, St Martin d'Hères, France — [3]ESRF, Grenoble, France

The surface dynamics at the nanometer scale of thin polymer films decorated with gold clusters was investigated using x-ray photon correlation spectroscopy (XPCS) in grazing incidence geometry. The scattering signal from polystyrene films (80-100 nm thick) with different molecular weights (34.4 and 220 kg/mol) and rather large nominal gold thicknesses (1-2 nm) was measured by a CCD as a function of time for temperatures in the range of 290 to 450 K. Capillary waves motion at the polymer surface as well as surface diffusion of the nanoparticles have already been observed for length scales of about 10 nm, leading to viscosity values much higher than the ones already known for the bulk. In this experiment we confirmed the large surface viscosity and investigated the q-parallel dependence of the relaxation time for different temperatures. q-parallel values from 0.1 to 1 nm^{-1} were measured simultaneously, thus leading to the direct observation of surface dynamics on nanometer length scales.

O 53.2 Mi 11:00 TU EB420

PE and NEXAFS study of self-assembled bacterial surface-layer proteins — •Denis Vyalikh[1], Alexander Kirchner[2], Steffen Danzenbächer[1], Michael Mertig[2], Wolfgang Pompe[2], Yuriy Dedkov[1], and Serguei Molodtsov[1] — [1]Inst. f. Festkörperphysik, TU Dresden — [2]Inst. f. Werkstoffwissenschaft, TU Dresden

Electronic structure of regular bacterial cell wall proteins (S layer) of *Bacillus sphaericus* was studied by photoemission (PE) and near-edge x-ray absorption fine structure (NEXAFS) spectroscopies [1]. Both the occupied and unoccupied valence electronic states were characterized and found to represent a series of PE and NEXAFS peaks, respectively, related to the molecular orbitals of individual amino acids. It was shown that the NEXAFS data could be interpreted applying a phenomenological "building block"model, whereas understanding of the valence-band PE structures can be achieved on the basis of electronic density-of-states calculations performed for rather small proteins. It was found that the π clouds of aromatic rings contribute both to the lowest unoccupied and the highest occupied molecular orbitals (LUMO and HOMO). The studied S layer reveals semiconductor-like behavior with a gap value of ~ 3 eV. The Fermi level is pinned close to the bottom of the LUMO.

We expect that the position of the Fermi level can be shifted across the gap by insertion of dopants into the pores in the S layers. First experiments on intercalation of alkali and transition metals into S layer are under way in our cooperation. The obtained results will be reported.

[1] D.V. Vyalikh *et al.*, Phys. Rev. Lett. (2004) in print

O 53.3 Mi 11:15 TU EB420

Radiotracer diffusion measurements of noble metal atoms in semiconducting crystalline organic films — •Michael Scharnberg[1], Jörn Kanzow[1], Klaus Rätzke[1], Stefan Meyer[2], Jens Pflaum[2], Rainer Adelung[1], and Franz Faupel[1] — [1]Lehrstuhl für Materialverbunde, CAU Kiel, Kaiserstr. 2, D-24143 Kiel — [2]3. Physikalisches Institut, Universität Stuttgart, Paffenwaldring 57, D-70569 Stuttgart

The application of organic field effect transistors (OFETs) for large scale low-cost electronic devices has lead to intense research. Diindenoperylene (DIP) thin films on SiO2 are a prominent system due to their high structural out-of-plane order. Preparation of top contacts might cause diffusion of metal atoms (typically Au or Ag) deep into the organic film changing the injection properties at the interface, which are of great importance for the device performance. Only by understanding the diffusion behaviour of metal in the organic layer, formation of well defined interfaces and control of their properties will become possible. Therefore, diffusion profiles for Ag [1] and Au diffusion in DIP films with different crystalline properties, e.g., Rocking widths, were obtained using a radiotracer technique. The results indicate similarities in the diffusion behaviour of noble metals in polymers and organic crystalline films. They will be discussed with respect to the crystalline structure of the DIP films.

[1] M. Scharnberg et al, APL 2004, in press

O 53.4 Mi 11:30 TU EB420

Crystal Face Resolved Oxidation of Pentacene with Ozone — •S. Rentenberger[1], H. Weiss[2], A. Vollmer[3], J. Niemax[4], J. Pflaum[4], I. Salzmann[5], J. P. Rabe[5], and N. Koch[5] — [1]TU-Graz, Institut f. Festkörperphysik, A-8010 Graz, Austria — [2]Universität Magdeburg, Lehrstuhl f. Physikalische Chemie, D-39106 Magdeburg — [3]BESSY GmbH., D-12489 Berlin — [4]Universität Stuttgart, 3. Physikalisches Institut, D-70550 Stuttgart — [5]Humboldt-Universität zu Berlin, Institut f. Physik, D-12489 Berlin

While the oxidation of pentacene by molecular oxygen proceeds very slowly, ozone (produced by illumination with ultraviolet light) leads to a rapid oxidation of this prototypical conjugated organic molecule, successfully used in flexible thin film transistors. We have studied the ozone-induced oxidation kinetics of pentacene thin films by infrared absorption spectroscopy in transmittance and reflection, and the accompanied evolution of the film morphology by atomic force microscopy. In order to selectively probe individual pentacene crystal faces, thin films were grown on silicon oxide [exposing the (ab) plane] and on highly oriented pyrolytic graphite [exposing the (bc) plane]. We find in both cases substantial loss of pentacene mass-thickness, indicating that ozone produces highly volatile reaction products, however, on a faster time scale for films grown on graphite.

O 53.5 Mi 11:45 TU EB420

A new approach to the determination of the transport gap in organic semiconductors using a combination of IPES and UPS — •Stefan Krause, Benedetta Casu, and Eberhard Umbach — Experimentelle Physik II, Universität Würzburg, Am Hubland, 97074 Würzburg

Organic semiconductors are in general believed to be strongly correlated systems. The value for the transport gap is somewhere between the measured value of optical absorption and the one, which one gets from the energetic distance of the HOMO in UPS and the LUMO in IPES. If one uses the peak positions of the HOMO and LUMO the gap is about 1 eV larger than the one of optical absorption. This is then explained with the strong correlation and polarization [1].

We compared the measurements of organic semiconductors with those of inorganic to find a hint on which side of these two boundaries one has to search. Surprisingly the data for the inorganic semiconductors showed the same trend and the UPS-IPES gap was much larger than the optical gap. This can no longer be explained with correlation because these materials are solids with strong covalent bonds and small (Mott-Wannier-) exciton binding energies. However, the distance of the peak onsets perfectly fits the optical data.

[1] E.V. Tsiper et al. Chem. Phys. Lett. 360 (2002), 47-52

O 53.6 Mi 12:00 TU EB420

The self-assembly of alkyl-trichlorosilanes on model surfaces of biphenylthiols — •Svetlana Stoycheva[1], Jörg Fick[1], Steffen Franzka[2], Nils Hartmann[2], Alexander Kornviakov[3], Avi Ulman[3], Michael Himmelhaus*[1], and Michael Grunze[1] — [1]Angewandte Physikalische Chemie, Universität Heidelberg — [2]Institut für Physikalische und Theoretische Chemie, Universität Essen — [3]Dept. of Chemical Engineering, Polytechnic University, Brooklyn, New York

Despite of its technological relevance, the self-assembly of monolayers of alkyl-trichlorosilanes onto oxidized metal or semiconductor surfaces is still not fully understood. Phenomena, such as island formation and polymerization, hamper the formation of densely packed and well-oriented self- assembled monolayers (SAM) in many cases. In particular, it has been found that the amount of surface-adsorbed water plays a crucial role for the process of film formation. In our study we have used rigid 4-mercaptobiphenyls (MBP) to prepare stable, molecularly engineered SAM surfaces, and used them as substrates for the study of the assembly mechanism of alkyltrichlorosilanes. SAM of 4-Methyl-4'-MBP, 4-Hydroxy-4'-MBP and MBP (as a reference system) as well as the bilayer assemblies were characterized by contact angle measurements, spectral ellipsometry, infrared reflection absorption spectroscopy, X-ray photoelectron spectroscopy, sum frequency generation, and atomic force microscopy. In combination with a frequency analysis based on ab initio calculations, insight into the structure of the MBP as well as a detailed picture of the film formation of the silane overlayer could be achieved.

O 53.7 Mi 12:15 TU EB420

Functionalized para-phenylene nanofibers — •Frank Balzer[1], Katharina Al-Shamery[2], Arne Luetzen[2], Manuela Schiek[2], Ralf Frese[3], and Horst-Günter Rubahn[3] — [1]Humboldt-Universität zu Berlin, Institut für Physik / ASP — [2]University of Oldenburg, Institute of Pure and Applied Chemistry, Oldenburg — [3]SDU Odense, Fysisk Institut, Denmark

Growth of mutually aligned, several tens to hundreds of μm long organic nanofibers from functionalized molecules has been demonstrated for the first time. The fibers from 4,4'''-Dimethoxy-1,1':4',1'':4'',1'''-quaterphenyl (MOP4) are grown on mica by vacuum sublimation and they resemble more the well organized growth of long para-hexaphenyl (p-6P) nanofibers as compared to the rather unorganized growth of short para-quaterphenyl (p-4P) aggregates. Atomic force microscopy reveals typical heights of the MOP4 nanofibers of a few ten nanometers and typical widths of a few hundred nanometers. The MOP4 fibers show intense, polarized blue light emission with well resolved higher order vibronic peaks and a morphology that is slightly different from that of p-6P nanofibers.

O 53.8 Mi 12:30 TU EB420

Electron-vibron coupling in the NEXAFS spectra of naphthalene in the condensed and gas phase — •Dominique Hübner[1], F. Holch[1], A. Schöll[1], R. Fink[2], K.C. Prince[3], S. Stranges[4], and E. Umbach[1] — [1]Univ. Würzburg, Exp. Phys. II — [2]Univ. Erlangen, Phys. Chem. II — [3]Sincrotrone Trieste — [4]CNR-Istituto di Metodologie Inorganiche e dei Plasmi

High-resolution NEXAFS spectroscopy is ideally suited to investigate the electronic structure of large organic molecules in both, the condensed and the gas phase. In ideal cases one observes distinct fine structures which are attributed to the coupling of electronic transitions to vibronic excitations [1]. We present NEXAFS data on naphthalene and deuterated naphthalene both in the gas and condensed phase. In order to identify vibronic modes, especially the C-H modes, in the electronic transitions deuterated naphthalene has been utitlized. In contrast to previous studies [1], a manifold of vibronic states efficiently couple to the core excitation which makes the analysis difficult.Comparison with benzene data sufficiently explain most of the structures. The differences between gas and condensed phase spectra are explained by Van-der-Waals like bonding in the condensed phase. The project is financed by BMBF (contracts 05 KS1 WWA5 and 05 KS4 WWC/2).

[1] A. Schöll et al. PRL 93, 146406 (2004)

O 53.9 Mi 12:45 TU EB420

Interaction of Self-Assembled Monolayers of Oligo(ethylene glycol)-Terminated Alkanethiols with Water studied by Vibrational Sum Frequency Generation (VSFG) — •Jörg Fick[1], Rongyao Wang[2], Sascha Herrwerth[1], Wolfgang Eck[3], Michael Himmelhaus*[1] und Michael Grunze[1,3] — [1]Angewandte Physikalische Chemie, Universität Heidelberg — [2]Department of Physics, National University of Singapore — [3]Institute for Molecular Biophysics, University of Maine

In einer kürzlichen Studie konnte nachgewiesen werden, daß die Proteinresistenz selbstaggregierender Monolagen (SAM) aus Oligoether-terminierten Alkanthiolen von verschiedenen Faktoren, wie der Hydrophilie der Molekül-Endgruppen und der Hydrophilie des Molekülinneren, abhängt. Außerdem wurde gezeigt, daß die laterale Packungsdichte der Moleküle einen Einfluß auf die Repulsion von Proteinen hat.

In diesem Beitrag analysieren wir mit Hilfe der Breitband-IR-Vis-Summenfrequenzerzeugung (BB-SFG) den Einfluß von Packungsdichte und Hydrophilie auf die Proteinresistenz der Filme, indem wir Konformations-änderungen der SAMs vor, während und nach Wasserkontakt in-situ verfolgen. Dabei zeigt sich, daß die Proteinresistenz nicht substratabhängig, sondern in der Tat ein reiner Dichteeffekt ist. Die BB-SFG-Resultate werden durch Ellipsometrie- und IR-Messungen ergänzt, mit deren Hilfe das Adsorptionsverhalten von Modelproteinen in den unterschiedlichen Präparationsstadien der Filme untersucht wurde. Darüber hinaus wurde ein Degradationsmechanismus für OEG-SAMs in wäßrigen Lösungen erforscht und aufgeklärt.