CPP 13 Selforganized and supramolecular assemblies II

Zeit: Montag 11:15–12:30 Raum: TU C243

CPP 13.1 Mo 11:15 TU C243

The interfacial structure of electrolyte solutions — •Thomas Krebs, Gunther Andersson, and Harald Morgner — Universität Leipzig, Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Linnéstrasse 2, 04103 Leipzig

The structure of the surface of salty liquid solutions plays an important role for reactions at the gas/liquid interface. Recently the question has been raised about the distribution of halide ions at liquid surfaces. MD Computer Simulations predict even segregation of the heavier halide ions to the surface in aqueous solution. This suggests a positive surface excess of the salt although the surface tension of the solution increases with salt concentration.

Neutral Impact Collision Ion Scattering Spectroscopy (NICISS) is a suitable method to determine concentration depth profiles of elements at liquid surfaces. We present data which show that halide ions can appear in the top layer of solutions in polar solvents. The topography around ions at the top surface layer can be evaluated. This is possible by applying NICISS in the angular resolved mode. Angle resolved measurements have been performed at solutions of Tetra-n-butylphosphonium bromide and potassium iodide in formamide and in glycerol.

CPP 13.2 Mo 11:30 TU C243

An experimental route to Hofmeister. — •Patrick Koelsch and Hubert Motschmann — Max-Planck-Institute of Colloids and Interfaces, Am Muehlenberg, 14476 Potsdam, Germany

The distribution of ions close to a charged wall is a classical problem in colloid and interface science. The complex interplay of electrostatics, dispersion forces, thermal motion, fluctuations, hydration, ion size effects and the impact of interfacial water structure makes it hard or even impossible to identify an universal law. The diversity of specific ion effects as manifested by the Hofmeister series of ions is a direct consequence of the subtle interplay of forces. Recently this field has attracted renewed attention as reflected by a special edition in Current Opinion of Colloid and Interface Science.

We already demonstrated, that the combination of nonlinear (surface Second Harmonic Generation SHG) and linear optical techniques (Ellipsometry) allows a direct determination of the prevailing ion distribution. A simple analytical expression was derived which can be used to retrieve the number of condensed counterions within the compact or so called Stern-layer. We applied this formalism on experimental data gained on aqueous cationic surfactants by varying the counterions in order to quantify specific ion effects at the interface following the Hofmeister series. In this contribution we will compare our experimental data with recently done simulations which take into account the polarizability or in other words the structure of water at interfaces.

CPP 13.3 Mo 11:45 TU C243

Addressing metal centers in complex supramolecules by STS — •M.S. Alam[1], S. Strömsdörfer[1], A.M. Ako[2], V.V. Dremov[1], M. Ruben[3], R.W. Saalfrank[2], L.K. Thompson[4], and P. Müller[1] — [1]Physikalisches Institut III, Universität Erlangen-Nürnberg — [2]Institut für Organische Chemie, Universität Erlangen-Nürnberg — [3]Institut für Nanotechnologie, FZ Karlsruhe — [4]Dept. of Chemistry, Memorial University, St. John's, NL, Canada

Investigating elementary structure formation processes of supramolecules on substrate surfaces is a rather complex task. As the contrast in scanning tunnelling microscopy (STM) is produced by the local density of electronic states, extracting information on the geometrical shape of a complex molecule is not straightforward. Using a home built STM under ambient conditions, we succeeded to combine high resolution topography mapping with simultaneous current-voltage characteristics (STS) measurements on single molecules deposited on highly oriented pyrolytic graphite (HOPG) surfaces. We present our recent results on Co 2x2 and Mn 3x3 grid molecules as well as on ring-shaped Fe ion chains (ferric wheels). Small, regular molecule clusters as well as separated single molecules were observed. One of the most interesting results is that the location of the metal ions in their organic matrix is directly addressable by STS.

CPP 13.4 Mo 12:00 TU C243

Interaction among Charged Membranes — •Beate Klösgen[1] and Viveka Alfredsson[2] — [1]University of Southern Denmark, Phys. Dept. and MEMPHYS, Denmark — [2]Lund University, Inst. Phys. Chem., Sweden

Charged membranes exhibit unspecific electrostatic interactions; especially the cationic ones have the potential for binding DNA which suggests an application in gene transfer systems. Yet, the pure electrostatics of composite systems of neutral and charged lipid, counterions and water is not fully understood. Results from interaction studies among charged membranes are presented. Electron microscopy (cryo-TEM, 120kV, $\Delta z \simeq -1\mu m$) experiments were done on vitrified SUVs ($r \simeq 50nm$) of neutral lipid (DOPC) and admixed cationic / anionic lipids of the same chain length (DOPG, E-DOPC), Cl- being the charge counterion. Lipid concentration of 1% (wt/wt) was constant in all vesicle suspensions; charge densities were adjusted to 1% or 10 % (charged lipid/total lipid). A crossover between adhesion and repulsion among adjacend membranes depending on membrane charge density was found. At least two opposing contributions must cause this balance. It may be speculated that the net attractive interaction at low charge density can be attributed to an entropic contribution by counterion release from the aqueous gap in the adhesion site, or to charge dependencies of fluctuation forces.

CPP 13.5 Mo 12:15 TU C243

Quantum chemical investigation of the adsorption of PTCDA on Ag(110) — •Afshin Abbasi, Reinhard Scholz, and Michael Schreiber — Institut für Physik, Technische Universität Chemnitz, Germany

The vibrational properties of a PTCDA molecule adsorbed to an Ag(110) surface have been investigated with different quantum chemical techniques, including Hartree-Fock based approaches and density functional theory. Keeping the atoms of the topmost Ag layer in the ideal lattice positions, a relaxed geometry for a PTCDA molecule was calculated with Hartree-Fock (HF). The anhydride oxygen atoms experience a strong interaction with the substrate, resulting in an Ag-O bond length of about 2.6 Å. The interaction with the metal substrates is energetically so favourable that an elastic energy of about 1 eV stored in the bended molecule is overcompensated. Within this geometry, the infrared (IR) activity along the substrate normal has been calculated. Above 1100 cm^{-1}, the IR activity of the adsorbed molecule results from vibrational modes which resemble the in-plane breathing modes of the free molecule, but due to the modified geometry, they acquire a dipole moment along the substrate normal. The positions and relative intensities of these modes are in excellent agreement with the HREELS data obtained in specular direction, giving the first microscopic interpretation of the modified vibrational fingerprint of the adsorbate [1].

[1] F.S. Tautz, S. Sloboshanin, J.A. Schaefer, R. Scholz, M. Sokolowski, V. Shklover, and E. Umbach, Phys. Rev. B **61**, 16933 (2000).