O 2 Organische Dünnschichten I

Zeit: Freitag 10:45–13:00 Raum: TU EB301

O 2.1 Fr 10:45 TU EB301

Investigating the stability of the tetracene/Al_2O_3-interface with high-resolution electron energy loss spectroscopy and LEED — •R. Temirov[1], A. Langner[2], M. Sokolowski[2], and F.S. Tautz[1] — [1]International University Bremen, School of Engineering and Science, PO Box 750761, D-28725 Bremen — [2]Institut für Physikalische und Theoretische Chemie, Universität Bonn, Wegelerstr. 12, D-53115 Bonn

Surprisingly, fluorescence of tetracene molecules in contact with a sapphire substrate is quenched, in spite of the fact that the high band gap of Al_2O_3 should provide an effective barrier to charge delocalisation [1]. The reappearance of luminescence after annealing thin tetracene layers to 240 K can be explained by a reduction of the tetracene/substrate interaction, either by molecular reorientation or dewetting of the interface. Here we report an HREELS investigation of the interface between thin epitaxial Al_2O_3-layers on $Ni_3Al(111)$ and tetracene. Our experiments show that under the current deposition conditions (thermal evaporation onto a sample at T=80K) at least some tetracene molecules are oriented with their molecular plane parallel to the substrate. The maximized contact area between molecule and substrate may be an important factor in understanding the observed luminescence quenching. Our data also suggest that after annealing, contact area is minimized by the formation of three-dimensional tetracene islands. [1] M. Schneider, E. Umbach, A. Langner, M. Sokolowski, Journal of Luminescence 110, 275-283 (2004).

O 2.2 Fr 11:00 TU EB301

Tripod Liganden für starre und geordnete selbstorganisierte Monolagen auf Gold — •T. Weidner[1,2], A. Krämer[3,2], U. Siemeling[3,2] und F. Träger[1,2] — [1]Institut für Physik, Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel — [2]Center for Interdisciplinary Nanostructure Science and Technology - CINSaT, Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel — [3]Institut für Chemie, Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel

Selbstorganisation maßgescheiderter Moleküle auf Oberflächen ist ein verbreitetes und vielversprechendes Konzept, hoch geordnete funktionelle monomolekulare Schichten auf Edelmetalloberflächen zu präparieren. Entscheidend für Anwendungen in Katalyse, Sensorik und Datenspeicherung ist es, eine definierte und stabile Anordnung der funktionellen Einheiten zu gewährleisten.

Um dieses Ziel zu erreichen, haben wir äußerst starre, tripodale Tris[(methylthio)-methyl]silyl Ankergruppen synthetisiert. Untersuchungen der Phenyl- und Biphenylderivate dieser "dreibeinig" aufgebauten Ankergruppe auf Goldsubstraten mit Infrarotspektroskopie und Rastertunnelmikroskopie, sowie der Adsorptions- und Ordnungskinetik mit optischer Frequenzverdopplung und Ellipsometrie zeigen deutlich, dass beide Verbindungen auf Gold adsorbieren. Darüber hinaus konnte die Entstehung sehr stabiler und geordneter Phenyl- und Biphenyl-Monolagen in situ verfolgt werden.

O 2.3 Fr 11:15 TU EB301

Molekulare Magnete auf Oberflächen — •Miriam Klusmann, Andrea Kahlen und Marika Schleberger — Universität Duisburg-Essen, Fachbereich Physik, 45117 Essen

Durch geeignete Präparationstechniken wurden die magnetischen Moleküle Ti4 und Mo72Fe30 auf die Schichtsubstrate Glimmer und HOPG aufgebracht. Untersuchungen mit den Rastersondenmethoden AFM (*Atomic Force Microscopy*, Rasterkraftmikroskopie) und STM (*Scanning Tunneling Microscopy*, Rastertunnelmikroskopie) zeigen eine Ausbildung von Ti4-Inseln auf Glimmer sowie die Selbstorganisation von Mo72Fe30 auf HOPG. Da das Lösungsmittel Dichlormethan, welches zur Deponierung von Ti4 auf Glimmer verwendet wird, einen ungünstigen Einfluss auf das Substrat nimmt, ist eine qualitative Auswertung der aus AFM-Messungen gewonnenen Topographie-Daten nur unter Berücksichtigung der simultan aufgezeichneten Signale der Frequenzverschiebung und der Dämpfung der Cantilever-Oszillation möglich. Die Adsorption von Mo72Fe30 ist abhängig von der Konzentration der Moleküle in Lösung, so dass sich verschiedene Strukturen auf dem HOPG-Substrat ausbilden - von Ringen über Ketten bis hin zu Einfach- oder Mehrfachlagen.

O 2.4 Fr 11:30 TU EB301

Aliphatic selenolates on gold and silver substrates — •Andrey Shaporenko[1], Avi Ulman[2], Andreas Terfort[3] und Michael Zharnikov[1] — [1]Angewandte Physikalische Chemie, Universität Heidelberg, Im Neuenheimer Feld 253, 69120 Heidelberg, Germany — [2]Department of Chemical Engineering, Polytechnic University, Brooklyn 11201, New York, USA — [3]Anorganische und Angewandte Chemie, Universität Hamburg, 20146 Hamburg, Germany

We studied self-assembled monolayers (SAMs) formed from didodecyl diselenide (C12SeSeC12) and didodecyl selenide (C12SeC12) on (111) Au and Ag substrates. C12SeSeC12 was found to form contamination-free, densely-packed, and well-ordered C12Se SAMs on both substrates, whereas the adsorption of C12SeC12 occurred only on Au and resulted in the formation of a SAM-like C12SeC12 film with a low packing density and a conformational disorder. The properties of the C12Se SAMs were compared with those of dodecanethiolate (C12S) SAMs. The packing density, orientational order, and molecular inclination in C12Se/Au and C12S/Au were found to be very similar. In contrast, C12Se/Ag exhibited significantly lower packing density, a lower degree of the conformational and orientational order, and a larger molecular inclination than C12S/Ag. The results suggest a sp^3 bonding configuration for the selenium atom on Au and Ag and indicate a larger corrugation of the headgroup-substrate binding energy surface in C12Se/Ag than in C12S/Ag.

O 2.5 Fr 11:45 TU EB301

Periodical density functional theory study of the bonding of aromatic organic molecules containing carboxylate group on metal surfaces — •Nicolae Atodiresei, Azadeh Farahzadi, Kurt Schroeder, and Stefan Blügel — Institut für Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich, Germany

The family of five-membered heterocycles and its derivates is of basic importance in chemistry and physics. Much work is now undertaken in molecular self-assembly experiments which lead to oriented growth of organic films. We study the structure of adsorbed carboxylic acids containing furan, thiophene, selenophene and tellurophene aromatic rings in a (2x1) cell on Cu(110) surface by ab initio calculations. In the stable configuration the molecules sit perpendicular in bridge position above the first Cu-surface layer with the carboxylate group oriented along to the $[1\bar{1}0]$ direction. In the gas phase the single molecule has a planar geometry with an extended π-system over the five-membered ring and carboxylate group. The adsorption of the molecules breaks this planarity. Due to the strong lateral interactions between the hydrogen atoms of neighboring adsorbed molecules the rings are rotated by $\sim 24°$ relative to the carboxylate group.

O 2.6 Fr 12:00 TU EB301

Growth of thin para-sexiphenyl films on Cu(110) and Cu(110)-(2x1)O — •K. Maschek, Y. Hu, L.D. Sun, M. Hohage, and P. Zeppenfeld — Institut für Experimentalphysik, Johannes-Kepler-Universität Linz, Austria

Para-sexiphenyl (P6P) has attracted considerable interest as a promising candidate for future organic opto-electronic applications. Its molecular structure consists of a linear chain of six linked benzene rings showing strong π bond delocalization in the direction of the chains. Previous research shows that the optical absorption of P6P films depends strongly on the molecular orientation. On the other hand, Reflectance Difference Spectroscopy (RDS) has been demonstrated to be a powerful tool to measure the optical anisotropy at normal incidence. Here, we present a RDS investigation of para-sexiphenyl thin film growth on Cu(110) and Cu(110)-(2x1)O. The RDS spectra show a pronounced anisotropy of the P6P films formed on both substrates at room temperature, indicating preferential orientation of P6P molecules on these two atomically well defined substrates: On Cu(110), the P6P molecular chains align in the $[1\bar{1}0]$ direction, i.e., along the Cu atomic rows, while on the Cu(110)-(2x1)O surface, the molecules align in the orthogonal [001] direction, i.e., along the Cu-O rows formed on Cu(110). Additionally, the evolution of the RDS signal at different photon energies during growth provides detailed information about the growth mode of P6P on both substrates.

O 2.7 Fr 12:15 TU EB301

Ab-initio investigation of organic molecules on metal surfaces:3-nitrothiophen/selenophen/tellurophen on Cu(110) — •Azadeh Farahzadi[1,2], Nicolae Atodiresei[1], Stefan Blügel[1], and Kurt Schroeder[1] — [1]Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich — [2]I.Physikalisches Institut, RWTH-Aachen Sommmerfeldstraße 14, 52074

The future of nanoelectronics may consist in hybrid structures build of organic molecules and inorganic materials. The interesting family of five-member heterocycles which includes thiophen/selenophen/tellurophen rings, plays an important role in constructing the charge carrier polymers. Based on the density functional theory (DFT) in the generalized gradient approximation (GGA), we have optimized the geometric structure of the single molecules, 3-nitrothiophen/selenophene/tellurophen and the dense-packed structure ((2×1) unit cell) of these molecules on the Cu(110) surface. In the stable configuration the molecules sit perpendicular to the surface with the nitro group ($-NO_2$) along the [110] direction. In the gas phase the single molecules have a planar geometry but the adsorption of the molecules breaks this planarity. We discuss the electronic structure and the binding energy of the molecule at the surface. The calculations have been carried out using the PAW-method EStCoMPP.

O 2.8 Fr 12:30 TU EB301

Transfer and amplification of chirality in hydrocarbon monolayers — •Karl-Heinz Ernst, Manfred Parschau, Roman Fasel, and Sara Romer — Empa-Materials Science and Technology, 8600 Duebendorf, Schweiz

We present a new form of chirality transfer and amplification observed in two-dimensional monolayers. In the first case, a special surface enantiomorphism is observed via STM after adsorption of the enantiomers of a helical aromatic hydrocarbon on Cu(111) at 50 K. Instead of crystallization into homochiral domains on the surface, racemic mirror domains are observed, i.e., they possess an equimolar content of left- and right-handed molecules. In this situation, a small excess of one chiral species is sufficient to create domains of a single handedness throughout the whole surface layer. In the second case, homochirality was induced in monolayers of achiral molecules after chiral doping. Achiral molecules can become chiral when adsorbed at surfaces because of the reduced symmetry in the molecule or the adsorbate lattice. Adsorbed on Cu(110), succinic acid forms equal numbers of left- and right-handed domains and the surface is globally achiral. Doping with small amounts of left- or right-handed tartaric acid, however, creates homochirality and the opposite mirror domains are not observed anymore in the LEED pattern. Our findings are explained by cooperative interactions and will be discussed in the frame of a one-dimensional random-field Ising model.

O 2.9 Fr 12:45 TU EB301

STM investigations of ordered monolayers of tetralactam macrocycles on Au(111) — •Iordan Kossev and Moritz Sokolowski — Institut für Physikalische und Theoretische Chemie, Universität Bonn, Wegelerstr. 12, 53115 Bonn, Germany

Rotaxanes and catenanes are of interest for the investigation on mechanically interlocked molecules [1]. A large tetralactam - macrocycle (905.05 amu), very often used as a building block for catenanes, was deposited onto the Au(111) surface in UHV from a thermal evaporation cell. STM images were taken for different coverages at room temperature. At a coverage around one monolayer, different long range ordered monolayer structures were observed with submolecular resolution on the terraces. After annealing to 400 K, in addition to the two dimensional structures, chains of well ordered molecules adsorbed at step edges were observed. We explain these STM images by structure models based on a weak interaction of the molecules to the Au(111) surface and a considerable intermolecular interaction due to hydrogen bonds. The macrocycles were kindly supplied by C. Schalley and F. Vögtle. This work was supported by the DFG (SFB 624).

[1] C. A. Schalley, K. Beizai, F. Vögtle, Acc. Chem. Res. 34 (2001) 465.