cyclic voltammetry. Simultaneous monitoring of the absorption spectra of the films reveals nearly reversible electrochromic behavior after some conditioning cycles caused by an irreversible structural change. Only one reduction and reoxidation peak can be observed. Different isosbestic points in different potential ranges indicate different reduced species. Electroneutrality of the films is preserved by intercalation of Li^+ ions. The influence of different film thickness and sweep rates on the cyclic voltammetry and spectral changes has been investigated. Due to the electron withdrawing effect of the substituents the redox potential is found to be shifted by about 0.2 V for $F_{64}PcCu$ towards more positive potentials relative to $F_{16}PcCu$. An increase of intermolecular coupling in $F_{16}PcCu$ compared with $F_{64}PcCu$ is concluded from an observed spectral broadening of the Q-band.

DS 43.3 Fri 12:00 H2

Monitoring photooxidation of acetone on TiO_2(110) using IR spectroscopy — •Youkun Gao[1], Mingchun Xu[1], Yuemin Wang[1], and Christof Wöll[2] — [1]Lehrstuhl für Physikalische Chemie I, Ruhr-Universität Bochum, 44801 Bochum, Germany — [2]Institut für Funktionelle Grenzflächen (IFG), Karlsruher Institut für Technologie, 76021 Karlsruhe, Germany

The photochemistry on semiconductor TiO_2 surfaces has recently received enormous attention from both fundamental and technological perspectives because of its extensive applications related to energy conversion and other associated processes with environmental impact. There is much interest in the heterogeneous photooxidation of acetone on TiO_2. Whereas acetone photooxidation has been extensively studied on TiO_2 powder samples there is, due to experimental difficulties, a general lack of information on single-crystal surfaces. In this work, we report the first IR studies of acetone photoreactions on the TiO_2(110) surface using reflection-absorption infrared spectroscopy (RAIRS). Exposing TiO_2 to acetone at 110 K leads to molecular (associatve) adsorption, forming mono- and multilayers. The dark reaction of acetone with oxygen molecules on this TiO_2 surface leads to the formation of η^2- diolate species. Irradiation with UV light leads to a conversion of this species to acetate via methyl radical ejection. Furthermore, we found that carbonate/bicarbonate is the final oxidation product after extended exposure to UV light. Finally, the quantum yield and photo-reaction cross section Q for photo-induced oxidation of acetone on differently modified TiO_2(110) surfaces were determined.

Topical Talk DS 43.4 Fri 12:15 H2

Molecular orientation in phthalocyanine films assessed by combined optical and magneto-optical investigations — •Georgeta Salvan[1], Michael Fronk[1], Björn Bräuer[1,2], Dietrich R. T. Zahn[1], Oliver G. Schmidt[3], and Jens Kortus[4] — [1]Chemnitz University of Technology, Physics Department, D-09107 Chemnitz, Germany — [2]SIMES Center, SLAC National Accelerator Laboratory, Stanford University, Stanford, CA 94309, USA — [3]Institute for Integrative Nanosciences, IFW Dresden, Helmholtzstr. 20, 01069 Dresden, Germany — [4]TU Bergakademie Freiberg, Theoretical Physics Department, D-09596 Freiberg, Germany

Magneto-optical Kerr effect (MOKE) is commonly used to study the magnetic properties of inorganic ferromagnetic layers or magnetic nanostructures. For the example of phthalocyanine thin films it will be shown that also paramagnetic and diamagnetic molecules can exhibit a strong MOKE signal in the visible to near ultraviolet spectral range. A numerical analysis of the energy dispersion of the real and imaginary part of the complex magneto-optical Kerr rotation angle and of the optical constants allows the determination of the magneto-optical material constant, the so-called Voigt constant. For phthalocyanines this is only about two orders of magnitude smaller compared to soft ferromagnetic materials such as Ni. The magnitude of the Voigt constant is found to be highly sensitive to the orientation of the molecules with respect to the substrate plane. This opens new possibilities to accurately determine the molecular orientation in organic thin films.

DS 43.5 Fri 12:45 H2

Environment-friendly photolithography using poly-(N-isopropylacrylamide)-based thermoresponsive photoresists — •Leonid Ionov[1], Nikolay Puretskiy[1], Georgy Stoychev[1], Svetlana Zakharchenko[1], Stefan Diez[2], and Manfred Stamm[1] — [1]Leibniz-Institut fuer Polymerforschung Dresden e.V., Dresden, Germany — [2]Max-Planck-Institute of Molecular Cell Biology and Genetics, Dresden, Germany

We report a novel approach for the temperature-triggered development of water-soluble photoresists based on photocleavable poly-(N-isopropylacrylamide) copolymers. These copolymers are soluble in aqueous environment below their Lower Critical Solution Temperature (LCST). Upon UV irradiation, the photocleavable groups are deprotected resulting in an increased LCST. Thus, the illuminated parts of spin-coated copolymer layers dissolve at higher temperatures than the surrounding areas, leading to pattern development. The photoresist can finally be completely removed at low temperature. We demonstrate the applicability of this novel photolithographic approach by the patterning of fluorescent proteins.

DS 43.6 Fri 13:00 H2

Avidin immobilization on mixed monomolecular template prepared by irradiation promoted exchange reaction — Nirmalya Ballav[1], Andreas Terfort[2], and •Michael Zharnikov[1] — [1]Angewandte Physikalische Chemie, Universität Heidelberg, 69120 Heidelberg, Germany — [2]Institut für Anorganische und Analytische Chemie, Goethe-Universität Frankfurt, Germany

An applicability of irradiation-promoted exchange reaction (IPER) to the fabrication of mixed self-assembled monolayers (SAMs) comprised of the protein-repelling matrix and moieties bearing binding sites for specific attachment of a target protein is demonstrated. As test systems, we took mixed films of oligoethyleneglycol (OEG) substituted alkanethiols (OEG-ATs) and biotin-substituted alkanethiols (BATs) on Au(111). Such SAMs are suitable for specific immobilization of avidin and its variants. The SAM composition was precisely controlled by varying the irradiation dose, which is a prerequisite for the fabrication of the respective patterns by electron-beam lithography. While the general trend in the immobilization of avidin onto the mixed OEG-AT/BAT SAMs prepared by IPER was found to be consistent with the earlier reports regarding the analogous films fabricated by the co-assembly method, the concentration of the BAT component in the mixed SAMs needed for the maximum surface coverage of the specific protein was found to be lower and the maximum avidin coverage higher in the case of IPER than for the co-assembly method. We ascribe these differences to the lack of phase segregation and better separation of the BAT species in the OEG-AT matrix in the case of IPER.

DS 43.7 Fri 13:15 H2

Structural Characterization of Self-assembled Monolayers of Pyridine-terminated Thiolates on Gold — •Jinxuan Liu[1], Björn Schüpbach[2], Asif Bashir[3], Osama Shekhah[1], Alexei Nefedov[1], Martin Kind[1], Andreas Terfort[2], and Christof Wöll[4] — [1]Lehrstuhl für Physikalische Chemie I, Ruhr-Universität Bochum, 44780 Bochum, Germany — [2]Institut für Anorganische und Analytische Chemie, Goethe-Universität Frankfurt am Main, 60325 Frankfurt, Germany — [3]Interface Chemistry and Surface Engineering, Max-Planck-Institut für Eisenforschung, 40237 Düsseldorf, Germany — [4]Institute of Functional Interfaces, Karlsruhe Institute of Technology (KIT), 76021 Karlsruhe, Germany

Self-assembled monolayers (SAMs) on Au from a homologous series of four pyridine-terminated organo thiols have been investigated using a variety of surface-analytical techniques (IR, XPS, NEXAFS, STM) and DFT calculations. For all pyridine-terminated thiols the immersion of Au-substrates in the corresponding ethanolic solutions was found to result in the formation of highly ordered and densely packed SAMs. For an even number of the methylene spacers between the SH group and the aromatic moieties the SAM unit-cell is rather large, $5\sqrt{3} \times 3$, whereas in case of an odd number of methylene units a smaller unit cell is adopted, $2\sqrt{3} \times \sqrt{3}$ R30°. The tilt-angle of the molecules amounts to 15°. In contrast to expectation, the pyridine-terminated organic surfaces exposed by the corresponding SAMs showed a surprisingly strong resistance with regard to protonation.

Topical Talk DS 43.8 Fri 13:30 H2

***In-silico* optimization of function and emissive properties of Silicon nanoparticles** — •Thomas Niehaus — Bremen Center for Computational Materials Science, Bremen, Germany

Excited-state properties of silicon quantum dots (SiQDs) up to diameters of 2 nm are studied using an approximate time-dependent density-functional theory method (TD-DFTB) [1] and compared with available experimental data. Several functionalizations ranging from simple hydrogen passivation up to capping with amine [2], allyamine [3] and propionic acid [4] groups are discussed. Signatures in vibrational and optical absorption spectra are revealed, which show the detailed effect of surface modification of the SiQDs. It is verified that the modification could be expected to not only reduce the surface oxidation rate but also maintain an efficient electronic transition feature