

## O 62: Posters: Surface Reactions and Dynamics, Nanostructures

Time: Wednesday 17:30–21:00

Location: P1

O 62.1 Wed 17:30 P1

**Formation of superhydrogenated PAHs through interaction with atomic hydrogen and hydrogenated carbonaceous grains** — ●JOHN THROWER<sup>1,2</sup>, EMIL FRIIS<sup>1</sup>, ANDERS SKOV<sup>1</sup>, BJARKE JØRGENSEN<sup>1</sup>, LOUIS NILSSON<sup>1</sup>, SAOUD BAUCHE<sup>1</sup>, RICHARD BALOG<sup>1</sup>, and LIV HORNEKAER<sup>1</sup> — <sup>1</sup>Department of Physics and Astronomy, Aarhus University, Aarhus, Denmark — <sup>2</sup>Present Address: Physikalisches Institut, Westfälische Wilhelms-Universität Münster, Germany

Processes occurring on dust grain surfaces play a crucial role in interstellar chemical evolution. In particular, H<sub>2</sub>, the most abundant molecule, is only formed efficiently through surface reactions. Polycyclic aromatic hydrocarbon (PAH) molecules account for up to 10% of the total carbon budget. It has been suggested that in warmer environments, e.g. photodissociation regions (PDRs), PAHs are involved in H<sub>2</sub> formation [1]. Building on previous DFT calculations [2], we present mass spectrometric investigations of the formation of superhydrogenated PAH molecules through H-atom addition to coronene (C<sub>24</sub>H<sub>12</sub>) which reveal abstraction reactions that release H<sub>2</sub> [3]. Furthermore, we demonstrate that hydrogenated graphitic surfaces can act as an addition source of H-atoms that can react with physisorbed PAH molecules, potentially releasing H and H<sub>2</sub> from the grain surface.

[1] E. Habart, F. Boulanger, L. Verstraete, *et al.*, *Astron. Astrophys.*, **414**, 531 (2004).

[2] E. Rauls and L. Hornekær, *Astrophys. J.*, **679**, 531 (2008).

[3] J. D. Thrower, B. Jørgensen, E. E. Friis, *et al.*, *Astrophys. J.*, **752**, 3 (2012).

O 62.2 Wed 17:30 P1

**Thermal desorption spectroscopy of astrophysically relevant molecules on olivine and single crystal forsterite** — ●TUSHAR SUHASARIA<sup>1,2</sup>, NADINE HEMING<sup>1</sup>, ROBERT FRIGGE<sup>1</sup>, BJÖRN SIEMER<sup>1</sup>, and HELMUT ZACHARIAS<sup>1,2</sup> — <sup>1</sup>Physikalisches Institut, University of Münster, Germany — <sup>2</sup>Graduate School of Chemistry, University of Münster, Germany

Chemical surface reactions on dust grains are a possible way of molecule formation in the Interstellar Medium (ISM). These grains typically consist of graphitic and silicate materials. At low temperatures in molecular clouds (T < 20 K) atoms and molecules freeze out and form ices around the dust grains [1]. Temperature programmed desorption (TPD) spectroscopy is an established method to define the binding energies between molecules and surfaces of astronomical interest. We have performed TPD measurements on several molecules like D<sub>2</sub>, CO, CH<sub>4</sub>, CO<sub>2</sub> and NH<sub>3</sub> adsorbed on single crystal forsterite (MgSiO<sub>4</sub>) and olivine (Mg<sub>x</sub>Fe<sub>1-x</sub>SiO<sub>4</sub>) surfaces. We determine the average binding energies, order and pre-exponential factors for such molecules on silicate surfaces and present a comparison of such properties on two silicate surfaces.

[1] Tielens A. G. G. M., 2005, the physics and chemistry of the interstellar medium, Cambridge University Press.

O 62.3 Wed 17:30 P1

**Carbon Dioxide Adsorption in Charged and Uncharged Carbon Nanotube Arrays** — ●MAHSHID RAHIMI<sup>1</sup>, JAYANT K. SINGH<sup>2</sup>, and FLORIAN MÜLLER-PLATHE<sup>1</sup> — <sup>1</sup>Technische Universität Darmstadt, Eduard-Zintl-Institut für Anorganische und Physikalische Chemie, Alarich-Weiss-Str. 4, D-64287 Darmstadt, Germany — <sup>2</sup>Department of Chemical Engineering, Indian Institute of Technology Kanpur, Kanpur-208016, India

Grand-canonical Monte Carlo simulations is carried out to understand the adsorption of CO<sub>2</sub> onto bundles of 3D aligned double-walled charged and uncharged carbon nanotubes of diameter 5 nm at 303 K. The simulation of partial adsorption isotherms, i.e. only inner tube volume, only interstices between tubes, and unrestricted, allow a breakdown of the experimental adsorption isotherms into contributions of different regions. The results for uncharged carbon nanotubes are compatible with microscopic observations of the majority of the inner tube volumes being accessible for CO<sub>2</sub>. Further, the unrestricted adsorption isotherm is quantitatively equivalent to the sum of inner and outer adsorption for the pressure range considered in this work, p < 40 bar, indicating no significant interference between inner and outer regions. The intertube distance, which is varied from 0 to 15 nm, dramatically affects the isosteric heat of adsorption and adsorption ca-

capacity. Excess adsorption is found to display a non-linear behavior with d, for unrestricted and outer cases.

O 62.4 Wed 17:30 P1

**Near ambient pressure XPS investigation of the oxidation and the CO oxidation on Pt(111)** — ●MATHIAS GRABAU<sup>1</sup>, SANDRA KRICK CALDERÓN<sup>1</sup>, LÁSZLÓ ÓVÁRI<sup>2</sup>, HANS-PETER STEINRÜCK<sup>1</sup>, and CHRISTIAN PAPP<sup>1</sup> — <sup>1</sup>Physikalische Chemie II, University of Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen, Germany — <sup>2</sup>MTA-SZTE Reaction Kinetics and Surface Chemistry Research Group, H-6720 Szeged, Rerrich Béla tér 1, Hungary

The oxidation of Pt(111) at oxygen pressures up to 1 mbar was followed *in situ* using (NAP)-XPS at temperatures between 300 and 700 K. The oxidation was found to proceed remarkably at temperatures of 300 and 500 K (oxygen coverage of 1.6 ML after 6 h at 300 K). The analysis of the data revealed varying saturation coverages found *in situ*, indicating a sensitive pressure- and temperature-dependent system. As a follow-up, the oxidation of CO by molecular oxygen on Pt(111) was investigated in the temperature range between 500 and 900 K using different reactant mixtures in continuous flow mode. Considerable reaction was observed at temperatures above 650 K under oxidizing conditions. Reaction onset at lower oxygen ratios was found for higher temperatures. Oxide formation under reaction conditions (T ≥ 650 K) was observed to lead to a lower catalyst activity up to complete inhibition of the CO oxidation reaction.

O 62.5 Wed 17:30 P1

**Microcalorimetric study of the hydrogen-to-water oxidation on solid-state Pt/TiO<sub>2</sub>/Ti emf cells** — ●ÖMER ÇAKABAY, MHAMED EL ACHHAB, and KLAUS SCHIERBAUM — Department of Materials Science, Institute for Experimental Condensed Matter Physics, Heinrich-Heine-University Düsseldorf

We study the hydrogen-to-water oxidation on Pt/TiO<sub>2</sub>/Ti layer structures in which the oxide is grown by a high-voltage electrochemical anodization. By means of microcalorimetry, we determine various kinetic parameters including the film and pore diffusion rates, the turn-over numbers, the activation energies and the reaction orders of hydrogen-to-water oxidation on platinum coated anodized titanium foils. By identifying these parameters, the experimental determination of the mass transport limitations as well as the temperature dependence of the activity of the catalyst are achieved.

O 62.6 Wed 17:30 P1

**CO oxidation at nanoporous gold: TPD, XPS, and DFT study** — SARAH RÖHE, LYUDMILA MOSKALEVA, ANDREAS SCHAEFER, ARNE WITTSTOCK, ●VOLKMAR ZIELASEK, and MARCUS BÄUMER — Institut für Angewandte und Physikalische Chemie, Universität Bremen

Nanoporous gold (np-Au) is an efficient catalyst for CO oxidation, even below RT. To gain insight into relevant mechanisms and surface species, we employed TPD and XPS in UHV directly at np-Au catalyst samples which were produced by leaching of silver from AgAu alloy and then activated for CO oxidation in a continuous-flow reactor. Supported by DFT calculations, the experiments indicate that the catalytic activity is based on a complex interplay of gold, silver, CO, and several oxygen species on and within the np-Au surface.

Residual silver is crucial for the ability of np-Au to chemisorb molecular oxygen, resulting in presumably atomic oxygen (O<sub>act</sub>) at the surface available for CO oxidation. TPD after exposing np-Au to CO at 105 K shows pronounced CO and CO<sub>2</sub> desorption at temperatures above 200 K, indicating an additional, more stable type of CO binding sites on np-Au as compared to pure gold. Only CO at these binding sites is oxidized by O<sub>act</sub>. DFT calculations demonstrate that the strong binding of CO to np-Au cannot be explained by the presence of silver residues. It can be conceived, however, that it is induced by the formation of O-Au-CO complexes at low-coordinated surface sites. In fact, besides silver and O<sub>act</sub>, we find various resident oxygen species on and within the np-Au surface. Their presence may be as crucial for the catalytic activity of np-Au as residual silver.

O 62.7 Wed 17:30 P1

**Electron dynamics of the topological insulator Sb<sub>2</sub>Te<sub>2</sub>S** — ●SOPHIA KETTERL<sup>1</sup>, THOMAS KUNZE<sup>1,2</sup>, THORSTEN U. KAMPEN<sup>2</sup>,

EVGENY CHULKOV<sup>3</sup>, and MARTIN WEINELT<sup>1</sup> — <sup>1</sup>FU Berlin, Germany — <sup>2</sup>SPECS GmbH, Germany — <sup>3</sup>UPV/EHU San Sebastian, Spain

The strength of the electron-phonon coupling in topological insulators is currently debated. Both strong and weak coupling constants have been reported [1,2].

We investigate the electron dynamics of the p-doped  $Sb_2Te_2S$  via time-resolved two-photon photoemission measurements with an angle-resolving time-of-flight spectrometer. p-doped  $Sb_2Te_2S$  exhibits a Dirac cone above the Fermi energy. In our experiment, the Dirac cone is populated by an infrared pump-pulse via direct absorption and interband scattering from the conduction band. In the Dirac cone we observe lifetimes on the picosecond timescale. The spectra hint at a stepwise relaxation via small-energy transfer processes. Cooling of the system leads to faster electron dynamics. This dynamics will be discussed in light of electron-electron and electron-phonon scattering.

[1] R. C. Hatch *et al.*, *Phys. Rev. B* **83**, 241303 (2011).

[2] Z.-H. Pan *et al.*, *Phys. Rev. Lett.* **108**, 187001 (2012).

O 62.8 Wed 17:30 P1

**Laser-triggered miniaturized electron gun for ultrafast low-energy electron diffraction** — ●GERO STORECK, SIMON SCHWEDA, MAX GULDE, SASCHA SCHÄFER, and CLAUDIUS RÖPERS — IV. Physical Institute, University of Göttingen, 37077 Göttingen, Germany

The time-resolved analysis of structural dynamics at surfaces will yield insight into a rich class of previously inaccessible effects, which are unique to quasi-two-dimensional systems. A main experimental challenge in the realization of optical pump/ electron probe schemes is the generation of short electron pulses at low energies and their undispersed propagation to the sample. Nanometric photocathodes were recently suggested to minimize spatial and temporal broadening and have been successfully implemented in a time-resolved diffraction experiment in a transmission geometry [1].

Here, we present the development of a compact pulsed electron gun for time-resolved low-energy electron experiments in backscattering diffraction. This will provide for a novel and versatile tool in ultrafast surface science.

[1] M. Gulde *et al.* (submitted).

O 62.9 Wed 17:30 P1

**Electronic surface structure of Au/Ge(001) and comparison with the pure Ge(001) substrate studied by 2PPE** — KRISTOF ZIELKE, ●KAMIL BOBOWSKI, CORNELIUS GAHL, and MARTIN WEINELT — Fachbereich Physik der Freien Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

For submonolayer gold coverage Au/Ge(001) has been shown to form nanowires which exhibit properties typical for a one-dimensional Luttinger liquid [1]. We have investigated the electronic structure of the Au/Ge(001) surface in dependency of gold coverage and annealing temperature by two-photon photoemission spectroscopy (2PPE). While the surface states  $D_{up}$  and  $D_{down}$  of the clean Ge(001) surface are suppressed upon gold adsorption, a new unoccupied state appears about 800 meV above  $E_F$  at normal emission. Additionally, time resolved investigations show a significant decrease in excited state lifetimes.

[1] C. Blumenstein *et al.*, *J. Phys.: Condens. Matter* **25**, 014015 (2013).

O 62.10 Wed 17:30 P1

**Exploring hot electron dynamics in the layered semiconductor 2H-MoS<sub>2</sub> by time- and angle-resolved photoelectron spectroscopy** — ●PETRA HEIN, KERSTIN HANFF, GERALD ROHDE, ANKATRIN STANGE, MICHAEL BAUER, LUTZ KIPP, and KAI ROSSNAGEL — Institute of Experimental and Applied Physics, University of Kiel, Germany

Pump-probe experiments with ultrashort pulses delivered by femtosecond laser systems provide important insights into the dynamics of condensed matter on fundamental time scales. In particular, high-harmonic extreme ultraviolet pulses can be used to investigate the temporal evolution of the electronic structure after excitation with an optical pump pulse. Previous time-resolved photoemission studies on layered transition-metal dichalcogenides (TMDCs) have focused on the dynamics of charge-density-wave and Mott insulating phases [1]. Here, we concentrate on the photo-induced electron dynamics in semiconducting TMDCs, with the indirect bandgap semiconductor

2H-MoS<sub>2</sub> serving as a model system. Specifically, we study the relaxation processes of the photo-excited electrons in dependence of the pump fluence, energy, and polarization. We also report the effects of alkali metal intercalation on the band structure and electron dynamics. Possible similarities of surface-intercalated 2H-MoS<sub>2</sub> and monolayer 2H-MoS<sub>2</sub> are discussed.

[1] S. Hellmann *et al.*, *Nat. Commun.* **3**, 1069 (2012).

O 62.11 Wed 17:30 P1

**Attosecond time resolved photoemission on solid surfaces** — ●SERGEJ NEB, FABIAN MERSCHJOHANN, PETER BARTZ, MATTHIAS HENSEN, CHRISTIAN STRÜBER, NORBERT MÜLLER, WALTER PFEIFFER, and ULRICH HEINZMANN — Universität Bielefeld, Universitätsstr. 25, 33615 Bielefeld

The availability of single attosecond (as) XUV pulses allows investigating ultrafast electron dynamics on the as time scale. For a (110) tungsten surface Cavalieri *et al.* reported that the photoemission from tungsten 4f states is delayed by about 100 as with respect to the electron emission from the valence band [1]. The physical origin of this delay is not yet understood and controversial theoretical models coexist. Further as-time-resolved photoemission studies using other surfaces help to resolve this controversy.

Here we report on as-time-resolved photoemission from a van-der-Waals crystal that exhibits a completely different electronic structure. XUV pulses with about 300 as duration are generated by high harmonic generation in a Ne target using 5 fs IR laser pulses with stable carrier-envelope phase. The layered structure of the investigated solid yields element specific photoelectrons emitted from different depth and thus helps resolving the physical origin of temporal delays in photoemission.

[1] A.L.Cavalieri *et al.*, *Nature* **449**, 1029 (2007)

O 62.12 Wed 17:30 P1

**Time- and angle-resolved XUV ARPES at sub-15 fs temporal resolution** — ●GERALD ROHDE, ARNE HENDEL, LEXIAN YANG, ANKATRIN STANGE, KERSTIN HANFF, CHRISTIAN SOHRT, LUTZ KIPP, KAI ROSSNAGEL, and MICHAEL BAUER — Institut für Experimentelle und Angewandte Physik der Christian-Albrechts-Universität zu Kiel

Time- and angle-resolved photoelectron spectroscopy (trARPES) provides a most direct access to ultrafast electronic processes in condensed matter systems. Application of XUV photon pulses generated in High-Harmonic Generation (HHG) light sources allows probing transient electronic structure within the entire Brillouin zone and beyond [1]. Typically, it is the pump pulse that limits the time-resolution of such experiments to values of  $\geq 30$  fs so that extremely fast phenomena such as characteristic melting times of electronic phases [2] or the thermalization of a nascent electron distribution [3] may remain unresolved.

Here we present a HHG-based trARPES setup exhibiting a substantially improved time-resolution. The optical pump-line of the experiment is operated using sub-6 fs pulses at a center wavelength of about 800 nm as generated in an amplifier-driven hollow-fiber chirped-mirror compressor. In the contribution, details of the compressor optimization procedure and its integration into the existing trARPES setup are described. First trARPES measurements on 1T-TiSe<sub>2</sub> are shown providing direct experimental evidence for a sub-15 fs time-resolution.

[1] T. Rohwer *et al.*, *Nature* **471**, 490 (2011)

[2] S. Hellmann *et al.*, *Nature Communications* **3**, 1069 (2012)

[3] G. Rohde *et al.*, *Eur. Phys. J.-Spec. Top.* **222**, 997 (2013)

O 62.13 Wed 17:30 P1

**Investigating Very Low Energy Electron Transmission through Thin Metallic Films** — ●DANIEL PANZER and GERD SCHÖNHENSE — Institut für Physik, Johannes-Gutenberg Universität, 55128 Mainz

The inelastic mean free path of electrons in matter is strongly energy dependent (it increases steeply at low energies  $<20$ eV [1]), and spin sensitive [2,3]. In the present work we use an imaging system that projects an electron optical image from a thermal or photoemitter onto an ultrathin metallic film and then watch the transmitted electrons using a standard Photo Emission Electron Microscope (PEEM) column. This allows for a wide range of combinations of different emitters and thin films. Thermionic emitters like BaO and Y<sub>2</sub>O<sub>3</sub> provide high intensity to rate transmission for thicker sample films or multi-layer systems. Threshold photoemission provides a smaller emission energy width to better evaluate transmission of samples like Au, Pt and Pd at different kinetic energies. A pulsed photoemitter in combination with a delay line detector facilitates time-of-flight measurements to distin-

guish between different scattering processes. A uniformly magnetized ferromagnetic film should eventually enable spin-filtering an electronic image coming from a spin-polarized photoemitter.

References:

- [1] M.P. Seah, W.A. Dench, Surf. a. Interface Analysis (1979), 1(1):2.
- [2] W. Weber, S. Riesen, H.C. Siegmann, Science 291 (2001), 1015
- [3] P. Dey, W. Weber, J. Phys.: Condens. Matter 23 (2011), 473201

O 62.14 Wed 17:30 P1

**Dynamical Study of Electron Transfer in Alkanethiolate Self-Assembled Monolayers Adsorbed at the Au(111) Surface** — ●VERONIKA PRUCKER<sup>1</sup>, PEDRO B. COTO<sup>1</sup>, ÓSCAR RUBIOPONS<sup>1</sup>, MICHEL BOCKSTEDTE<sup>1</sup>, HAOBIN WANG<sup>2</sup>, and MICHAEL THOSS<sup>1</sup> — <sup>1</sup>Institut für Theoretische Physik, Interdisziplinäres Zentrum für Molekulare Materialien (ICMM), Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstr. 7/B2, D-91058 Erlangen, Germany — <sup>2</sup>Department of Chemistry and Biochemistry, MSC 3C, New Mexico State University, Las Cruces, New Mexico 88003, USA

In this contribution, we present a dynamical ab-initio study of electron transfer (ET) in a series of self-assembled monolayers consisting of nitrile substituted short-chain alkanethiolate molecules on gold substrates. Employing a model Hamiltonian, which is parametrised by first principles electronic structure calculations [1], and dynamical simulations, we analyse the main factors underlying the ET process. In accordance to experiments [2,3], we demonstrate the dependence of the ET process on the molecular chain length and on the symmetry of the donor state, which allows to control the electron injection times even in the case of nearly degenerate donor states [4]. Additionally, we discuss the influence of electronic-vibrational coupling on the ET process.

- [1] I. Kondov *et al.*, J. Phys. Chem. C 111, 11970 (2007).
- [2] F. Blobner *et al.*, J. Phys. Chem. Lett. 3, 436 (2012).
- [3] P. Kao *et al.*, J. Phys. Chem. C 114, 13766 (2010).
- [4] V. Prucker *et al.*, J. Phys. Chem. C, accepted (2013).

O 62.15 Wed 17:30 P1

**Femtosecond time-resolved two-photon photoemission spectroscopy of C<sub>6</sub>H<sub>5</sub>F/Cu(111)** — ●ISHITA AGARWAL, ISABELLA AVIGO, MANUEL LIGGES, PING ZHOU, and UWE BOVENSIEPEN — Faculty of Physics, University of Duisburg-Essen, Duisburg

The electron dynamics at a metal-organic interface is studied with two-photon photoemission (2PPE) spectroscopy. We report here binding energies, band dispersion, and lifetimes of unoccupied metal-molecular interface states for up to 3 monolayers (ML) of mono-fluorobenzene (C<sub>6</sub>H<sub>5</sub>F) adsorbed on Cu(111). For all coverages, an unoccupied electronic state with a binding energy of  $3.67 \pm 0.05$  eV above the Fermi level ( $E_F$ ) was found. In addition, between 1 and 2 ML, a second unoccupied feature with a binding energy of  $3.54 \pm 0.05$  eV above  $E_F$  was observed. Using angle-resolved spectroscopy the band dispersion of these unoccupied states was studied and an effective mass of  $(0.76 \pm 0.20) \times m_e$  and  $(0.8 \pm 0.2) \times m_e$  was found, respectively. Time-resolved 2PPE measurements indicate an ultrashort lifetime of about 10 fs. Overall, the observations resemble previous coverage dependent 2PPE studies of C<sub>6</sub>F<sub>6</sub>/Cu(111)[1] and C<sub>6</sub>H<sub>6</sub>/Cu(111)[2] which suggest a structural influence on the unoccupied electronic structure at the interface. Funding by the DFG through BO1823/5-1 is gratefully acknowledged.

- [1] D.Velic, *et al.*, J. Chem. Phys., **109**, 9155, (1998)
- [2] C.Gahl, *et al.*, Faraday Discuss., **117**, 191, (2001)

O 62.16 Wed 17:30 P1

**Spin Effects in Ultrafast Charge Transfer Measurements on Ar/Co Interfaces using a TOF-Mott-Polarimeter** — ●TOBIAS SAUNDERMANN<sup>1</sup>, NORBERT MÜLLER<sup>1</sup>, ULRICH HEINZMANN<sup>1</sup>, JOHANNES BAUER<sup>2</sup>, RUNYUAN HAN<sup>2</sup>, PETER FEULNER<sup>2</sup>, and WILFRIED WURTH<sup>3</sup> — <sup>1</sup>Molecular and Surface Physics, Bielefeld University — <sup>2</sup>Physik-Department E20, TU München — <sup>3</sup>Physik-Department, University of Hamburg

Using the principle of the core hole clock method [1] the spin dependent charge transfer is studied from resonantly excited physisorbed Ar atoms into an in plane magnetized Co adlayer on W(110). For exciting the  $Ar2p_{3/2} \rightarrow 4s$  resonance circularly as well as linearly polarized synchrotron radiation of energy  $h\nu = 244.55\text{eV}$  is used (BESSY beamline UE56/II PGM2, single bunch mode). Emitted electrons are energy and spin analyzed by means of a TOF spectrometer followed by a spherical Mott polarimeter [2] operated in retarding mode at 45 keV

scattering energy. Excitation by circularly polarized radiation results in a spin polarization up to  $35\% \pm 5\%$  of the Auger electrons following the decay of the excited oriented Ar  $2p_{3/2}$  holes. With excitation by linearly polarized radiation smaller spin polarization effects appear for autoionization emission channels. These effects result from a spin dependent charge transfer from excited unpolarized Ar 4s states to empty Co conduction band states with minority spin preferred.

- [1] D. Menzel, Chem. Soc. Rev., 37 (2008)
- [2] G. Snell *et al.*, Phys. Rev. Lett. 76, 3923 (1996)

O 62.17 Wed 17:30 P1

**Circular dichroism of the unoccupied topological surface state of SnSb<sub>2</sub>Te<sub>4</sub>** — ●SEBASTIAN OTTO and THOMAS FAUSTER — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, D-91058 Erlangen, Germany

Time- and angle-resolved two-photon photoemission is used to study the electronic structure and dynamics at the surface of SnSb<sub>2</sub>Te<sub>4</sub>. Circular dichroism is used to map the spin structure of the topological surface state. Due to the intrinsic p-doping the topological surface state is centered at  $0.32 \pm 0.03$  eV above the Fermi level with a group velocity of  $3.4$  eVÅ. The circular dichroism pattern of the Dirac cone shows a strong dependence on the polarization of the probe pulse while the polarization of the pump pulse has no significant effect. This stands in good agreement with time-resolved measurements showing a transient population of the topological surface state dominated by refilling from the conduction band minimum.

O 62.18 Wed 17:30 P1

**Structured hetero-material nanorod arrays** — ●ERIC JEHNES, VERA HOFFMANN, FABIAN PATROVSKY, MATTHIAS BÖHM, and LUKAS M. ENG — Institute of Applied Photophysics, TU Dresden, D-01062 Dresden, Germany

Metal nanorod arrays grown in anodic aluminium oxide (AAO) show distinct plasmonic resonances [1] that cover a wide range of future applications - for instance in optical sensors, biosensors, nanoantennas, waveguides, etc.. In order to improve their applicability additional structuring is needed both laterally, horizontally and radially.

We show such an approach by laser interference lithography, electrochemical deposition and multiple etching steps. Our processing results in core-shell and segmented nanorods composed of gold, silver, cobalt and/or nickel. The lateral structuring creates nanorod arrangements of dense lines covering a large area.

- [1] R. Kullock *et al.*, J. Opt. Soc. Am. B, 27, 1819

O 62.19 Wed 17:30 P1

**Tunable Silicon Nanowire Arrays Based on A New Method to Transfer Large Area of Ultra-Thin Alumina Membranes** — ●AHMED AL-HADDAD<sup>1,2</sup>, RANJITH VELLACHERI<sup>1</sup>, SAMAR TARISH<sup>1,2</sup>, YAN ZHENG<sup>1</sup>, LIAOYONG WEN<sup>1</sup>, YANG XU<sup>1</sup>, and YONG LEI<sup>1</sup> — <sup>1</sup>Institute for Physics and IMN MacroNano (ZIK), Ilmenau University of Technology, Prof. Schmidt Str. 26, 98693 Ilmenau, Germany. — <sup>2</sup>Department of Physics, College of Science, The University of Mustansiriyah, Baghdad, Iraq.

A new effective method was developed to transfer large area ultra-thin alumina membrane (UTAM) with Au thin film as supporting layer to Si wafer. UTAM was prepared by a two-step anodization of aluminum foil with controllable thicknesses (100-400nm), followed by the transportation to Si wafer using a special cell and the removal of the backside Al and barrier Al<sub>2</sub>O<sub>3</sub> layer. Several drops of DI water were added on Si before placing the UTAM to increase the adhesion between UTAM and Si surface. Furthermore, ordered Au nanodots arrays on Si surface were obtained by physical vapor deposition of Au with a thickness of 20 nm, which could be further used for. Moreover, the obtained Au grid from supporting UTAM was used for metal-assisted chemical etching to fabricate Si nanowires arrays. Furthermore, the structure and surface morphology were examined by Raman spectroscopy and scanning electron microscopy, respectively.

O 62.20 Wed 17:30 P1

**Structuring of nanorods for sensing applications** — ●RICO EISSMANN, ANDREAS HILLE, and LUKAS M. ENG — Institut für Angewandte Photophysik, Technische Universität Dresden, D-01062 Dresden, Germany

Metal nanorod arrays are elegant for various sensing applications. The fabrication of nanorod arrays is an established technique. [1] In this study graded nanorod arrays, having a variably tuned rod diameter,

are investigated. In combination with integrating such graded nanorod arrays on CCD/CMOS chips it allows for very small sensor applications.

The optical and plasmonic properties of those graded nanorod arrays are calculated with the multiple multipole method [2]. The distinct plasmonic behavior of nanorods with different geometric parameters (volume, rod length and distance) allows to use them as an optical filter on light-sensitive electronic devices, and moreover to record spectrally selected wavelengths.

[1] P. Evans et al. Growth and properties of gold and nickel nanorods in thin film alumina. doi:10.1088/0957-4484/17/23/006

[2] C. Hafner. Post-modern Electromagnetics: Using Intelligent Maxwell Solvers. John Wiley & Sons, New York, 1999

O 62.21 Wed 17:30 P1

**C<sub>60</sub> fullerenes on noble gas layers (Ar/Xe): Photoelectron spectroscopy with ultraviolet light** — ●DOMINIK WOLTER, CHRISTOPH SCHRÖDER, NATALIE MIROSLAWSKI, and HEINZ HÖVEL — Fakultät Physik / DELTA, Technische Universität Dortmund, 44221 Dortmund, Germany

We have investigated C<sub>60</sub> clusters deposited and measured at temperatures between 10 K and 13 K on 60 monolayers of xenon (Xe) with 10 monolayers of argon (Ar) on top using ultraviolet photoelectron spectroscopy. The noble gas layers were adsorbed at 45 K (Xe) and 10 K (Ar) on copper(111), silver(111) and gold(111) substrates. To get a well ordered surface the first layer of each gas was adsorbed at slightly higher temperatures (75 K for Xe and 25 K for Ar). We used an Ar-gas discharge lamp ( $h\nu = 11.6$  eV) with a heatable LiF-window to suppress the satellite lines [1]. To extract the signal of the fullerenes we measured the spectra for the rare gas covered substrate before deposition and subtracted them from measurements after the deposition. The observed shift of the C<sub>60</sub> spectra depending on substrate and the noble gas layers is of importance for the interpretation of UPS on mass selected metal clusters on similar surfaces.

[1] M. Budke and M. Donath, Appl. Phys. Lett. **92**, 231918 (2008); S. Suga, et al., Rev. Sci. Instruments **81**, 105111 (2010)

O 62.22 Wed 17:30 P1

**Simulations with FEFF of XANES spectra on Ag clusters deposited in PDMS and silica aerogel** — ●STEFANIE ROESE, DAVID ENGEMANN, and HEINZ HÖVEL — Fakultät Physik / DELTA, Technische Universität Dortmund, 44227 Dortmund

For many applications of clusters such as catalysis the knowledge of geometrical structure, size and electronic properties is essential.

Depositing Ag clusters produced in a supersonic expansion into silica aerogel or PDMS can prevent the clusters from coalescence. Silica aerogel is a very porous compound of SiO<sub>2</sub> nanoparticles containing up to 99 % empty space. PDMS is a polymer in which the clusters are dispersed by deposition.

The L<sub>2</sub> and L<sub>3</sub> edge of the Ag clusters is investigated with XANES carried out at the synchrotron radiation sources ESRF (ID 26) and DELTA (BL 8).

The experimental data are compared to ab initio multiple scattering calculations [1] for different cluster sizes and structures. The calculations include information about the geometric and electronic structure of the deposited clusters and also about their chemical environment. We examine cluster structures modeled with a Gupta potential [2] and compare the calculated XANES spectra to the measured ones.

The focus is here on the number of next neighbors and the next-neighbor distances to investigate the geometrical structure of the Ag clusters.

[1] J. J. Rehr et al., Phys. Chem. Chem. Phys., **12**, 5503-5513 (2010)

[2] W. Huang et al., Chem. Phys. Lett., **507**:199-202 (2011)

O 62.23 Wed 17:30 P1

**Optical measurements and simulations for cluster plasmons in various environments** — ●DAVID ODENTHAL, DAVID ENGEMANN, and HEINZ HÖVEL — Fakultät Physik/DELTA, Technische Universität Dortmund, 44227 Dortmund

The research on clusters, consisting from a few up to some hundreds silver atoms, shall shed light on their behaviour compared to a solid-state body or a single atom. Positioning clusters into various environments is necessary to apply their special properties, for instance their reactivity in catalysis.

To investigate the properties of clusters on surfaces, various amounts of clusters were deposited into silica aerogel (chem. SiO<sub>2</sub>). Aerogel is a highly porous compound which contains mainly air (up to 99

vol.-%) and it is highly transparent for the wavelengths used in the experiments. The samples were irradiated with light ranging from ultraviolet to visible, so that cluster plasmons [1] were excited and the extinction spectrum was recorded. The results were then compared with theoretical models, so that physical variables like the thickness of a surrounding shell could be determined.

[1] U. Kreibig and M. Vollmer. *Optical Properties of Metal Clusters*. Springer-Verlag Berlin Heidelberg, 1995.

O 62.24 Wed 17:30 P1

**Two-photon photoemission spectroscopy: The effect of cluster superlattices on the electronic structure of Ir(111)/graphene** — ●KIRA JOCHMANN, FLORIAN KNALL, and THORSTEN M. BERNHARDT — University of Ulm, Institute of Surface Chemistry and Catalysis, 89069 Ulm, Germany

A single graphite layer - namely graphene - supported by a metal crystal surface provides an ideal template for the ordered growth of regular cluster nanostructures with equally spaced and sized clusters. The ability to synthesize such ideal model systems opens completely new opportunities for fundamental research.

Two-photon photoemission (2PPE) spectroscopy is a method to experimentally gain an insight into the unoccupied electronic structure of these systems. The rather high work function of an iridium single crystal surface decreases with increasing graphene coverage, which enables the possibility to detect image potential state electrons by 2PPE at a laser wavelength of 266 nm [1].

In this contribution we report the influence of an Ir cluster superlattice on the overall workfunction and the image potential states, observed on the Ir(111)/graphene system as a function of Iridium coverage. Furthermore the influence of these nanostructures on the lifetime of the image potential states can be monitored by the means of time-resolved 2PPE.

[1] D. Niesner, Th. Fauster, J. I. Dadap, N. Zaki, K. R. Knox, P.-C. Yeh, R. Bhandari, R. M. Osgood, M. Petrović, M. Kralj, Phys. Rev. B **85**, 081402 (2012).

O 62.25 Wed 17:30 P1

**Initial growth of heteromolecular layers studied by LEEM** — ●CAROLINE HENNEKE, DANIEL SCHWARZ, JONAS VAN BEBBER, and CHRISTIAN KUMPF — Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany, and Jülich Aachen Research Alliance (JARA)-Fundamentals of Future Information Technology

One crucial issue for the performance of organic materials in electronic devices is the ability to specifically design the interfaces between different active layers according to their functional purpose. Heteromolecular films are of highest interest in this context, in particular their initial growth and the structure formation of the first molecular layer since this layer acts as a template for further growth.

We have investigated a prototypical donor-acceptor system containing copper-II-phthalocyanine (CuPc) and 3,4,9,10-perylene-tetracarboxylic-acid dianhydride (PTCDA) molecules adsorbed in mixed films on low-index noble metal surfaces. Kinetic processes like thin film growth, the formation of the organic mixed layer, and the transitions between different phases were studied in real time with LEEM. The lateral structure of the different phases was investigated with LEED.

O 62.26 Wed 17:30 P1

**Simulation of angle-resolved photoemission cross-sections for organic/metal interfaces** — ●DARIO KNEBL, DANIEL LÜFTNER, BERND KOLLMANN, and PETER PUSCHNIG — Karl-Franzens-Universität Graz, Institut für Physik

Several combined experimental / theoretical investigations have demonstrated a close relation between the angle-resolved photoemission (ARPES) intensity of oriented organic molecular films and the Fourier transform of the molecular orbital. So far, experimental ARPES data has been accounted for by neglecting the interaction of molecule with the underlying metal substrates. The remaining small differences have been tentatively attributed to modifications of the molecular states due to molecule-substrate hybridization, though alternative explanations, e.g., light polarization effects or the failure of the simple plane-wave final state approximation could not be excluded. Here we calculate ARPES intensity maps for the prototypical PTCDA/Ag(110) interface by explicitly considering molecule-substrate interactions within ab-initio density functional calculations. In order to take into account the free mean path of photo-emitted

electrons, we modify the final state plane wave by introducing an exponential decay term of the final state. We perform careful convergence studies with respect to the number of metallic layers and the number of k-points, and compare our results to ARPES measurements. Thereby, we shed light on the molecule-metal hybridization and reveal limitations of the plane-wave final state approximation for such molecular films.

O 62.27 Wed 17:30 P1

**STM investigations of functional platform adlayers on Au(111) surfaces** — ●ANDREAS BLOEDORN<sup>1</sup>, SONJA KUHN<sup>1</sup>, FRAUKE CLAUSSEN<sup>1</sup>, ULRICH JUNG<sup>1</sup>, SANDRA ULRICH<sup>2</sup>, RAINER HERGES<sup>2</sup>, and OLAF MAGNUSSEN<sup>1</sup> — <sup>1</sup>Institut für Experimentelle und Angewandte Physik, Universität Kiel, 24098 Kiel, Germany — <sup>2</sup>Otto Diels-Institut für Organische Chemie, Universität Kiel, 24098 Kiel, Germany

Functionalized adsorbate layers are of great interest for advanced nanosystems containing molecular switches, motors, or light harvesting systems. We employ triazatriangulenium (TATA) [1,2,3] or trioxatriangulenium (TOTA) [4] ions for attaching functional molecules to a metal surface. These molecular platforms can be functionalized at the central carbon atom as well as by alkyl side chains. Using this versatile concept, it is possible to control the orientation and distance of the functional group with respect to the surface and the intermolecular distance.

Here, detailed STM investigations of TATA adlayers with alkyl side chains from propyl to dodecyl on Au(111) surfaces are presented, showing that the favoured hexagonal superstructure varies with the alkyl chain length. Furthermore, results on functionalized TATA derivatives containing azobenzene derivatives or porphyrins are shown.

This work was supported by the Deutsche Forschungsgemeinschaft via SFB 677.

[1] Baisch et al., *J. Am. Chem. Soc.* (2009), 131, 442. [2] Kuhn et al., *PCCP* (2010), 12, 4481. [3] Kubitschke et al., *Eur. J. Org. Chem.* (2010), 5041. [4] Kuhn et al., *Chem. Commun.*, (2011), 47, 8880-8882.

O 62.28 Wed 17:30 P1

**Self-assembled molecular triangles with a central pillar unit pointing towards the third dimension** — ●STEFAN-SVEN JESTER, ANNA JOCHEMICH, EVA SIGMUND, and SIGURD HÖGER — Universität Bonn, Kekulé-Institut für Organische Chemie und Biochemie, Gerhard-Domagk-Str. 1, 53121 Bonn, Germany

Shape-persistent molecular triangles with an intraannular unit pointing towards the third dimension are designed, synthesized and investigated. The molecules self-assemble at the solution/solid interface on HOPG to form highly ordered patterns. *In situ* scanning tunneling microscopy gives an insight into the driving forces for supramolecular self-assembly. The molecular design and substitution pattern is consistent with our previously published set of molecular triangles, squares, pentagons, and hexagons. [1] Consequent with our expectation, the intraannular substituted triangular molecules mix with the hexagons to form periodic cocrystals. [1] S.-S. Jester, E. Sigmund, S. Höger *J. Am. Chem. Soc.* **2011**, 133, 11062.

O 62.29 Wed 17:30 P1

**IV-Analysis of organic adsorbates investigated by MCP-LEED** — ●INA KRIEGER<sup>1</sup>, OLIVER BAUER<sup>1</sup>, GEORG HELD<sup>2</sup>, and MORITZ SOKOLOWSKI<sup>1</sup> — <sup>1</sup>Institute for Physical and Theoretical Chemistry, University of Bonn, Wegelerstraße 12, 53115 Bonn, Germany — <sup>2</sup>University of Reading, Department of Chemistry, Whiteknights, Reading, RG6 6AD, UK

OVER the last years, the adsorption geometries of some large aromatic molecules on metal surfaces could be determined by the normal incidence wave technique (NIXSW). However, NIXSW is rather elaborate and requires synchrotron radiation. In addition, any substrate reconstruction is difficult to access by NIXSW. Hence we investigate whether LEED-IV analysis, the conventional method for the determination of adsorption sites of adsorbates, is suitable for this purpose. We have chosen PTCDA on Ag(100) as a test systems, because this adsorption geometry had been determined in detail by NIXSW and DFT before [1]. We find reasonable agreement of experimental and theoretical IV curves and support for the surface buckling predicted by DFT. In addition, we discuss current problems of the experiment and the theoretical evaluation. Supported by the DFG.

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O 62.30 Wed 17:30 P1

**First Steps Towards Anchoring Large Functional Organic Molecules on MgO(100)** — ●QURATULAIN TARIQ, MICHAEL RÖCKERT, MATTHIAS FRANKE, HANS-PETER STEINRÜCK, and OLE LYTKEN — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, 91058 Erlangen, Egerlandstraße 3, Germany

The emerging field of organic/oxide interfaces has a huge scientific and technological potential in molecular electronics, solar energy conversion, catalysis or sensor development. At the microscopic level, however, oxide bonding sites, interaction mechanisms, bonding geometries and structure formation processes at organic/oxide interfaces are among the most poorly understood and least controlled aspects of such systems. Controlled growth of nanostructured films requires selective bonding between particular linker groups and specific surface sites. Such linkers may also generate a defined molecular contact to larger functional molecular entities such as porphyrins or fullerenes. By an appropriate choice of the linker groups, the bonding sites, orientation, density and ordering of such systems could in principle be controlled. In present study, we will be investigating the surface interactions, thermal stability and transformations of the benzonitrile (C<sub>6</sub>H<sub>5</sub>-CN) and catechol (C<sub>6</sub>H<sub>4</sub>(OH)<sub>2</sub>) on MgO(100) thin films on Ag(100) as a function of temperature and coverage, by means of x-ray photoemission spectroscopy (XPS) and temperature programmed desorption (TPD).

O 62.31 Wed 17:30 P1

**Highly strained bicyclophanes on HOPG** — GABI OHLENDORF<sup>1</sup>, CHRISTIAN W. MAHLER<sup>1</sup>, ●STEFAN-S. JESTER<sup>1</sup>, GREGOR SCHNAKENBURG<sup>2</sup>, STEFAN GRIMME<sup>3</sup>, and SIGURD HÖGER<sup>1</sup> — <sup>1</sup>Universität Bonn, Kekulé-Institut für Organische Chemie und Biochemie, Gerhard-Domagk-Str. 1, 53121 Bonn, Germany — <sup>2</sup>Universität Bonn, Institut für Anorganische Chemie, Gerhard-Domagk-Str. 1, 53121 Bonn, Germany — <sup>3</sup>Universität Bonn, Mulliken Center for Theoretical Chemistry, Institut für Physikalische und Theoretische Chemie, Beringstrasse 4, 53115 Bonn, Germany

Architectures with aromatic units aligned perpendicularly to the graphite surface are rarely observed but may become of interest when functionalization towards the volume phase is desired. Recently, our group reported on a convenient synthesis of complex phenyl substituted *p*-phenylene oligomers without the need of common transition metal catalyzed cross-coupling reactions requiring complex protective group strategies. Based on these oligophenylenes, bicyclic components are obtained in very good yields. As confirmed by state-of-the-art DFT calculations, the molecules have a planar bicyclic unit with a perpendicular center which seems to be a promising structural unit to reach the purpose of three-dimensional growth on surfaces. Self-assembled monolayers of the bicyclophanes at the solid/liquid interface of 1-phenyloctane and HOPG are visualized by scanning tunneling microscopy (STM). [1] G. Ohlendorf, C. W. Mahler, S.-S. Jester, G. Schnakenburg, S. Grimme, S. Höger *Angew. Chem. Int. Ed.* **2013**, 125, 12308.

O 62.32 Wed 17:30 P1

**Adsorption Dynamics of Tetrahydrofuran on Si(001)** — ●MARCUS LIPPONER<sup>1</sup>, MICHAEL DÜRR<sup>1,2</sup>, and ULRICH HÖFER<sup>1</sup> — <sup>1</sup>Fachbereich Physik, Philipps-Universität Marburg — <sup>2</sup>Institut für Angewandte Physik, Justus-Liebig-Universität Giessen

The functionalization of semiconductor surfaces by means of organic molecules is of great interest due to possible applications in the field of nanoelectronics. However, only little information is available on the reaction dynamics of organic molecules on semiconductor surfaces. Recent STM/XPS experiments from our group have shown that tetrahydrofuran (THF), which is a cyclic ether molecule and is used as a typical organic solvent, shows a complex surface chemistry on Si(001). These experiments suggest that initial reaction with the silicon surface occurs via an electron lone pair of the oxygen atom by forming a dative bond with the lower atom of the Si dimer.

On this poster, we show results from molecular beam experiments of THF on Si(001): With increasing kinetic energy of the impinging molecules, we find a decrease of the initial sticking coefficient as it is typical for a non-activated reaction channel. However, the decrease is much less pronounced than e.g. in the case of C<sub>2</sub>H<sub>4</sub>/Si(001), pointing towards a more efficient energy dissipation in the case of THF/Si(001). With increasing surface temperature a decrease of the initial sticking coefficient is observed, which gives information on the energetics of the datively bound intermediate state.