

## O 90: Surface Dynamics: Experiments

Time: Thursday 10:30–12:45

Location: WIL C107

O 90.1 Thu 10:30 WIL C107

**Adsorption Dynamics of Methanol on Si(001) Studied by Means of Molecular Beam Techniques** — ●TAMAM BOHAMUD<sup>1</sup>, MARCEL REUTZEL<sup>1</sup>, MICHAEL DÜRR<sup>1,2</sup>, and ULRICH HÖFER<sup>1</sup> — <sup>1</sup>Philipps-Universität, 35037 Marburg — <sup>2</sup>Justus-Liebig-Universität, 35392 Giessen

Understanding the reaction of organic molecules on semiconductor surfaces is a fundamental step on the way to hybrid structures with high functionality. For this reason, the adsorption of organic molecules with different functional groups on silicon surfaces has been studied in detail. In most cases, the adsorption dynamics are governed by a metastable intermediate state [1,2]. For methanol, such an intermediate state was also proposed but could not be observed experimentally yet.

In this contribution, we make use of molecular beam experiments to investigate the adsorption dynamics of methanol on Si(001). The initial sticking probability  $s_0$  was measured both as a function of surface temperature and kinetic energy of the impinging molecules. It was found that  $s_0$  decreases with increasing surface temperature, indicating adsorption via an intermediate state. The dependence of  $s_0$  on the kinetic energy of the incoming molecules deviates from a simple non-activated adsorption behavior. This is discussed both in terms of strong coupling between intermediate and final state as well as in terms of additional reaction channels accessible at higher kinetic energy.

[1] M. Lipponer et al., Chem. Phys. Lett. 624, 69 (2015)

[2] M. Lipponer et al., Surf. Sci. 651, 118 (2016)

O 90.2 Thu 10:45 WIL C107

**Surface-morphology transition between step-flow growth and step bunching** — ●KONRAD BELLMANN<sup>1</sup>, UDO W. POHL<sup>1</sup>, ALEXANDER SABELFELD<sup>1</sup>, CHRISTIAN KUHN<sup>1</sup>, TIM WERNICKE<sup>1</sup>, and MICHAEL KNEISSL<sup>1,2</sup> — <sup>1</sup>Technische Universität Berlin, Institute of Solid State Physics — <sup>2</sup>Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, Berlin

Epitaxially grown opto-electronic devices rely on smooth interfaces with step-flow morphology. The surface-morphology transition between step-flow growth and step bunching will be theoretically discussed by comparing two different boundary conditions to solve the differential equation for surface diffusion. Favored smooth surfaces rely on vicinal terraces which are characterized by a mean terrace width and terrace-edge conditions. An energy diffusion-barrier at the terrace edge, the Ehrlich-Schwöbel barrier, influences the adatom incorporation towards the lower terrace edge. The first approach simply considers an asymmetric equilibrium adatom-density at the edges which offers a simple analytic morphology transition relation. The second more-physical approach considers an asymmetric adatom-incorporation flux at the edges. Both approaches yield a similar qualitative behavior. However, the morphology transition does not only rely on the two adatom-incorporation rates at the edges and the surface diffusion, but also on the adatom-mean resident time on the surface. Finally, the morphology transition between step-flow growth and step bunching is experimentally confirmed by homoepitaxial growth of AlN.

O 90.3 Thu 11:00 WIL C107

**On the reduction behavior of CeO<sub>2</sub> (100) and (111) surfaces** — ●JOHANNA HACKL<sup>1</sup>, TOMAS DUCHOŇ<sup>2</sup>, DAVID NIKOLAUS MÜLLER<sup>1</sup>, DANIEL MARIUS GOTTLÖB<sup>3</sup>, IMTIAZ KHAN<sup>1</sup>, STEFAN CRAMM<sup>1</sup>, SLAVOMIR NEMŠÁK<sup>1</sup>, and CLAUDIUS MICHAEL SCHNEIDER<sup>1</sup> — <sup>1</sup>Peter Grünberg Institut PGI-6, Forschungszentrum Jülich, Germany — <sup>2</sup>Department of Surface and Plasma Science, Charles University in Prague, Czech Republic — <sup>3</sup>SPEC, CEA, CNRS, Université Paris Saclay, F-91191 Gif-sur-Yvette, France

Ceria has an ability to store and release oxygen by changing its oxidation state reversibly between CeO<sub>2</sub> and Ce<sub>2</sub>O<sub>3</sub>. This gives ceria unique catalytic properties with many applications. DFT calculations predict a strong dependence of oxygen vacancy formation energies for different CeO<sub>2</sub> surface orientations. Particularly the (100) surface is expected to have a lower oxygen vacancy formation energy than the (111) surface. In the present work CeO<sub>2</sub> islands with (111) and (100) surfaces are simultaneously grown in-situ onto a Cu (111) substrate. The island formation is observed and characterized with low energy electron

microscopy (LEEM) and micro-LEED. Using laterally resolved x-ray absorption spectroscopy (XAS) performed in a photoemission electron microscope (PEEM) the partial reduction of CeO<sub>2</sub> to Ce<sub>2</sub>O<sub>3</sub> in an H<sub>2</sub> environment is observed in-situ and in real-time, directly comparing the reduction kinetics of the (111) and the (100) islands. Spectra of the Ce M5 edge show a more pronounced reduction state of cerium for the (100) islands. This behavior can be connected to a higher catalytic activity of CeO<sub>2</sub> (100) for some types of the oxidizing reactions.

O 90.4 Thu 11:15 WIL C107

**Surface Phase Behavior of [PPh<sub>4</sub>][Tf<sub>2</sub>N] / Cs[Tf<sub>2</sub>N]- and [PPh<sub>4</sub>][Tf<sub>2</sub>N] / Ni[Tf<sub>2</sub>N]<sub>2</sub> Low-Temperature Molten Salt Mixtures** — PATRICK SCHREIBER<sup>1</sup>, MARLENE SCHEUERMEYER<sup>2</sup>, ●RADHA G. BHUIN<sup>1</sup>, PETER WASSERSCHIED<sup>2</sup>, HANS-PETER STEINRÜCK<sup>1</sup>, and FLORIAN MAIER<sup>1</sup> — <sup>1</sup>Lehrstuhl für Physikalische Chemie II, FAU, Erlangen, Germany — <sup>2</sup>Lehrstuhl für Chemische Reaktionstechnik, FAU, Erlangen, Germany

We report on surface investigations using a new class of organic/inorganic molten salt mixtures based on a [PPh<sub>4</sub>][Tf<sub>2</sub>N] compound. Depending on composition, these mixtures combine low melting points with exceptionally high thermal stability, and thus, exhibit considerably enlarged reaction windows compared to conventional ionic liquids.[1] To elucidate their surface behavior, temperature-dependent angle-resolved XPS investigations were performed using our unique spectrometer DASSA (Dual Analyzer System for Surface Analysis).[2] The DASSA comprises an UHV chamber equipped with two electron analyzers for simultaneous electron detection at 0° and 80°. We follow temperature-induced changes in bulk and surface composition for mixtures of [PPh<sub>4</sub>][Tf<sub>2</sub>N]/Cs[Tf<sub>2</sub>N] and [PPh<sub>4</sub>][Tf<sub>2</sub>N]/Ni[Tf<sub>2</sub>N]<sub>2</sub>. Interestingly, the Cs-containing mixture in the liquid state favors the presence of [Cs]<sup>+</sup> at the surface on expense of the bulky [PPh<sub>4</sub>]<sup>+</sup> ions. RGB and HPS thank the ERC for financial support through an Advanced Investigator Grant to HPS. References: [1] Scheuermeyer et al., New J. Chem., 40, 7157, 2016. [2] Niedermaier et al., Rev. Sci. Instrum., 87, 045105, 2016.

O 90.5 Thu 11:30 WIL C107

**The effect of chemical pressure on Ag<sup>+</sup> cation substitution in CdSe nanocrystals** — ●URKO PETRALANDA, LUCA DE TRIZIO, LIBERATO MANNA, and SERGEY ARTYUKHIN — Istituto Italiano di Tecnologia, Via Morego 30, Genova (Italy)

Cd<sup>2+</sup> cations in CdSe nanocrystals experience, at ambient conditions, a fast and total replacement by Ag<sup>+</sup> cations when exposed to the latter in an appropriate solvent [1,2]. A promising mechanism proposed to describe the cation exchange (CE) reactions is the so called kick-out mechanism [3,4], where the exchanged ions are considered to diffuse through interstitials. Within this framework, we use a tight binding model based on ab initio calculations to investigate the effect of chemical pressure on the CE reaction energy barrier and discuss the role played by different energy contributions.

[1] E. M. Chan, M. A. Marcus, S. Fakra, M. ElNaggar, R. A. Mathies, A. P. Alivisatos, J. Phys. Chem. A, 111, 12210 (2007). [2] L. De Trizio, L. Manna, Chem. Rev. 116, 10852 (2016). [3] U. Gösele, W. Frank, A. Seeger, Appl. Phys. 23, 361 (1980). [4] F. D. Ott, L. L. Spiegel, D. J. Norris, S. C. Erwin, Phys. Rev. Lett. 113, 156803 (2014).

O 90.6 Thu 11:45 WIL C107

**Surface explosion of tartaric acid diastereomers on a Cu(111) surface in ultrahigh vacuum** — ●ALEXANDRA RIEGER and KARL-HEINZ ERNST — Nanoscale Materials Science, Swiss Federal Laboratories for Materials Testing and Research (EMPA), Überlandstrasse 129, CH-8600 Dübendorf, Switzerland

Tartaric acid (TA) comes as three diastereomers: the two enantiomers L-TA and D-TA as well as the achiral meso form m-TA. We have studied the adsorption of m-TA, L-TA and the racemic mixture of L- and D-TA on a Cu(111) and on a Pd(110) surface. Using thermally desorption spectroscopy (TDS), we have investigated the thermally induced auto-catalytic decomposition reaction, the so-called surface explosion, which leads to decomposition into carbon dioxide, water and hydrogen within a very narrow temperature interval. This allows identification of structural differences in the monolayer of the isomers. X-ray pho-

toelectron spectroscopy was used in order to identify the adsorption mode as a function of coverage. Using low-energy electron diffraction (LEED), we have investigated how the molecules self-assemble on a Cu(111) and on a Pd(110) surface.

O 90.7 Thu 12:00 WIL C107

**Photodesorption of CO from Si(100)** — ●MICHAEL LACKNER, DANIEL LUCASSEN, and ECKART HASSELBRINK — Universität Duisburg-Essen, Fakultät für Chemie, 45141 Essen

Velocity distributions of photodesorbed molecules can provide substantial insights into the desorption dynamics.

CO adsorbed on Si(100) is desorbed by a pulsed UV laser (266/355 nm). Time of flight spectra of these desorbed CO molecules are measured with a mass spectrometer, yielding velocity distributions. We observe at least two desorption channels. The yield in these solely depends on photon wavelength.

Furthermore cross sections were determined by a similar measurement setup. Here, the total signal decays double exponentially and depends on photon exposure.

O 90.8 Thu 12:15 WIL C107

**Kinetic controlled hierarchical self-assemblies of all-trans-retinoic acid on Au(111)** — ●CHAO LI and YONGFENG WANG — Key laboratory for the physics and chemistry of nanodevices, Department of Electronics, Peking University, Beijing 100871, China

Kinetic controlled hierarchical self-assemblies of all-trans-retinoic acid on Au(111) are investigated by low-temperature scanning tunneling microscopy (STM) in ultra-high vacuum. The dominant molecular hierarchical superstructure can be selectively controlled to dimer,

tetramer, or pentamer patterns, which are stabilized by hydrogen bonds and vdW interactions.

O 90.9 Thu 12:30 WIL C107

**A test experiment to determine the long term behaviour of surface work functions** — ●MATTHIAS WECKER and KATRIN COLLABORATION — Karlsruhe Institute of Technology (KIT), ITeP/TLK, Postfach 3640, 76021 Karlsruhe

The Karlsruhe Tritium Neutrino (KATRIN) experiment aims to determine the effective mass of neutrinos with a sensitivity of  $200 \text{ meV}/c^2$  (90% C.L.). This requires the precise measurement of the  $\beta$ -spectrum from tritium-decay close to the endpoint at 18.6 keV. The energy is analysed with the Main Spectrometer, a electrostatic high-pass filter with a filter width of 0.93 eV. The filter voltage of 18.6 kV has to be known with 60 mV accuracy. Thus, the plasma potential in the windowless gaseous tritium source (WGTS), where the  $\beta$ -electrons are produced, has to be known with the same precision. The rear end of the WGTS is electrically terminated by the Rear Wall, a gold-coated stainless steel disk. Superconducting solenoids around the beam-pipes produce a strong magnetic field (3.6 - 6 T) that guides the  $\beta$ -electrons to the spectrometer. The field also connects the plasma in the WGTS with the Rear Wall. Thus, inhomogeneities and fluctuations in the potential of the Rear Wall directly translate into an uncertainty of the WGTS potential, thus limiting the ultimate sensitivity of KATRIN. Exposure to ambient air before its subsequent operation in vacuum can lead to such changes of the work function. This talk introduces a new experiment at KIT for the in-situ determination of the work function. Initial results will be presented. We acknowledge the support of KSETA, the BMBF (05A14VK2) and the Helmholtz Association.