

HL 83: Focus Session: Functionalization of Semiconductors II

Organizers: Kerstin Volz, Sangam Chatterjee (Universität Marburg), Michael Dürr (Universität Giessen)

Time: Thursday 14:45–17:15

Location: H16

Invited Talk

HL 83.1 Thu 14:45 H16

Electronic properties and applications of functionalized wide gap semiconductors — ●MARTIN STUTZMANN — Walter Schottky Institut and Physics Department, Technical University of Munich, 85748 Garching, Germany

Wide band gap semiconductors such as SiC, GaN and diamond are well suited for applications in bioelectronics and photochemistry due to their stability, their particular surface chemistry, and the possibility to change their work function by surface termination, alloying, or substitutional doping. In addition, inorganic, organic or biological surface functionalization can be used to enhance the specific properties for the targeted application. In this presentation we will review some recent examples of such applications: specific enzyme-based biosensors, the detection of cellular action potentials with electrolyte-gated field effect transistors, bio-photovoltaics with supported bacterial reaction centers, and the electronic control of photocatalytic reactions.

HL 83.2 Thu 15:15 H16

Frequency Conversion Properties of SnS-Clusters — ●NILS W. ROSEMAN¹, JENS EUSSNER², ULRICH HUTTNER¹, ANDREAS BEYER¹, KERSTIN VOLZ¹, STEPHAN W. KOCH¹, MACKILLO KIRA¹, STEFANIE DEHNEN², and SANGAM CHATTERJEE¹ — ¹Faculty of Physics and Materials Science Center, Philipps-Universität Marburg, Renthof 5, D-35032 Marburg, Germany — ²Faculty of Chemistry and Materials Sciences Center, Philipps-Universität Marburg, Hans-Meerwein-Straße, D-35043 Marburg, Germany

Clusters based on at least one element of the chalcogenide family exhibit a large variety of physical properties. These arise mainly due to their diverse assembly of the cluster atoms resulting in highly complex electronic landscapes. Hence, such materials are expected to show an intriguing linear response and even more so significant nonlinear optical properties. Here, we present a SnS-based cluster that exhibits an extreme optical nonlinearity.

30 min. Coffee Break

HL 83.3 Thu 16:00 H16

Functionalization of III/V semiconductor surfaces with small organic molecules — ●PATRICK VOGT — Institut für Festkörperphysik, TU Berlin, Hardenbergstr. 36, 10623 Berlin; Germany.

Hybrid materials consisting of interfaces between organic layers and solid semiconductors form the basis for novel applications in sensing, biophysics and nanotechnology. The understanding of the fundamental properties that determine the interaction between organic materials and semiconductor surfaces, however, is still insufficient. This presentation summarizes our current understanding of the functionalization of differently reconstructed, carefully prepared GaAs, InP and GaP (001) surfaces with organic reagents. The functionalization is characterized by x-ray photoelectron spectroscopy, scanning tunneling microscopy, and by reflectance anisotropy spectroscopy in a spectral range between 1.5 and 5 eV.

HL 83.4 Thu 16:30 H16

Diethyl Ether on Si(001) - An Experimental Study on Adsorption Configurations and Energy Barriers — ●MARCEL REUTZEL¹, GERSON METTE¹, MARCUS LIPPONER¹, MICHAEL DÜRR^{1,2}, and ULRICH HÖFER¹ — ¹Philipps-Universität, 35037 Marburg — ²Justus-Liebig Universität, 34392 Gießen

The functionalization of semiconductor surfaces with organic molecules has attracted much interest, especially with respect to the challenges arising from the miniaturization in semiconductor device physics. It is thus important to understand the basic adsorption processes of different functional groups on these surfaces.

Here, we present an experimental study of the adsorption config-

urations and the underlying potential energy curve of diethyl ether on Si(001): At low temperature, diethyl ether adsorbs in a datively bonded intermediate state, as observed by means of STM and XPS experiments. By thermal activation, the ether is cleaved; covalently attached Si-C₂H₅ and Si-O-C₂H₅ fragments are observed on two neighboring dimer rows [*J. Phys. Chem. C* **119**, 6018 (2015)]. Using optical second-harmonic generation, the surface mediated ether cleavage reaction was followed in realtime. Conversion rates were measured as a function of surface temperature; the barrier $\epsilon_a = 0.38 \pm 0.05$ eV ($\nu_a = 10^{4 \pm 1}$ s⁻¹) was determined. Using molecular beam techniques, the initial sticking probability was measured as a function of surface temperature. From the difference between binding energy ϵ_d and conversion barrier ϵ_a , the binding energy $\epsilon_d = 0.62 \pm 0.08$ eV ($\nu_d = 10^{7 \pm 1.3}$ s⁻¹) was determined [*J. Phys. Chem. Lett.* **6**, 3971 (2015)].

HL 83.5 Thu 16:45 H16

Ab initio study on precursor reactivity in CVD growth: GaP on Si — ●ANDREAS STEGMÜLLER and RALF TONNER — Fachbereich Chemie, Philipps-Universität, 35032 Marburg

Successful growth of high-quality III/V semiconductor materials via CVD or MOVPE is (kinetically) constrained by precursor decomposition chemistry and transport.[1] As *in situ* experimental evidence is scarce DFT calculations were applied being an important means to grasp elementary processes during growth.

The molecular reactivity of commonly applied precursors triethylgalane (TEGa), tertiary butylphosphine (TBP) and higher homologues was screened and fundamental mechanisms were elucidated.[2,3] The insight gained can be utilized to optimize the decomposition behaviour by chemical design in order to reduce energy barriers and, thus, growth temperatures necessary for growth of metastable materials.[4] The influence of the Si substrate on precursor decomposition was investigated for various alkyl compounds of groups 13 and 15 (III/V) applying periodic models of the hydrogen-passivated Si(001)H surface.

[1] A. Brauers, *J. Cryst. Growth*, **107**, 281-289, 1991.

[2] Andreas Stegmüller et al., *Phys. Chem. Chem. Phys.*, **16**, 17018-17029, 2014.

[3] Andreas Stegmüller et al., *Inorg. Chem.*, **54**, 6363-6372, 2015.

[4] Andreas Stegmüller et al., *Chem. Vap. Depos.*, **21**, 161-165, 2015.

HL 83.6 Thu 17:00 H16

In situ controlled MOVPE-preparation of As-modified Si(100) surfaces and single-domain GaP heteroepitaxy — ●OLIVER SUPPLIE^{1,2}, MATTHIAS M. MAY^{1,2}, AGNIESZKA PASZUK¹, ANDREAS NÄGELEIN¹, PETER KLEINSCHMIDT¹, SEBASTIAN BRÜCKNER^{1,2}, and THOMAS HANNAPEL^{1,2} — ¹TU Ilmenau, Institut für Physik, FG Photovoltaik — ²HZB, Institute Solar Fuels

III-V/Si(100) tandem absorber structures are promising for high-efficiency direct solar watersplitting [1]. MOVPE-processing commonly involves arsenic, either supplied directly via precursors or in form of residuals. Annealing of Si(100) in TBAs and background As results in an As-modified surface with a characteristic reflection anisotropy spectroscopy (RAS) signal. We show that its spectral features emerge at different stages of a two-step annealing process. LEED patterns of the final surface show a preferential A-type, (1 × 2) reconstructed surface with dimer rows in parallel to the step edges. These are also clearly visible in STM images. XPS evidences the presence of As at the surface, but also atomic exchange across the interface. Subsequent pseudomorphic GaP heteroepitaxy leads to single-domain GaP/Si(100) surfaces, which are free of antiphase disorder. The sublattice orientation of the GaP film is inverted compared to GaP grown on H-terminated Si [2]. The atomic structure of the heterointerface is more complex than in the abrupt Si-P case [3] for As-free systems.

[1] M. M. May et al., *Nat. Commun.* **6**, 8256 (2015).

[2] O. Supplie et al., *Phys. Rev. B* **90**, 235301 (2014).

[3] O. Supplie et al., *J. Phys. Chem. Lett.* **6**, 464 (2015).