O 30: Phenomena at Semiconductor Surfaces

Time: Tuesday 12:00–14:00 Location: MA 041

O 30.1 Tue 12:00 MA 041

Vibrational relaxation of CO stretching excitation on Si(100): DFT study — •Sung Sakong and Peter Kratzer — Fachbereich Physik, Universität Duisburg-Essen, Duisburg, Germany

On semiconductor and insulator surfaces, the vibrational lifetime of adsorbates can be very long and the vibrational energy is predominantly dissipated to phonons, because electron-hole pair excitations are not allowed. Recently, the lifetime of the CO stretch vibration on Si(100) has been measured to be 2.3 nano seconds (Laß *et al.*, J. Chem. Phys. **123** 051102 (2005)).

We have performed density functional theory calculations within the framework of the generalized gradient approximation for the energy dissipation of the CO vibrational mode on the Si(100) surface. In this scheme, the vibrational relaxation is controlled by the anharmonic coupling between vibrational modes and the interaction between vibrations and phonons. In DFT, vibrational excitations of the adsorbate are accurately described by the multi-dimensional potential energy surface which includes anharmonic coupling between vibrations. And the phonon properties of the underlying Si substrate are calculated with the force field method to treat a large slab. From this information, the coupling between anharmonic vibrations and the phonon continuum is calculated within perturbation theory, thus the transition rate is derived by Fermi's Golden Rule. The calculated lifetime is in qualitative agreement with the experiments and the suggested microscopic decay channels of the stretching mode of C-O into lateral shift/bending quanta and a phonon satisfy energy conservation.

O 30.2 Tue 12:15 MA 041

Cyclopentene (C5H8) on InP(001)(2x4): adsorption structure — •R. Passmann[1,2], P. Favero[3], T. Bruhn[1,2], W. Braun[4], W. G. Schmidt[5], M. Kneissl[1], W. Richter[6], N. Esser[1,2], and P. Vogt[1] — [1]TU Berlin, Institut für Festkörperphysik, Hardenbergstr. 36, 10623 Berlin, Germany — [2]ISAS - Institute for Analytical Sciences, Department Berlin, Albert-Einstein-Str. 9, 12489 Berlin, Germany — [3]Instituto de Física da Universidade de Brasília, Brazil — [4]BESSY GmbH, Albert-Einstein-Str. 15, 12489 Berlin, Germany — [5]Universität Paderborn, Warburger Str. 100, 33098 Paderborn, Germany — [6]Universita Tor Vergata, Via della Ricerca Scientifica 1, 00133 Roma, Italy

In this study we report on the modification of the InP(001)(2x4) surface upon C5H8 exposure, observed by reflectance anisotropy spectroscopy (RAS), synchrotron based PES (SXPS) and LEED. The samples were prepared in ultra high vacuum and the reconstruction formation was controlled by LEED and RAS. The characteristic features at 1.8 eV in the RAS spectra related to the InP(2x4) surface is reduced during the deposition of the molecules and shifted towards higher photon energies. SXPS measurements of the C1s, In4d and P2p core level confirm a covalent bonding of the C5H8 molecules to the top In-P mixed dimer. The molecules can be desorbed at 400°C and the (2x4) reconstruction can be restored. The comparison to DFT total energy calculations supports an interaction between C5H8 and the top-layer dangling bonds. From these results a structural model for the absorption of C5H8 on the InP(2x4) surface is proposed.

O 30.3 Tue 12:30 MA 041

Adsorption of small organic ring molecules on GaAs(001) c(4x4) - Structural and electronic properties — •T. Bruhn[1,2], R. Passmann[1,2], C. Friedrich[1], G. Gavrila[3], T.A. Nilsen[5], W. Braun[4], D.R.T. Zahn[3], B.O. Fimland[5], W. Richter[6], M. Kneissl[1], N. Esser[1,2], and P. Vogt[1] — [1]TU Berlin, Institut für Festkörperphysik, Hardenbergstr.36, 10623 Berlin, Germany — [2]ISAS Berlin, Albert-Einstein-Str.9, 12489 Berlin, Germany — [3]TU Chemnitz, Institut für Physik, 09107 Chemnitz, Germany — [4]BESSY GmbH, Albert-Einstein-Str.15, 12489 Berlin, Germany — [5]NUST, NO-7491 Trondheim, Norway — [6]Universita Tor Vergata, Via della Ricerca Scientifica 1, 00133 Roma, Italy

For a selective implementation of functional organic units in semiconductor devices, a detailed understanding of the electronic and structural properties of the interface is indispensable. In a first step, we have investigated the influence of the adsorption of small ring molecules (Cyclopentene (C_5H_8) and 1,4-Cyclohexadiene (C_6H_8)) on the GaAs $c(4 \times 4)$ surface. The samples were prepared in UHV and investigated with reflectance anisotropy spectroscopy (RAS), soft x-ray photoelectron spectroscopy (SXPS) and scanning tunneling microscopy (STM). Measurements of the C 1s, Ga 3d and As 3d core levels exhibit a covalent bonding of the molecules to the topmost As dimers. A significant influence on the surface band bending could be observed. Furthermore, the results indicate that the adsorption process depends on functional units of the adsorbed molecules. A structure model of the interface formation is suggested for the first time.

O 30.4 Tue 12:45 MA 041

Terephthalic acid (TPA) on Si(111)-7×7 and Si(111)-$\sqrt{3} \times \sqrt{3}$-Ag surfaces — •Takayuki Suzuki, Theresa Lutz, Giovanni Costantini, and Klaus Kern — Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, D-70569 Stuttgart

We have carried out STM measurements of terephthalic acid (TPA) deposited on Si(111)7×7 and Si(111)$\sqrt{3} \times \sqrt{3}$-Ag surfaces. Due to a strong molecule-substrate interaction, TPA molecules do not form any ordered molecular layer but adsorb randomly on the Si(111)7×7 surface with several binding motifs. On the contrary, the interaction of TPA with the Si(111)$\sqrt{3} \times \sqrt{3}$-Ag surface is much weaker allowing for the formation of an ordered layer stabilized by intermolecular hydrogen bonds. The TPA overlayer is characterized by a modulation of about 2nm in period along the $\langle \bar{1}\bar{1}2 \rangle$ direction. This periodicity is not uniform but appears wider in some places and narrower in the others. The wide and the narrow regions have a parallelogram $\begin{pmatrix} 3 & 0 \\ -2 & 7 \end{pmatrix}$ and a rectangular $\begin{pmatrix} 3 & 0 \\ -3 & 6 \end{pmatrix}$ unit cell comprising 5 and 4 TPA molecules, respectively. This study demonstrates the viability of silver passivated silicon surfaces as optimal substrates for supramolecular self-organisation.

O 30.5 Tue 13:00 MA 041

Bistability of single cyclooctadiene molecules on Si(001) induced by inelastic electron tunneling — •Christophe Nacci, Jérôme Lagoute, Xi Liu, and Stefan Fölsch — Paul Drude Institute for Solid-State Electronics, Hausvogteiplatz 5-7, 10117 Berlin, Germany

The tip-induced switching of single 1,5 cyclooctadiene molecules (COD) on Si(001) was studied by low-temperature scanning tunneling microscopy. COD (C_8H_{12}) is a cyclic alkene with a twisted boat double-degenerate configuration which adsorbs in two different structures: the so-called bridge structure and the upright structure, with the bridge structure being the prevalent conformation [1]. Time spectroscopy of the tunnel current with the tip positioned over the molecule adsorbed in the bridge structure reveals fluctuations between two levels of current reminiscent to statistical telegraph noise. This behavior is interpreted as a reversible dynamic switching of the adsorbed molecule between two degenerate conformations triggered by inelastic single-electron excitation. First measurements on COD adsorbed in the upright structure reveal a significantly different noise response with an enhanced quantum yield and a lifted degeneracy of the current level population probabilities.

[1] J. H. Cho et al. Phys. Rev. B **64**, 241306 (2001)

O 30.6 Tue 13:15 MA 041

Investigations of Ga atom wire formation on Si(112) — •Moritz Speckmann[1], Thomas Schmidt[1], Jan-Ingo Flege[1,2], and Jens Falta[1] — [1]Institute of Solid State Physics, University of Bremen, 28334 Bremen — [2]National Synchrotron Light Source, Brookhaven National Laboratory, Upton, New York 11973, USA

High index surfaces are of strong interest in today's research because they are supposed to be a candidate for self-assembling systems, e. g. nano wires. In this work the adsorption of Ga on Si(112) has been investigated with different surface sensitive techniques. The stepped silicon surface consists of (111)- and (337)-facets. Because of the lower surface energy at the step edges growth of metals, e.g. Ga or Al, results in quasi-1D metal quantum wires along the direction of the step edges.

STM and LEED images clearly reveal a Ga:Si(112)-(6 × 1)-reconstruction with Ga atom rows along the step edges in $[1\bar{1}0]$-direction. Using XPEEM experiments performed at NSLS,

Brookhaven and comparing with the Ga:Si(111)-($\sqrt{3} \times \sqrt{3}$)-reconstruction we were able to determine the coverage of the Ga:Si(112)-(6×1)-reconstruction. Our results correspond to 10 Ga atoms per (6×1) unit cell and therefore confirm the model by Snijders et al. (Phys. Rev. B, **72**, 2005). Furthermore we performed x-ray standing waves experiments at HASYLAB, Hamburg. The obtained positions of the Ga atoms again show a strong agreement with the proposed positions in the model.

O 30.7 Tue 13:30 MA 041

Self-assembled films of Lead Phthalocyanine on GaAs(001) surfaces — •V. Rackwitz[1], R. Passmann[1,2], M. Kneissl[1], N. Esser[1,2], and P. Vogt[1] — [1]TU Berlin, Institute of Solide State Physics, Hardenbergstr. 36, 10623 Berlin, Germany — [2]ISAS Berlin, Albert-Einstein-Str. 9, 12489 Berlin, Germany

The influence of the atomic surface structure on the adsorption process of organic molecules on semiconductor surfaces is not yet fully understood. However, the interface arrangement of such hybrid systems is crucialy important for applications in sensors and electronic devices.

In this work we present our results on the adsorption of the non-planar lead phthalocyanines (PbPc) on the three main GaAs(001) reconstructions the c(4×4), (2×4) and (4×2). The interface formation is investigated by Reflections Anisotropy Spectroscopy (RAS), Atomic Force Microscope (AFM) and Auger Electron Spectroscopy (AES). The results shows that intra-molecular contributions resulting from the PbPc dominate the RAS spectrum upon deposition on the c(4×4) and (4×2) but not on the (2×4). The film thickness in all three cases is approximately 20nm as determined by AFM. We interpret the anisotropies of the PbPc layers as resulting from the inital atomic structure of the GaAs(001) surfaces.

O 30.8 Tue 13:45 MA 041

Investigation of crucial interfaces for III-V multi-junction solar cells — •Ulf Seidel, Henning Döscher, and Thomas Hannappel — Hahn-Meitner-Institut, Glienicker Str. 100, 14109 Berlin, Germany

Currently high efficiency III-V multi-junction solar cells are grown epitaxially on Ge(100)-substrates, which are simultaneously utilized for the low band gap subcell. Our concept is the replacement of Ge in these devices by a more efficient InGaAsP/InGaAs tandem solar cells integrated on Si(100) substrates. According structures contain many different layers of III-V semiconductors, which were prepared in this work via MOVPE. For the best performance of the solar cells sharp hetero-interfaces are necessary. Here, the investigation of two interfaces is presented in detail: (1) InGaAs/GaAsSb that is needed in the tunnel junction of our low band gap multi-junction solar cell and (2) Si/GaP that is needed for the epitaxy of our III-V solar cells on silicon(100) substrates instead of InP(100). Both interfaces were characterized in-situ during the MOVPE-growth with reflectance difference spectroscopy (RDS) and after a contamination free transfer in ultra high vacuum with X-ray photoelectron spectroscopy (XPS), low energy electron diffraction (LEED) and scanning tunnelling microscopy. Additionally AFM micrographs were recorded.