O 38: Semiconductor Substrates

Time: Tuesday 18:15–21:00 Location: Poster A

O 38.1 Tue 18:15 Poster A

Sulfur Dioxide Adsorption in Carbon Nanotube Studied by Molecular simulation and a Simple Analytical Model — •Yongbiao Yang, Mahshid Rahimi, Michael Böhm, and Florian Müller-plathe — TU Darmstadt, 64287 Darmstadt, Germany

Sulfur dioxide (SO2) is one of the main toxic gases which can result in acid rain, thus removing SO2 from atmosphere currently becomes an important subject both in industry and in science. Grand-canocical Monte Carlo method and a simple analytical model are used to understand the adsorption of SO2 onto bundles of 3D aligned double-walled carbon nanotubes (DWCNT) of different diameters and different intertube distances at 300 K. At molecular level, SO2 is found to adsorb to CNT with oxygen atoms nearer to CNT wall than sulfur atoms whether for inner or outer adsorption. It is also found condensation happens at a lower pressure compared to bulk case of SO2. For outer adsorption, the adsorption type changes from type I to type IV when intertube distance is increased from 0 nm to 2 nm. This trend is even more remarkable with CNTs of relatively larger diameter. Finally we show that the simulation data of adsorption isotherm can be well discribed by a simple analytical model.

O 38.2 Tue 18:15 Poster A

Study of the ZnO surface by XSW: elucidating the position of adsorbed oxygens — •Antoni Franco-Cañellas[1], Jens Niederhausen[2], Martin Oehzelt[2,3], Tien-Lin Lee[4], Alexander Gerlach[1], Norbert Koch[2,3], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, Tübingen, Germany — [2]Institut für Physik, Humboldt-Universität zu Berlin, Germany — [3]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, BESSY II, 12489 Berlin, Germany — [4]Diamond Light Source, UK

For its promising applications in optoelectronics and sensing devices, zinc oxide (ZnO) has attracted significant attention in the last decades. Of particular interest in this context are devices based on the combination of ZnO with different organic semiconductor materials. It is well known that for these heterostructures the characterization of the interface is of paramount importance to understand and tune the properties of the final device [1]. In this work we focus on the study of the ZnO surface, for different terminations, using the X-ray standing wave technique (XSW) [2] and photoelectron spectroscopy. Particularly, the adsorption site of the hydroxil (OH-) groups is resolved. These results will help to elucidate how the OH-groups affect deposited organic layers. Furthermore, they can provide information on surface-driven phenomena, which are specially important for ZnO nanostructures with high surface-to-volume ratio.

[1] Y. Xu et al. Phys. Rev. Lett., 111 (2013) 226802.

[2] A. Gerlach et al., in The Molecule-Metal Interface (eds N. Koch, N. Ueno and A. T. S. Wee), Wiley-VCH, Weinheim, Germany (2013).

O 38.3 Tue 18:15 Poster A

First-principles study of covalent and noncovalent functionalization of single-walled carbon nanotubes with diisocyanates — •Jakub Goclon[1], Mariana Kozlowska[2], Pawel Rodziewicz[2], and Bernd Meyer[1] — [1]Interdisciplinary Center for Molecular Materials and Computer-Chemistry-Center, FAU Erlangen-Nürnberg, Germany — [2]Institute of Chemistry, University of Bialystok, Poland

Using density functional theory (DFT) we investigated the covalent and noncovalent functionalization of (6,0) and (10,0) single-walled carbon nanotubes (SWCNTs) with 4,4'-methylene diphenyl diisocyanate (MDI) and toluene-2,4-diisocyanate (TDI) molecules. MDI and TDI are frequently utilized in the production of polyurethanes [1], which can be used in hybrid polymer–CNTs composites and coatings. Such hybrid materials are much more resistant to wear than the pure polymers [2].

The structural and electronic properties of MDI-SWCNT(6,0)/(10,0) and TDI-SWCNT(6,0)/(10,0) were scrutinized. We have also analyzed the changes in the electronic band structure of the SWCNTs caused by the amide bond formation after the covalent and noncovalent functionalization. Additionally, the MDI–MDI and TDI–TDI mutual interactions on the carbon nanotube surface were investigated.

[1] S. A. Madbouly, J. U. Otaigbe, *Prog. Polm. Sci.* **34**, 1283 (2009).
[2] H.-J. Song, Z.-Z. Zhang, X.-H. Men, *Eur. Polym. J.* **43**, 4092 (2007).

O 38.4 Tue 18:15 Poster A

Opening of subsurface dangling bond triplets via atomic manipulation — Jan Berger[1,2], Evan Spadafora[1], •Pingo Mutombo[1], Pavel Jelinek[1,3], and Martin Švec[1] — [1]Institute of Physics, Academy of Sciences of the Czech republic, Prague, Czech Republic — [2]Czech Technical University, Prague, Czech Republic — [3]Osaka University,Osaka, Japan

Atomic manipulation of the delta-doped B:Si(111)-($\sqrt{3}\times\sqrt{3}$)R30° surface was performed using a low temperature nc-AFM based on the Kolibri sensor. Through a controlled vertical displacement of the probe, a Si adatom was removed in order to create a vacancy. We succeeded to place precisely a Si atom back into the vacancy site, thus showing that this process is completely reversible. The manipulations also lead to the rearrangement of the atoms at the tip apex by sharpening it, thus allowing for a deeper look into the vacancy site. It is shown that the removal of a Si adatom exposes subsurface Si dangling bond (DB) triplets, surrounding the substitutional B dopant in the first bilayer. DFT simulations reproduced the experimental findings and suggest that the tip is likely terminated by two Si atoms at the apex. Interestingly, the closing of the vacancy was possible only when the manipulation was performed with the tip placed off-center the vacancy site.

O 38.5 Tue 18:15 Poster A

Characterization of Dy induced reconstructions on Si(111) — •Frederic Timmer[1], Robert Oelke[1], Stephan Appelfeller[2], Henrik Wilkens[1], and Joachim Wollschläger[1] — [1]Physics Department, Osnabrück University, Germany — [2]Institute of Solid State Physics, TU Berlin, Germany

Epitaxial thin films of rare earth silicides are of particular interest because of their possible application as low-resistivity contacts to n-type Si [1]. Therefore the growth of Dy on Si(111) in the monolayer regime has been investigated in-situ by Spot Profile Analysis Low Energy Electron Diffraction (SPA-LEED), Surface X-Ray Diffraction (SXRD) and Auger Electron Spectroscopy (AES).
Dy coverages of 0.1ML - 3ML were deposited by Physical Vapor Deposition (PVD) at different substrate temperatures. A plethora of reconstructions were observed by SPA-LEED, including the $(2\sqrt{3}\times 2\sqrt{3})$, $(\sqrt{3}\times\sqrt{3})$ and (1×1) reconstructions known by literature [1]. In addition we observed a spot splitting for the $(2\sqrt{3}\times 2\sqrt{3})$-spots due to the periodically arrangement of domain boundaries.
The in-situ SXRD studies were carried out at the ID03 beamline of ESRF. Dy was deposited by PVD on the Si(111) substrate at 600°C until the $(2\sqrt{3}\times 2\sqrt{3})$ reconstruction signal yielded maximum intensity. Subsequently 30 surface rods and 8 crystal truncation rods were recorded in order to determine the atomic structure of the reconstruction.

[1] I.Engelhardt et al., Surf. Sci. 600 (2006) 755-761

O 38.6 Tue 18:15 Poster A

Point defects and diffusion on Bi2Te3 surfaces — •Mert Taskin[1], Ilker Oztoprak[1], Dilek Yildiz[1], Carl Willem Rischau[2], Cornelis J. van der Beek[2], Alberto Ubaldini[3], and Oguzhan Gurlu[1] — [1]Istanbul Technical University, Istanbul, Turkey — [2]Ecole Polytechnique, Palaiseau, France — [3]Université de Genéve, Geneva, Switzerland

Bi2Te3 was shown to be a topological insulator besides being a thermoelectric material, yet the knowledge on the atomic scale defects and their effect on the local electronic structure is still incomplete. Bi2Te3 has rhombohedral crystal structure and bonds between the atoms of Bi/Te1 are the strongest in the lattice. In contrast, Te1/Te1 interface has just van der Waals bonds in between them. Consequently the crystals can be cleaved on this plane and the Te1 surface can be imaged with scanning tunneling microscopy (STM) with out need for further surface preparation. Despite its inertness, point defects were observed on the Te1 surface. In addition to these defects we have observed vacancy defects and clusters on the Te1 surface. In order to understand the nature of these defects, we performed time lapse STM imaging by means of which we have observed their diffusion. Moreover, bias dependent images have shown that the defects were not of single type.

O 38.7 Tue 18:15 Poster A

Surface Analysis of MOVPE-prepared GaP(111)B — •Peter Kleinschmidt[1], Pingo Mutombo[2], Oleksandr Romanyuk[2], Marcel Himmerlich[3], Weihong Zhao[1], Andreas Nägelein[1], Matthias Steidl[1], Agnieszka Paszuk[1], Sebastian Brückner[1], Oliver Supplie[1], Stefan Krischok[3], and Thomas Hannappel[1] — [1]Photovoltaics Group, Institute of Physics, Technische Universität Ilmenau, 98684 Ilmenau, Germany — [2]Institute of Physics, Academy of Sciences of the Czech Republic, Cukrovarnicka 10, 162 00 Prague 6, Czech Republic — [3]Technical Physics I, Institute of Physics, Technische Universität Ilmenau, 98684 Ilmenau, Germany

We have investigated the MOVPE-prepared GaP(111)B surface by LEED, XPS, and STM as well as ab intio DFT. We obtained atomically resolved occupied-state STM images, characterized by large, atomically flat terraces. Most areas on these terraces exhibit no discernable order, in agreement with the (1×1) LEED pattern we obtained. However, locally, the STM images also show $(\sqrt{3} \times \sqrt{3})$ and c(2×4) ordering. Our measurements indicate P-induced surface states. The different surface reconstructions were analyzed by ab initio DFT and relative surface formation energies of the Ga-rich and P-rich structures were derived. The most energetically favorable structures were used for STM image simulations and compared with the experimental STM images.

O 38.8 Tue 18:15 Poster A

Ordered growth of hexagonal molecules on hexagonal surfaces: a new type of epitaxy? — •Falko Sojka, Matthias Meissner, Tobias Huempfner, Roman Forker, and Torsten Fritz — Friedrich Schiller University, Institute of Solid State Physics, Helmholtzweg 5, 07743 Jena, Germany

We analyzed the growth of diverse monolayers of organic molecules with hexagonal symmetry on different hexagonal surfaces using coronene and hexa-peri-hexabenzocoronene (HBC). By compensating geometric distortions and other systematic errors in low-energy electron diffraction (LEED), high-precision determination of the epitaxial matrices using numerical fitting routines is feasible [1, 2]. The LEED studies are complemented by other methods like low temperature scanning tunneling microscopy (LT-STM) and differential reflectance spectroscopy (DRS) [3].

We found well-defined ordered structures which are, however, partially in contrast to the literature. Within error margins the lattice alignment cannot be assigned to any known type of epitaxy [4] and may therefore point towards a new type of epitaxy.

References: [1] F. Sojka et al., Rev. Sci. Instrum. 84, 015111 (2013).
[2] F. Sojka et al., Ultramicroscopy 133, 35-40 (2013).
[3] R. Forker et al., Annu. Rep. Prog. Chem., Sect. C: Phys. Chem. 108, 34-68 (2012).
[4] S.C.B. Mannsfeld et al., Phys. Rev. Lett. 94, 056104 (2005).

O 38.9 Tue 18:15 Poster A

Nanostructuring and Dye-Functionalization of Diamond Electrodes for Photoelectrochemical Applications — •Nina Felgen[1], Christo Petkov[1], Philipp Reintanz[2], Alberto Pasquarelli[3], Thomas Hantschel[4], Menelaos Tsigkourakos[5], Ulrich Siemeling[2], Johann Peter Reithmaier[1], and Cyril Popov[1] — [1]Institute of Nanostructure Technologies and Analytics, Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, Germany — [2]Institute of Chemistry, Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, Germany — [3]Institute of Electron Devices and Circuits, University of Ulm, Germany — [4]IMEC, Leuven, Belgium — [5]Instituut voor Kern- en Stralingsfysica, K.U. Leuven, Belgium

Diamond is a prospective electrode material for a number of applications providing efficient electron transport, high stability of electrolytic performance with time, a possibility for dye-sensitizing with photosensitive molecules, etc. Boron-doped diamond (BDD) films have been prepared by hot filament chemical vapor deposition (HFCVD) and structured by reactive ion etching with oxygen plasma applying a gold mask lithographically defined or composed of random droplets. Further, the nanostructured BDD surfaces were modified by O2 or NH3 plasma and grafted with different phthalocyanines. The modified and functionalized BDD were tested as electrodes for photoelectrochemical measurements.