HL 73: Heterostructures and Interfaces (Joint session of HL and O, organized by HL)

Time: Thursday 9:30–13:15 Location: H17

HL 73.1 Thu 9:30 H17

Silicon p-n junctions prepared by group-V in-diffusion in CVD ambient — •Agnieszka Paszuk, Oliver Supplie, Marek Duda, Anja Dobrich, Peter Kleinschmidt, Sebastian Brückner, and Thomas Hannappel — Technische Universität Ilmenau, Institut für Physik, Fachgebiet Photovoltaik, Gustav-Kirchhoff-Str. 5, 98693 Ilmenau, Germany

Integration of III-V materials with Si substrates is promising for high-efficiency tandem solar cells. Preparation of Si bottom cell in MOCVD environment requires control over the doping. Phosphorus (P) in-diffusion into crystalline Si is a complex process, but has been shown suitable to form a working emitter [1,2]. Arsenic (As) in-diffusion on the other hand is interesting since Si surfaces terminated with As enable the prepareation of B-type GaP/Si(111)[3] and As-based planar graded buffer layers. Here, we focus on As and P in-diffusion and its impact on the Si surface (controlled by in-situ reflection anisotropy spectroscopy). Diffusion of As and P into Si is carried out by annealing the substrates under TBAs or TBP. We investigated the diffusion in dependence on duration and temperature of the annealing step, precursor source, reactor pressure and post diffusion annealing. Annealing the Si surface in presence of the precursors results in surface roughening and a disordered surface. Subsequent annealing without precursor supply leads to a re-ordered dimerized surface. [1] E. García-Tabarés et al., 8th International Conference on Concentrating Photovoltaic Systems (2012). [2] R. Varache et al., Energy Procedia 77, 493 (2015). [3] A. Paszuk et al., Appl. Phys. Lett. 106, 231601 (2015).

HL 73.2 Thu 9:45 H17

Interfacial Doping of a MoS2 Monolayer in a 2D Heterostructure — •Mahfujur Rahaman[1], Gerd Plechinger[2], Raul D. Rodriguez[1], Christian Schüller[2], Tobias Korn[2], and Dietrich R.T. Zahn[1] — [1]Semiconductor Physics, Technische Universität Chemnitz,09126 Chemnitz, Germany — [2]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, D-93040 Regensburg, Germany

We report on the interfacial doping of the transition metal dichalcogenide MoS2 monolayer in contact with GaSe and graphite (HOPG). Photoluminescence (PL) results suggest that the PL emission of MoS2 monolayer on top of GaSe is dominated by neutral excitons. This is in contrast to MoS2 in contact with HOPG where trions dominate the PL due to n-type doping. Raman spectroscopy investigations indicate e- doping of the MoS2 monolayer on top of HOPG reflected by the change in A1g out-of-plane mode. Finally, the carrier concentration of MoS2 monolayers for both interfaces is quantitatively determined by Kelvin probe force microscopy (KPFM). Our results pave the way for simple, scalable, and patterned doping in order to modify the electrical and optical properties of MoS2 monolayers and other 2D materials by engineering the graphite substrate.

HL 73.3 Thu 10:00 H17

Epitaxial growth and conductivity mechanisms of $[LaNiO_3/LaAlO_3]_{10}$ superlattices — •Haoming Wei, Michael Lorenz, and Marius Grundmann — Universität Leipzig, Institut für Exp. Physik II, Germany

$LaNiO_3$ (LNO) is an interesting material exhibiting Pauli paramagnetic metallic behavior in a wide temperature range. New properties can emerge in the LNO-based superlattices (SLs) by modifying the orbital, electronic, and magnetic structure of bulk LNO [1]. We have grown LNO, $LaAlO_3$ (LAO) films, and [LNO (d nm)/LAO (2 nm)]$_{10}$ SLs by plused laser deposition [2]. Sharp reflection high-energy electron diffraction patterns and atomic force microscopy images confirm an atomically flat surface. Reciprocal space maps reveal the in-plane lattice match of the SLs to the substrates. X-ray reflectivity data with strong Bragg reflections indicate abrupt interfaces of SLs with interfacial roughness in the order of one unit cell. A clear quantum confinement effect on the electronic properties including a metal-insulator transition (MIT) of the LNO/LAO SLs is demonstrated for decreasing LNO thickness. Single LNO films and SLs with LNO thickness of 4 nm show metallic behaviour at all temperatures. The SL with 2 nm thick LNO shows MIT due to the quantum interference of electronic waves. Strong localization appears when the LNO thickness of SLs reduced to 1.2 nm and two-dimensional variable range hopping is the main conduction mechanism.

[1] M. K. Stewart et al. J. Appl. Phys. 110, 033514 (2011).
[2] H. M. Wei et al. Appl. Phys. Lett. 106, 042103 (2015).

HL 73.4 Thu 10:15 H17

How can band offsets in III-V nanowires be determined correctly by scanning tunneling spectroscopy? — •Philipp Ebert[1], Pierre Capiod[2], Tau Xu[2], Adrian Díaz Álvarez[2], Xiang-Lei Han[2], David Troadec[2], Jean-Philippe Nys[2], Maxime Berthe[2], Liverios Lymperakis[3], Jörg Neugebauer[3], Isabelle Lefebvre[2], Sébastien Plissard[2,4], Philippe Caroff[2,5], Rafal Dunin-Borkowski[1], and Bruno Grandidier[2] — [1]Peter Grünberg Institut, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [2]IEMN, CNRS, UMR 8520, Dept. ISEN, 59046 Lille, France — [3]Max-Planck Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany — [4]CNRS-LAAS, Univ. de Toulouse, 31400 Toulouse, France — [5]Dept. of Electronic Materials Engineering, Australian National University, Canberra, ACT 0200, Australia

Scanning tunneling spectroscopy (STS) allows the determination of band gaps and band offsets at interfaces between different polytypes or materials of III-V semiconductor nanowires (NWs). However, STS is mostly wrongly interpreted in literature: The commonly high step density at the sidewall surfaces of III-V NWs leads to extrinsic surface states that induce a pinning of the Fermi energy within the fundamental band gap. Since the pinning level is different on every polytype/material, the relative band edge positions between different NW segments are extrinsically determined. Therefore, we developed a new methodology to accurately determine band offsets between different NW segments by using a thin overgrown shell with wider band gap, assuring identical pinning of the overgrown and the pure segment.

HL 73.5 Thu 10:30 H17

Atomic-Scale Electronic Structures across $BiFeO_3/La_{0.7}Sr_{0.3}MnO_3$ Heterointerfaces — •Ya-Ping Chiu[1,2], Bo-Chao Huang[3], Pu Yu[4], Chia-Seng Chang[3], and Ying-Hao Chu[3,5] — [1]Dept. of Physics, National Taiwan Normal University, Taipei 116, Taiwan — [2]Dept. of Physics, National Sun Yat-sen University, Kaohsiung 804, Taiwan — [3]Institute of Physics, Academia Sinica, Taipei 115, Taiwan — [4]State Key Laboratory of Low-Dimensional Quantum Physics, Dept. of Physics, Tsinghua University, and Collaborative Innovation Center of Quantum Matter, Beijing 100084, China — [5]Dept. of Materials Science and Engineering, National Chiao Tung University, Hsinchu 300, Taiwan

Atomic-level evolution of electronic structures across $BiFeO_3/La_{0.7}Sr_{0.3}MnO_3$ complex oxide heterointerfaces has been demonstrated by cross-sectional scanning tunneling microscopy and spectroscopy in this work. Analysis of scanning tunneling spectroscopy results exploits how the change in the terminated interface brings the influence to the electrostatic configurations across the $BiFeO_3/La_{0.7}Sr_{0.3}MnO_3$ heterointerfaces. Spatially unit-cell-by-unit-cell resolved electronic states at the atomic level reveal that the control of material interfaces at the atomic level determines the ferroelectric polarization in $BiFeO_3$. The precise electronic information therefore provides a clear realization about the electronic state at these complex-oxide heterointerfaces, which is crucial to understand and design a host of novel functionalities at complex oxide heterointerfaces.

30 min. Coffee Break

HL 73.6 Thu 11:15 H17

Ultrafast multi-terahertz nanoscopy of strained vanadium dioxide nanobeams — •Markus A. Huber[1], Markus Plankl[1], Max Eisele[1], Robert E. Marvel[2], Fabian Sandner[1], Tobias Korn[1], Christian Schüller[1], Richard F. Haglund[2], Rupert Huber[1], and Tyler L. Cocker[1] — [1]Department of Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Department of Physics and Astronomy and Interdisciplinary Materials Science Program, Vanderbilt University, Nashville, Tennessee 37235-1807, USA

Long regarded as a model system for studying insulator-to-metal transitions, vanadium dioxide features a rich phase diagram including at least three insulating states and one metallic state. Recently, the effects of strain on the transition temperature and nanoscale domain

structure have been brought into focus. In this regard scattering-type near-field microscopy in the multi-terahertz regime [10-100 THz] has been proven to be a valuable tool for imaging the spatial heterogeneity of the transition. However, so far no time-resolved near-field studies have been undertaken. Here, we show the local pump-probe behavior of a single-crystalline vanadium dioxide nanobeam upon near-infrared photoexcitation. We probe with an ultrafast multi-terahertz pulse and see a modulation of the photoconductivity along the c_R-axis of the wire. This modulation qualitatively matches the different switching susceptibilities inside the wire upon thermal heating. We therefore propose that the switching susceptiblity is built into the wire already at room-temperature, most likely by strain.

HL 73.7 Thu 11:30 H17

Structural and optical characterization of hybrid ZnO/polymer nanostructures fabricated by spin coating — •Stephanie Bley[1], Alejandra Castro-Carranza[1], Linus Krieg[2], Tobias Voss[2], and Jürgen Gutowski[1] — [1]Institute of Solid State Physics, Semiconductor Optics, University of Bremen, 28359 Bremen — [2]Institute of Semiconductor Technology, Braunschweig University of Technology, 38106 Braunschweig

Hybrid core-shell nanowires with inorganic ZnO cores and organic p-conductive polymer shells have shown to possess a huge potential for the realization of efficient light-emitting or photovoltaic devices. A controlled deposition of the polymer shell is required to tailor the electronic and optical properties.

We show that spin-coating of planar ZnO layers and nanowires with poly(3,4-ethylenedioxythiophene) (PEDOT) is suitable to form hybrid heterojunctions. A thin polystyrene passivating interlayer is deposited in the hybrid structure. Its thickness is systematically modified to study its impact on defect state passivation, confirmed by the optical and electrical performance of the heterojunction. SEM and TEM characterization of the hybrid ZnO/polymer nanostructures show that conformal coating is possible. PL measurements confirm that the general optical properties of the ZnO have not been significantly changed after the coating process. A reduction of the defect luminescence of the ZnO is found for the passivated samples.

HL 73.8 Thu 11:45 H17

Photoelectrochemical investigation of TiO_2-coated InGaN/GaN nanowires under visible light irradiation — •Paula Neuderth[1], Adina Frank[1], Pascal Hille[1], Christian Reitz[2], Jörg Teubert[1], Jörg Schörmann[1], Roland Marschall[3], and Martin Eickhoff[1] — [1]I. Physikalisches Institut, Justus-Liebig-Universität Gießen, Gießen, Germany — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology (KIT), Eggenstein-Leopoldshafen, Germany — [3]Physikalisch-Chemisches Institut, Justus-Liebig-Universität Gießen, Gießen, Germany

Composite structures of InGaN/GaN nanowire heterostructures with a thin anatase titania coverage were prepared by combination of molecular beam epitaxy and atomic layer deposition and investigated with respect to their photoelectrochemical properties. The bandgap of InGaN can be adjusted in the visible regime which makes it suitable for solar-driven photocatalytic reactions such as solar water splitting. In these nanocomposite structures an anodic photocurrent under visible excitation was gained. However, the presence of a thin (2 - 10 nm) anatase titania film increases the photocurrent significantly although direct generation of carriers in the titania is not possible. The influence of the titania coating on charge separation, charge transfer and surface recombination will be discussed by comparison to photoluminescence measurements in electrochemical environment.

HL 73.9 Thu 12:00 H17

Disorder and Interface Properties in III-N-V-quantum wells — •Sebastian Gies, Sarah Karrenberg, Tatjana Wegele, Phillip Springer, Christian Fuchs, Andreas Beyer, Martin Zimprich, Wolfgang Stolz, Kerstin Volz, Stephan W. Koch, and Wolfram Heimbrodt — Philipps-University Marburg, 35032 Marburg, Germany

Nitrogen containing quantum well (QW) structures are an interesting material for solar cells and lasers. Because of the band anticrossing between the N-impurity and the GaAs conduction band the band gap is pushed towards 1.55 μm. Otherwise N introduces a huge disorder. The influence of this disorder on QW-interfaces (IF) and optical properties is scarcely studied. However, IFs are an important part of any device and influence strongly the charge carrier confinement and the transport properties. We investigate the quaternary Ga(NAsP) pseudomorphically grown on silicon. This material is a promising light source for optoelectronic integration on silicon. The important disorder parameters are revealed using photoluminescence (PL) spectroscopy, while the material's structure is characterized via transmission electron microscopy and X-ray diffraction. The conjunction of these methods allows us to uncover the complex interplay between N-incorporation and optical and structural properties. Furthermore, type-II excitons in (GaIn)As/Ga(NAs)-heterostructures are studied. The conjunction of experiment and microscopic theory allows us not only to determine the band alignment in the heterostructures, but also to directly analyze the influence of the IF on disorder and optical properties.

HL 73.10 Thu 12:15 H17

Hybrid structures of semi-metals, excitonic insulators and superconductors — •Dario Bercioux[1,2] and Sebastian Bergeret[1,3] — [1]Donostia International Physics Center (DIPC), E-20018 San Sebastián, Spain — [2]IKERBASQUE, Basque Foundation of Science, 48011 Bilbao, Spain — [3]Centro de Física de Materiales (CFM-MPC) Centro Mixto CSIC-UPV/EHU, E-20018 Donostia-San Sebastian, Spain

Excitonic insulars are a condensate phase of matter investigated since the sixties [1]. They remain so far an elusive phase in solid state systems. Recent experiments on HgTe quantum wells with a width of circa 20 nm [2] hints at their observation. However, there is no common agreement on this point [3]. Combinations of excitonic insulators with superconductors should show evidence of Andreev processes due to the combination of two different type of condensates [4]. Here, we present results for hybrid structures combining semi-metals, excitonic insulators and superconductors and discuss phenomena related to the interplay between the two distinct condensates.

[1] D. Jérome, T. M. Rice, & W. Kohn, W., Phys. Rev. **158**, 462 (1967).
[2] G. M. Minkov, *et al.*, Phys. Rev. B **88**, 155306 (2013).
[3] M. Knap, J. D. Sau, B. I. Halperin, & E. Demler, Phys. Rev. Lett. **113**, 186801 (2014).
[4] F. Dolcini, *et al.*, Phys. Rev. Lett. **104**, 027004 (2010).

HL 73.11 Thu 12:30 H17

A functional renormalization group approach for treating interactions in disordered electron systems — •Christian Seiler and Ferdinand Evers — Institut für Theoretische Physik, Universität Regensburg, Deutschland

We propose an approach to treat the effects of interactions in disordered electron systems on a numerical level. The idea is to solve the non-interacting disorder problem for a given disorder realization exactly. We then use the functional renormalization group method to introduce interactions on a perturbative level. In contrast to usual applications of the fRG, we formulate it in terms of the eigenfunctions of the disordered non-interacting Hamiltonian. The main advantage of our approach is that we are able to treat disorder exactly from a numerical point of view, while the fRG enables us to characterize interaction-induced phase transitions that the system undergoes in an unbiased manner. This allows us to study the phase diagram of a model system without being restricted in the strength of the disorder.

HL 73.12 Thu 12:45 H17

***Ab initio* Anderson localisation in Si:P** — •Edoardo G. Carnio[1], Nicholas D. M. Hine[1], David Quigley[1,2], and Rudolf A. Römer[1,2] — [1]Department of Physics, The University of Warwick, Coventry CV4 7AL, UK — [2]Centre for Scientific Computing, The University of Warwick, Coventry CV4 7AL, UK

The Anderson metal-insulator transition (MIT) has long been studied, but there is still no agreement on its critical exponent when comparing experiments and theory. In this work, we employ *ab initio* methods to study the MIT that occurs in phosphorus-doped silicon (Si:P) when the density of the dopants is increased. Our strategy consists in using ONETEP, an implementation of linear scaling DFT, to model an effective potential between the P atoms, which is used in a Monte Carlo simulation to randomly distribute the impurities in the host material. We then combine these spatial configurations with the DFT data into an effective tight-binding Hamiltonian for a system of Si:P close to the critical concentration of the MIT. In this way we characterise the MIT in Si:P including the *ab initio* determined possible spatial correlations in P and the electronic interactions between the donated electrons. The extent of the resulting electronic states is characterised by the participation numbers and their scaling.

HL 73.13 Thu 13:00 H17

General DFT+NEGF approach for modeling metal-semiconductor interfaces — •DANIELE STRADI[1], UMBERTO MARTINEZ POZZONI[2], ANDERS BLOM[2], MADS BRANDBYGE[1], and KURT STOKBRO[2] — [1]DTU Nanotech, Technical University of Denmark, DK-2800 Kgs. Lyngby, Denmark — [2]QuantumWise A/S, Freubjergvej 3, Postbox 4, DK-2100 Copenhagen, Denmark

Metal-semiconductor (M-SC) contacts play a pivotal role in a broad range of technologically relevant devices. Still, their characterization remains a delicate issue, as the present understanding relies either on simplified analytical models [1], or on simulations describing the interface using simple slab models [2]. We model realistic M-SC interfaces by using the DFT+NEGF method as implemented in the Atomistix ToolKit (ATK) simulation software [3]. An accurate description of the interface is achieved by using a meta-GGA functional [4], and an effective scheme to account for the presence of doping in the SC side. The present approach has the advantages of (i) treating the system using the appropriate boundary conditions and (ii) allowing for a direct comparison between theory and experiments by simulating the I-V characteristics of the interface. We apply this methodology to an Ag/Si interface relevant for solar cell applications, and test the reliability of traditional strategies [1,2] to describe its properties [5]. [1] Physics of Semiconductor Devices: 3rd edition (Wiley, 2006); [2] Phys. Rev. B 35, 8154 (1987); [3] Atomistix ToolKit version 2015.0, QuantumWise A/S (www.quantumwise.com); [4] Phys. Rev. Lett. 102, 226401 (2009); [5] D. Stradi et al. In preparation