Semiconductor Physics Division
Fachverband Halbleiterphysik (HL)

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Overview of Invited Talks and Sessions

(lecture rooms FOE Anorg., POT 006, POT 051, POT 151, and POT 251; posters P1, P3, and P4)

Intersectional Symposium "Artificial Optical Materials" (SYOM)

Orginzation: Ralf B. Wehrspohn (Fraunhofer Institute for Mechanics of Materials Halle), Kurt Busch (Karlsruhe Institute of Technology), Jörg Schilling (Martin-Luther-Universität Halle-Wittenberg)

SYOM 1.1	Mon	14:30–15:00	HSZ 01	**Photonic Metamaterials and Transformation Optics: Recent Progress** — •Martin Wegener
SYOM 1.2	Mon	15:00–15:30	HSZ 01	**Keeping a tight focus on matter** — •Philip St. J. Russell
SYOM 1.3	Mon	15:30–16:00	HSZ 01	**The Physics of Photonic Crystals LEDs** — •Claude Weisbuch, Elison Matioli
SYOM 1.4	Mon	16:15–16:45	HSZ 01	**Using nanophotonic structures to overcome conventional limits in solar energy conversion** — •Shanhui Fan
SYOM 1.5	Mon	16:45–17:15	HSZ 01	**Plasmonic nanocavities: New design concepts and determination of the complete mode spectrum using electron-beam spectroscopies** — •Stefan A. Maier

SKM-Symposium "Semiconductor Nanophotonics: Quantum Optics and Devices" (SYNP)

Orginzation: Jürgen Christen (Otto-von-Guericke-Universität Magdeburg), Oliver Benson (Humboldt-Universität zu Berlin)

SKM-SYNP 1.1	Wed	14:30–15:00	TRE Ma	**Quantum Optics on Photonic Chips** — •Dirk Englund, Brendan Shields, Hongkun Park, Mikhail Lukin, Kelley Rivoire, Jelena Vuckovic, Fariba Hatami
SKM-SYNP 1.2	Wed	15:00–15:30	TRE Ma	**Two-photon Interference from Separate Quantum Dots** — Edward Flagg, Andreas Muller, Sergey Polyakov, Alexander Ling, Alan Migdall, •Glenn S. Solomon
SKM-SYNP 1.3	Wed	15:30–16:00	TRE Ma	**Coherent optoelectronic control of a single exciton qubit** — •Artur Zrenner, Steffen Michaelis de Vasconcellos, Simon Gordon, Dirk Mantei, Wadim Quiring, Mohannad Al-Hmoud, Torsten Meier, Max Bichler, Andreas D. Wieck, Dirk Reuter
SKM-SYNP 1.4	Wed	16:15–16:45	TRE Ma	**Generation of non-classical states of light with site- and potential-controlled pyramidal quantum dots** — •Eli Kapon
SKM-SYNP 1.5	Wed	16:45–17:15	TRE Ma	**Semiconductor Devices for Quantum Photonics** — •Andrew Shields, Anthony Bennett, Mark Stevenson, Cameron Salter, Raj Patel, Ian Farrer, Christine Nicoll, David Ritchie

Focused Session HL 32 & HL 42 "Inorganic/Organic Semiconductor Hybrid Structures"

Organization: Fritz Henneberger (Humboldt-Universität zu Berlin), Norbert Koch (Humboldt-Universität zu Berlin)

HL 32.1	Tue	10:15–10:45	POT 151	**Self-assembled monolayers on zinc oxide** — •Craig L. Perkins
HL 32.2	Tue	10:45–11:15	POT 151	**Inorganic/organic semiconductor heteroepitaxy - towards new hybrid systems for optoelectronics and photonics** — •Sylke Blumstengel
HL 32.3	Tue	11:30–12:00	POT 151	**Electrostatic Field Driven Alignment of Organic Oligomers on ZnO Surfaces** — •Fabio Della Sala, Sylke Blumstengel, Fritz Henneberger
HL 32.4	Tue	12:00–12:30	POT 151	**The incorporation of metal nanostructures at organic/inorganic semiconductor interfaces** — •Dietrich RT Zahn, Michael Ludemann, Ovidiu Gordan, Philipp Schäfer, Georgeta Salvan
HL 42.1	Tue	14:15–14:45	POT 151	**Interfacial charge-carrier energetics probed by electromodulated absorption spectroscopy: implication for organic-inorganic hybrid photovoltaic devices** — •Peter Ho
HL 42.2	Tue	14:45–15:15	POT 151	**Organic layers on Si, SiC, and diamond substrates: structural and electronic properties** — •Martin Stutzmann, Ian D. Sharp, Jose Antonio Garrido, Martin S. Brandt

Focused Session HL 80 "Novel Green Laser Diodes"

Organization: Andreas Hangleiter (Technische Universität Braunschweig), Tim Wernicke (Technische Universität Berlin)

HL 80.1	Thu	14:30–15:00	POT 51	**GaN-based green laser diodes grown on c-plane GaN substrate** — •Shinichi Nagahama
HL 80.2	Thu	15:00–15:30	POT 51	**Room-temperature CW operation of BeZnCdSe green laser diode** — •shigehisa tanaka, jun-ichi kasai, sumiko fujisaki, ryouichi akimoto, takeshi kikawa, shinji tsuji, haruhiko kuwatsuka, toshifumi hasama, hiroshi ishikawa
HL 80.3	Thu	15:30–16:00	POT 51	**Growth and properties of semi-polar GaN on patterned silicon substrate** — •Nobuhiko Sawaki
HL 80.4	Thu	16:15–16:45	POT 51	**Advantages of Using Semipolar Orientation for Making Green InGaN QW Laser Diodes.** — •Dmitry Sizov, Rajaram Bhat, Kechang Song, Chung-en Zah
HL 80.5	Thu	16:45–17:15	POT 51	**Optical gain of green (Al,In)GaN laser diodes** — •Ulrich Schwarz

Further Invited Talks of the division HL

HL 1.1	Mon	10:15–10:45	FOE Anorg	**Self-organized quantum dots as single and entangled photon emitters** — •Erik Stock, Waldemar Unrau, Anatol Lochmann, Andrei Schliwa, Murat Öztürk, Askhat Bakarov, Aleksandr Toropov, Ilia Derebrezov, Vladimir Haisler, Dieter Bimberg
HL 13.1	Mon	12:45–13:15	FOE Anorg	**Semiconductor quantized current and voltage standard** — •Bernd Kaestner
HL 14.1	Mon	13:00–13:30	POT 06	**Why does a thin Layer of CdS on top of CdTe, and other thin-film solar cells improve their efficiency dramatically** — •Karl W. Boer
HL 27.1	Mon	17:00–17:30	POT 51	**Intraexciton terahertz nonlinear optics in quantum wells** — •Martin Wagner, Harald Schneider, Dominik Stehr, Stephan Winnerl, Aaron M. Andrews, Stephan Schartner, Gottfried Strasser, Manfred Helm
HL 56.1	Wed	14:30–15:00	POT 51	**Cross-sectional Scanning Tunneling Microscopy on Semiconductor Nanostructures** — •Holger Eisele
HL 58.1	Wed	14:30–15:00	POT 251	**Transport spectroscopy on non-equilibrium spin and charge states in self-organized quantum dots** — •Martin Geller

Sessions

HL 1.1–1.1	Mon	10:15–11:00	FOE Anorg	**Invited Talk: Erik Stock**
HL 2.1–2.6	Mon	10:15–11:45	POT 51	**Electronic Structure Theory**
HL 3.1–3.6	Mon	10:15–11:45	POT 151	**III-V-Compounds: GaAs and related Materials**
HL 4.1–4.12	Mon	10:15–13:30	POT 251	**Carbon: Diamond, Nanotubes, and Graphene**
HL 5.1–5.8	Mon	10:15–12:30	POT 06	**Innovative Systems and Devices**
HL 6.1–6.5	Mon	10:30–13:00	TRE Ma	**SKM Symposium: Elementary Processes in Organic Photovoltaics (SYOP)**
HL 7.1–7.6	Mon	11:00–12:30	FOE Anorg	**Single Photon Sources and Qbits**
HL 8.1–8.4	Mon	11:00–13:00	GER 37	**Joint Focussed Session: Thin Film Chalcogenide Photovoltaics I**
HL 9.1–9.4	Mon	11:15–13:00	WIL A317	**Joint Focussed Session: Transparent Conductive Oxides I**
HL 10.1–10.6	Mon	11:15–13:00	TRE Phy	**Joint Focussed Session: Theory and Computation of Electronic Structure: New Frontiers I**
HL 11.1–11.5	Mon	12:00–13:15	POT 51	**Transport: mainly Theory**
HL 12.1–12.6	Mon	12:00–13:30	POT 151	**Quantum Dots and Wires: Arsenides**
HL 13.1–13.1	Mon	12:45–13:15	FOE Anorg	**Invited Talk: Bernd Kästner**
HL 14.1–14.1	Mon	13:00–13:30	POT 06	**Invited Talk: Karl W. Böer**
HL 15.1–15.12	Mon	14:00–17:30	ZEU 222	**Joint Session: Organic Semiconductors I: Solar Cells A**
HL 16.1–16.10	Mon	14:30–17:15	FOE Anorg	**Microcavities**
HL 17.1–17.8	Mon	14:30–16:45	POT 51	**Nitrides: Growth and Characterization**
HL 18.1–18.4	Mon	14:30–15:30	POT 151	**Quantum Hall Effect**
HL 19.1–19.13	Mon	14:30–18:00	POT 251	**Silicon and Germanium**
HL 20.1–20.5	Mon	14:30–15:45	POT 06	**Innovative Materials**
HL 21.1–21.5	Mon	14:30–17:15	HSZ 01	**Symposium: Artificial Optical Materials (SYOM)**
HL 22.1–22.5	Mon	14:30–17:00	TRE Ma	**SKM Symposium: Spin Caloric Transport (SYST)**
HL 23.1–23.3	Mon	14:45–15:45	GER 37	**Joint Focussed Session: Thin Film Chalcogenide Photovoltaics II**
HL 24.1–24.6	Mon	16:00–17:30	GER 37	**Joint Focussed Session: Thin Film Chalcogenide Photovoltaics III**
HL 25.1–25.9	Mon	15:45–18:15	POT 151	**Transport**
HL 26.1–26.7	Mon	16:00–17:45	POT 06	**Interfaces and Surfaces**
HL 27.1–27.1	Mon	17:00–17:30	POT 51	**Invited Talk: Martin Wagner**
HL 28.1–28.5	Mon	17:30–18:45	POT 51	**THz Physics**
HL 29.1–29.4	Mon	17:45–18:45	FOE Anorg	**Organic Photovoltaics II: mainly Phtalocyanine**
HL 30.1–30.6	Tue	10:15–11:45	FOE Anorg	**Nano Wires: Growth and Characterization**
HL 31.1–31.12	Tue	10:15–13:30	POT 51	**III-V-Compounds: Nitrides**
HL 32.1–32.6	Tue	10:15–13:00	POT 151	**Focussed Session: Inorganic/Organic Semiconductor Hybrid Structures I**
HL 33.1–33.12	Tue	10:15–13:30	POT 251	**Spin-dependent Transport I**
HL 34.1–34.9	Tue	10:30–13:00	HSZ 02	**Joint Session: Solid State Photon Sources**
HL 35.1–35.9	Tue	10:30–13:00	ZEU 222	**Joint Session: Organic Semiconductors II: Solar Cells B**
HL 36.1–36.5	Tue	11:15–13:15	WIL B122	**Joint Focussed Session: Transparent Conductive Oxides II**
HL 37.1–37.6	Tue	11:15–13:00	TRE Phy	**Joint Focussed Session: Theory and Computation of Electronic Structure: New Frontiers II**
HL 38.1–38.5	Tue	12:00–13:15	FOE Anorg	**Polaritons and Polariton Lasing**
HL 39.1–39.7	Tue	13:30–15:15	FOE Anorg	**Photovoltaics: Chalcopyrites I**
HL 40.1–40.5	Tue	14:00–15:15	ZEU 222	**Joint Session: Organic Semiconductors III: Aggregation and Nanostructures**
HL 41.1–41.4	Tue	14:15–15:15	POT 51	**Nitrides: InGaN**
HL 42.1–42.2	Tue	14:15–15:15	POT 151	**Focussed Session: Inorganic/Organic Semiconductor Hybrid Structures II**
HL 43.1–43.3	Tue	14:30–15:15	POT 251	**Spin-dependent Transport II**
HL 44.1–44.100	Tue	18:00–21:00	P3	**Poster Session I**
HL 45.1–45.20	Tue	18:00–21:00	P1	**Joint Poster Session**
HL 46.1–46.12	Wed	10:15–13:30	FOE Anorg	**Organic Photovoltaics I**
HL 47.1–47.5	Wed	10:15–11:30	POT 51	**GaN on Si**
HL 48.1–48.12	Wed	10:15–13:30	POT 151	**ZnO: Devices**
HL 49.1–49.8	Wed	10:15–12:15	POT 251	**Photonic Crystals and Metamaterials**
HL 50.1–50.5	Wed	10:30–13:00	TRE Ma	**SKM Symposium: Topological Insulators (SYTI)**

HL 51.1–51.7	Wed	11:15–13:00	TRE Phy	**Joint Focussed Session: Theory and Computation of Electronic Structure: New Frontiers III**
HL 52.1–52.6	Wed	11:45–13:15	POT 51	**Nonpolar and Semipolar Nitrides**
HL 53.1–53.4	Wed	12:30–13:30	POT 251	**Optical Properties I**
HL 54.1–54.10	Wed	14:00–17:00	ZEU 222	**Joint Session: Organic Semiconductors IV: Excitations and Charges**
HL 55.1–55.12	Wed	14:30–17:45	FOE Anorg	**Photovoltaics: mainly Technology and Photon Management**
HL 56.1–56.1	Wed	14:30–15:00	POT 51	**Invited Talk: Holger Eisele**
HL 57.1–57.4	Wed	14:30–15:30	POT 151	**ZnO: Optical Properties**
HL 58.1–58.1	Wed	14:30–15:00	POT 251	**Invited Talk: Martin Geller**
HL 59.1–59.5	Wed	14:30–17:15	TRE Ma	**SKM Symposium: Semiconductor Nanophotonics - Quantum Optics and Devices (SYNP)**
HL 60.1–60.5	Wed	15:00–16:15	POT 251	**Quantum Dots: Transport**
HL 61.1–61.7	Wed	15:00–17:00	TRE Phy	**Joint Focussed Session: Theory and Computation of Electronic Structure: New Frontiers IV**
HL 62.1–62.6	Wed	15:15–16:45	POT 51	**Nitrides: Advanced Characterization Techniques**
HL 63.1–63.10	Wed	15:45–18:30	POT 151	**II-VI-Compounds**
HL 64.1–64.11	Wed	16:30–19:30	POT 251	**Quantum Wires: Transport**
HL 65.1–65.4	Wed	17:00–18:00	POT 51	**Nitrides: AlGaN**
HL 66.1–66.8	Wed	17:15–19:15	GER 38	**Joint Session: Plasmonics and Nanophotonics**
HL 67.1–67.6	Wed	18:00–19:30	FOE Anorg	**OLEDs and OFETs**
HL 68.1–68.12	Thu	10:15–13:30	FOE Anorg	**Photovoltaics: Chalcopyrites II**
HL 69.1–69.5	Thu	10:15–11:30	POT 51	**Nitrides: LEDs**
HL 70.1–70.13	Thu	10:15–13:45	POT 151	**Quantum Dots and Wires: Theory**
HL 71.1–71.11	Thu	10:15–13:15	POT 251	**Quantum Dots: Optical Properties**
HL 72.1–72.6	Thu	10:15–11:45	GER 38	**Joint Session: Organic Electronics and Photovoltaics I**
HL 73.1–73.4	Thu	12:00–13:00	GER 38	**Joint Session: Organic Electronics and Photovoltaics II**
HL 74.1–74.9	Thu	10:30–13:00	HSZ 02	**Joint Session: Quantum Optics of Solid State Photon Sources**
HL 75.1–75.6	Thu	11:15–13:00	TRE Phy	**Joint Focussed Session: Theory and Computation of Electronic Structure: New Frontiers V**
HL 76.1–76.6	Thu	11:45–13:15	POT 51	**Nitride-based Green Lasers**
HL 77.1–77.8	Thu	14:00–16:00	GER 38	**Joint Session: Organic Electronics and Photovoltaics III**
HL 78.1–78.6	Thu	16:15–17:45	GER 38	**Joint Session: Organic Electronics and Photovoltaics IV**
HL 79.1–79.10	Thu	14:30–17:15	FOE Anorg	**Photovoltaics: Mainly Silicon**
HL 80.1–80.5	Thu	14:30–17:15	POT 51	**Focussed Session: Novel Green Laser Diodes**
HL 81.1–81.10	Thu	14:30–17:15	POT 151	**Graphene: Transport**
HL 82.1–82.10	Thu	14:30–17:15	POT 251	**Ultrafast Phenomena**
HL 83.1–83.6	Thu	15:00–16:30	TRE Phy	**Joint Focussed Session: Theory and Computation of Electronic Structure: New Frontiers VI**
HL 84.1–84.7	Thu	17:15–19:15	TRE Phy	**Joint Focussed Session: Theory and Computation of Electronic Structure: New Frontiers VII**
HL 85.1–85.130	Thu	18:00–21:00	P4	**Poster Session II**
HL 86.1–86.11	Fri	10:15–13:15	FOE Anorg	**Quantum Dots: Growth and Characterization**
HL 87.1–87.12	Fri	10:15–13:30	POT 51	**ZnO: Growth and Defects**
HL 88.1–88.12	Fri	10:15–13:30	POT 151	**Lasers**
HL 89.1–89.12	Fri	10:15–13:30	POT 251	**Optical Properties II**
HL 90.1–90.5	Fri	10:30–13:00	BAR 205	**Intersectional Joint Session: Nano Plasmonic**
HL 91.1–91.5	Fri	11:15–12:45	TRE Phy	**Joint Focussed Session: Theory and Computation of Electronic Structure: New Frontiers VIII**

Annual General Meeting of the Semiconductor Physics Division

Thursday 17:15–18:00 POT 051

- Bericht
- Wahl
- Verschiedenes

HL 1: Invited Talk: Erik Stock

Time: Monday 10:15–11:00 Location: FOE Anorg

Invited Talk HL 1.1 Mon 10:15 FOE Anorg

Self-organized quantum dots as single and entangled photon emitters — •Erik Stock[1], Waldemar Unrau[1], Anatol Lochmann[1], Andrei Schliwa[1], Murat Öztürk[1], Askhat Bakarov[2], Aleksandr Toropov[2], Ilia Derebrezov[2], Vladimir Haisler[2], and Dieter Bimberg[1] — [1]Institut für Festkörperphysik, TU-Berlin, 10623 Berlin, Germany — [2]Institute of Semiconductor Physics, 630090 Novosibirsk, Russia

We realized a highly efficient single photon source (SPS) based on on a single electrically driven InGaAs/GaAs QD. Our resonant cavity light emitting diode (RLED) generates single polarized photons at a repetition rate of 1 GHz [1] exhibiting a second order correlation function $g(2)(0) = 0$. The operating temperature can be increased up to 80 K still preserving non-classical light emission.

To study the photon characteristic of the RCLED we used superconducting single photon detectors (SSPD). Photon cross correlation measurements on the exciton (X) and biexciton (XX) luminescence emission results in a time delay of less than 70 ps [2].

A promising candidate for the generation of entangled photons are QD grown on (111) GaAs substrate. Mikro-photoluminescence spectroscopy on single QDs demonstrates a fine structure splitting < 10 μeV limited by the spectral resolution of our setup [3]. This work was partly funded by the SFB 787.

[1]D. Bimberg et al., IEEE Photonics Journal 1, 58 (2009) [2]E. Stock, et al Semicond. Sci. Technol. 26, 014003 (2011) [3]E. Stock et al., Appl. Phys. Lett. 96, 093112 (2010)

15 min. break

HL 2: Electronic Structure Theory

Time: Monday 10:15–11:45 Location: POT 51

HL 2.1 Mon 10:15 POT 51

Quasiparticle band offsets at heterojunctions from GW superlattice calculations — •Christoph Freysoldt, Chandrima Mitra, and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung, Düsseldorf

The alignment of electronic bands at heterointerfaces is a key parameter for the performance of a variety of electronic devices. Theoretical calculations are an important aid in disentangling the underlying mechanisms and in designing better interfaces. Yet, the predictive capability of modern electronic structure theory's workhorse, namely density functional theory (DFT), is limited due to the band gap problem in standard functionals. Many-body perturbation theory in the GW approximation offers a systematic way to improve upon DFT, but for practical purposes, many additional approximations must be employed that affect the absolute alignment of the GW self-energy. This severely restricts the possibility to obtain quasiparticle corrections for the heterointerface band offset from separate bulk calculations. We propose an alternative route which circumvents the transferability issues of absolute GW corrections. For this, relative GW corrections are determined for a superlattice. By choosing electronic marker levels in the valence band that are spatially well localized within either AlN or GaN, and by then correcting for the intraband dispersion of self-energy effects, we extrapolate the GW corrections of the band edges. Our results for zincblende AlN/GaN and AlP/AlAs show that using absolute GW corrections from separate bulk calculations gives errors of up to 40 % compared to the full GW calculation.

HL 2.2 Mon 10:30 POT 51

Many Body calculations of Band offsets in III-V semiconductors heterostructures — •Pierre-Yves Prodhomme and Gabriel Bester — Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, 70569 Stuttgart, Germany.

Band offset are widely used to predict quantum properties of solid states. However most of the time these quantities are not calculated directly but rather rely on model for taking into account the effect of structure deformation on the band structure and a transitivity relation is assumed. Here we calculate directly the band offset of III-V heterostructures within the Many Body Perturbation Theory (in particular the GW approximation) for different strained unit cells in the stack. We propose different conditions under which the DFT computation and the deformation potential model are sufficient to obtain accurate band offsets in the case of III-V semiconductors. The validity of the transitivity relation according to the type of deformation and the type of semiconductor is discussed.

HL 2.3 Mon 10:45 POT 51

Vibrational properties of colloidal quantum dots — •Peng Han and Gabriel Bester — Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany.

To investigate the effects of carrier relaxation and dephasing via electron phonon coupling, the vibrational properties of the III-V semiconductor quantum dots are studied by density-functional perturbation theory (DFPT). Based on our calculation, decreasing the quantum dots diameters from 3.4 to 2.6 nm results in a blue shift of the longitudinal acoustic and optical vibration modes. The surface vibration modes are found to appear in the gap between the acoustic and the optical branches. In addition, the vibrational properties of the InAs/InP core/shell quantum dots are studied by projecting the vibrational eigenmodes onto the core and the shell atoms separately. The longitudinal acoustic modes of the core and shell atoms are found to be merged together, while the other modes remain distinct.

HL 2.4 Mon 11:00 POT 51

Optimized basis sets for coarse-grained electronic structure calculations of point defects — •Björn Lange, Christoph Freysoldt, and Jörg Neugebauer — Max-Planck Institut für Eisenforschung GmbH, 40237 Düsseldorf, Deutschland

Density-functional theory is a powerful tool to study the properties of point defects in the supercell approach. Yet, the size limitations make a description of the extended tails of defect states, especially for shallow defects, cumbersome. Atomic orbital basis sets are the method of choice to coarse-grain electronic structure calculations, but are in general not flexible enough for describing the unusual bonding situations, which occur in point defects. We employ a newly developed method that, based on a variational principle, allows to generate small atomic basis sets which optimally mimic the Kohn-Sham wavefunctions with a plane-wave basis set. We show that these basis sets accurately reproduce the underlying plane-wave calculation. We analyze how the atomic orbitals close to the defect are modified in comparison to their bulk counterparts. We are able to extend basis sets generated from small supercells and to reproduce the bandstructure of larger cells. Using this approach we construct and solve a reliable sparse model Hamiltonian for a shallow defect test system containing $10^3..10^4$ atoms.

HL 2.5 Mon 11:15 POT 51

EPR parameters of the dangling bond defect in crystalline and amorphous silicon: A DFT-study — •Gernot Pfanner, Christoph Freysoldt, and Jörg Neugebauer — Max-Planck Institut für Eisenforschung, Max-Planck-Strasse 1, D-40237 Duesseldorf

Thin-film a-Si:H solar cells are considered as low-cost alternatives to bulk crystalline silicon (c-Si) solar cells. A disadvantage of these devices is that their efficiency is severely limited by light-induced defects (Staebler-Wronski effect). In this context, electron-paramagnetic resonance (EPR) is a key technique to probe for the local atomic structure of defects with unpaired spins such as the silicon dangling bond. However, the assignment of the EPR signal to a specific defect structure requires comparison to theoretical models.

Using density-functional theory, we address structure-property relationships by combining systematic studies for idealized dangling-bond models in c-Si with a statistical analysis of a variety of dangling bonds in a-Si:H supercells. Our studies reveal the influence of the local ge-

ometry on sp-hybridization and delocalization. Yet, the structural variability of a-Si:H cannot be captured by these idealized defect models alone. Rather, our calculations indicate that a relatively broad distribution of dangling-bond like structures gives rise to the experimental signal supporting a recent re-evaluation of EPR parameters from multifrequency EPR.

HL 2.6 Mon 11:30 POT 51

Holographic view on nanostructure wave functions — •Gabriel Bester[1], Jie Peng[1], Wen Lei[2], Christian Notthoff[2], Axel Lorke[2], Dirk Reuter[3], and Andreas Wieck[3] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, 70569 Stuttgart, Germany — [2]Department of Physics and CeNIDE, University of Duisburg-Essen, Lotharstraße 1, 47048 Duisburg, Germany — [3]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, Universitätsstraße 150, 44780 Bochum, Germany

In this contribution we demonstrate the possibility to influence the shape of the wave-functions in semiconductor quantum dots by the application of an external magnetic field B_z. The states of the so-called p-shell, which show distinct orientations along the crystal axes for $B_z = 0$ can be modified to become more and more circularly symmetric with increasing field. Their changing probability density can be monitored using magneto-tunneling wave function mapping. Calculations of the magneto-tunneling signals are in good agreement with the experimental data and explain the different tunneling maps of the p^+ and p^--states as a consequence of the different sign of their respective phases.

W. Lei *et al.*, Phys. Rev. Lett. **105**, 176804 (2010).

HL 3: III-V-Compounds: GaAs and related Materials

Time: Monday 10:15–11:45 Location: POT 151

HL 3.1 Mon 10:15 POT 151

Dynamic nuclear polarization in n-GaAs - free versus localized electrons — •Jie Huang[1], Yuansen Chen[1], A. Ludwig[2], D Reuter[2], A. D. Wieck[2], and Gerd Bacher[1] — [1]Werkstoffe der Elektrotechnik and CeNIDE, Universität Duisburg-Essen, Bismarckstr. 81, D-47057 Duisburg, Germany — [2]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, Universitätsstr. 150,D-44780 Bochum, Germany

In spin dependent information processing using III-V semiconductors, the large electron-nuclear coupling plays an important role, e.g. in affecting the electron spin coherence through the hyperfine interaction. In our experiment, optically injected spin-polarized electrons are used to generate a dynamic nuclear polarization (DNP) in bulk n-GaAs. This results in a tiny variation of the electron Larmor precession frequency, which is probed by time resolved Kerr rotation. A saturated Overhauser field on the order of several 10 mT is obtained, depending on the helicity of the pump beam. Our experimental data indicate a significant difference of the DNP time constant for localized and itinerant electrons. This is explained by considering a model involving Fermi contact hyperfine interaction, spin exchange between donor electrons and itinerant electrons and nuclear spin diffusion.

HL 3.2 Mon 10:30 POT 151

Electron g-Factor Anisotropy in Symmetric (110)-oriented GaAs/AlGaAs Quantum Wells — •Jens Hübner[1], Huynh Thanh Duc[3], Sergej Kunz[1], Stefan Oertel[1], Michal Pochwala[3], Dieter Schuh[2], Thorsten Meier[3], and Michael Oestreich[1] — [1]Institute for Solid State Physics, Leibniz Universität Hannover, Appelstr. 2, D-30167 Hannover, Germany — [2]Institute for Experimental and Applied Physics, Universität Regensburg, D-93040 Regensburg, Germany — [3]Department of Physics, Universität Paderborn, Warburger Str. 100, D-33098 Paderborn, Germany

We demonstrate by spin quantum beat spectroscopy that in undoped GaAs/AlGaAs quantum wells even a symmetric spatial wavefunction gives rise to an asymmetric in-plane electron Landé-g-factor if the quantization axis is aligned along the [110] crystal axis. This observation emphasizes the specific symmetry sensing properties of the spin degree of freedom. Choosing the [110] quantization axis lowers the symmetry of the two dimensional system from D_{2d} to C_{2v} symmetry by removal of a mirror plane. This is similar to graded [001] quantum wells, however in the [110] case the spatial part of the wavefunction remains symmetric and only the spin dependent part, i.e., the Dresselhaus and Zeeman contributions, senses the symmetry reduction. This shows that the electron spin is a perfect meter variable to map out the internal –otherwise hidden– symmetries of a given system. The measurements are very well described within 14×14 band $\mathbf{k} \cdot \mathbf{p}$ theory and identify the intermixture of different $\mathbf{k}$-dependent Zeeman-split terms as the source for the anisotropy.

HL 3.3 Mon 10:45 POT 151

Excitonic electron spin relaxation in a (110)-GaAs quantum well — •Stefan Oertel[1], Jens Hübner[1], Dieter Schuh[2], Werner Wegscheider[3], and Michael Oestreich[1] — [1]Universität Hannover, Inst. f. Festkörperphysik, Abt. Nanostrukturen — [2]Universität Regensburg, Inst f. Experimentelle und Angewandte Physik — [3]Solid State Physics Laboratory, ETH Zürich

We detect excitonic signatures within the many body electron hole system in a specially designed 9 and 4 nm (110)-GaAs triple quantum well structure using the electron spin relaxation time τ_s as an exciton marker. The intricate exciton spin relaxation mechanism is much better resolved in these structure due to the lack of the dominant and concealing Dyakonov-Perel spin relaxation mechanism for spins aligned along this growth direction. Time- and polarization resolved photoluminescence spectroscopy yields τ_s over a large density and temperature regime. The measured spin relaxation time τ_s is in good agreement with calculations based upon the theoretical exciton spin relaxation time and the exciton fraction within the electron hole system according to the so called Saha equation.

HL 3.4 Mon 11:00 POT 151

Hole spin initialization mechanisms in 2D hole systems at low temperatures — •Michael Kugler[1], Stephan Furthmeier[1], Tobias Korn[1], Pawel Machnikowski[2], Michael Griesbeck[1], Marika Hirmer[1], Dieter Schuh[1], Werner Wegscheider[3], and Christian Schüller[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Germany — [2]Institute of Physics, Wrocław University of Technology, Poland — [3]Solid State Physics Laboratory, ETH Zurich, Switzerland

For the realization of scalable solid-state quantum-bit systems, spins in semiconductor quantum dots are promising candidates. A key requirement for quantum logic operations using holes is the generation of a resident hole spin polarization (RHSP).

Here, we report on two different mechanisms that lead to a RHSP of hole ensembles, confined in so-called natural quantum dots, in narrow GaAs/AlGaAs quantum wells at low temperatures after optical excitation. The first mechanism is driven by relaxation of the hole spins in the first few ps after excitation and leads to a RHSP pointing in the opposite direction than the optically generated hole spins after carrier recombination. It is enhanced by increased temperature, excitation density and excess carrier energy provided by detuning the laser from resonant excitation. The second mechanism is driven by applying a magnetic field and having hole and electron spins precess at different frequencies defined by their g-factors. This leads to a modified recombination behavior and therefore again to a RHSP. The interconnected electron and hole spin dynamics are well reproduced theoretically.

HL 3.5 Mon 11:15 POT 151

Optical detection of electrically-injected spin-polarization — •Roland Völkl[1], Tobias Korn[1], Andreas Einwanger[1], Mariusz Ciorga[1], Dieter Schuh[1], Werner Wegscheider[2], Dieter Weiss[1], and Christian Schüller[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, 93040 Regensburg — [2]ETH Zürich,8093 Zürich, Schweiz

An essential issue of spintronics is an effective spin injection into semiconductors. Here, we present experiments in which spin-polarized electrons are injected into n-bulk GaAs using a p+-(Ga,Mn)As/n+-GaAs Esaki diode structure.

To probe such a spin polarization, the Hanle-MOKE technique is applied. Hereby the originally in-plane oriented spins are rotated out of the plane by applying a magnetic field. The spin component perpen-

dicular to the sample plane is measured by detecting the Kerr rotation of a linearly polarized laser. The laser beam is focused through a microscope objective. Thus, a spot size around 1um is achieved. While moving the sample under the laser spot the spin polarization can be mapped. 1D as well as 2D mappings show a diffusion length of about 10 um. The spin polarization was also probed at a fixed position depending on the bias of the Esaki diode. The injected spin-polarized electrons polarize the nuclei via hyperfine interaction. By using a circularly polarized laser, additional, optically-injected spin-polarized electrons can be used to probe the local nuclear fields. Financial support by the DFG via SFB 689 is gratefully acknowledged.

HL 3.6 Mon 11:30 POT 151

Carbon doped GaAs/AlGaAs heterostructures with high mobility two dimensional hole gas — •Marika Hirmer[1], Dominique Bougeard[1], Dieter Schuh[1], and Werner Wegscheider[2] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, D 93040 Regensburg, Germany — [2]Laboratorium für Festkörperphysik, ETH Zürich, 8093 Zürich, Switzerland

Two dimensional hole gases (2DHG) with high carrier mobilities are required for both fundamental research and possible future ultrafast spintronic devices. Here, two different types of GaAs/AlGaAs heterostructures hosting a 2DHG were investigated. The first structure is a GaAs QW embedded in AlGaAs barrier grown by molecular beam epitaxy with carbon-doping only at one side of the quantum well (QW) (single side doped, ssd), while the second structure is similar but with symmetrically arranged doping layers on both sides of the QW (double side doped, dsd). The ssd-structure shows hole mobilities up to $1.2 * 10^6$ cm^2/Vs which are achieved after illumination. In contrast, the dsd-structure hosts a 2DHG with mobility up to $2.05 * 10^6$ cm^2/Vs. Here, carrier mobility and carrier density is not affected by illuminating the sample. Both samples showed distinct Shubnikov-de-Haas oscillations and fractional quantum-Hall-plateaus in magnetotransport experiments done at 20mK, indicating the high quality of the material. In addition, the influence of different temperature profiles during growth and the influence of the Al content of the barrier $Al_xGa_{1-x}As$ on carrier concentration and mobility were investigated and are presented here.

HL 4: Carbon: Diamond, Nanotubes, and Graphene

Time: Monday 10:15–13:30 Location: POT 251

HL 4.1 Mon 10:15 POT 251

Dynamical Decoupling of a single electron spin at room temperature — •Florian Dolde[1], Boris Naydenov[1], Liam T. Hall[2], Chang Shin[3], Helmut Fedder[1], Lloyd C.L. Hollenberg[2], Fedor Jelezko[1], and Jörg Wrachtrup[1] — [1]3. Physikalisches Institut and Research Center SCOPE, University of Stuttgart, Stuttgart 70659, Germany — [2]Centre for Quantum Computer Technology, School of Physics, University of Melbourne, Victoria 3010, Australia — [3])National Biomedical Center for Advanced ESR Technology, Dept of Chemistry and Chemical Biology, Cornell University, Ithaca, NY 14853, USA

The negatively charged Nitrogen-Vacancy center (NV) in diamond attracted a lot of interest lately due to the possibility of optical spin state read out of a single center and the possibility of coherent manipulations with microwaves at room temperature. Due to these unique properties the NV is an excellent candidate for room temperature quantum information processing and very sensitive magnetometry using an atom sized sensor. Here we report the increase of the coherence time T^2 of a NV by using dynamical decoupling. We show that the Carr-Purcell-Meiboom-Gill (CPMG) pulse sequence can prolong the T^2 of a single Nitrogen-Vacancy center in diamond up to 2.44 ms compared to the Hahn echo measurement where $T^2 = 390$ μs. Moreover, by performing spin locking experiments we demonstrate that with CPMG the maximum possible T^2 is reached. An application for detecting low magnetic field is demonstrated, improving the sensitivity by about a factor of two compared to the Hahn echo method.

HL 4.2 Mon 10:30 POT 251

Towards two electronic spin entangelment — •Ingmar Jakobi, Florian Dolde, Boris Naydenov, Helmut Fedder, Fedor Jelezko, and Jörg Wrachtrup — 3 Physikalisches Institut and Research Center SCOPE, University of Stuttgart, Stuttgart 70659, Germany

The negatively charged Nitrogen-Vacancy center (NV) in diamond attracted a lot of interest lately due to the possibility of optical spin state read out of a single center and the possibility of coherent manipulations with microwaves at room temperature. Due to these unique properties the NV is an excellent candidate for room temperature quantum information processing. We conducted a systematic search with ground state depletion measurements (GSD) and double electron electron resonance experiments (DEER) on implanted samples in order to identify NV pairs with a suitable distance with a strong dipolar coupling allowing for entanglement experiments.

HL 4.3 Mon 10:45 POT 251

Controlling the charge state of nitrogen-vacancy centers in diamond — •Moritz Hauf[1], Bernhard Grotz[2], Boris Naydenov[2], Markus Dankerl[1], Magalí Ros[1], Fedor Jelezko[2], Jörg Wrachtrup[2], Martin Stutzmann[1], Friedemann Reinhard[2], and José Garrido[1] — [1]Walter Schottky Institut, TU München, Garching — [2]3rd Physics Institute, University of Stuttgart

Nitrogen-vacancy defects (NV) in the diamond lattice have been extensively studied as they can act as single photon emitters with absolute photo-stability. Furthermore, they have found applications in novel fields like quantum computation and single spin magnetometry. In this context, it is of great interest to understand the effect of diamond surface termination and gain control over the charge state of NV centers in diamond. We have shown that by changing the diamond surface termination from oxygen to hydrogen, the fluorescence of the negatively charged NV (NV^-) can be suppressed, depending on the implantation energy and dose used for the creation of NV centers in diamond by low-energy nitrogen implantation. This effect is attributed to the band bending that occurs at hydrogen-terminated diamond surfaces. A two-dimensional hole gas is formed at the surface, converting the NV^- to either neutral or even positively charged NV centers. Self-consistent numerical simulations can reproduce the surface band bending and the concurrent disappearance of the NV^- fluorescence. Finally, we have demonstrated that electrostatic control of the charge state of single NV centers can be achieved by using surface-conductive diamond devices and an external gate electrode.

HL 4.4 Mon 11:00 POT 251

Electron transfer in diamond- and graphene-based hybrid systems — •Roberta Caterino, Franz Fuchs, Andreas A. Reitinger, Martin Stutzmann, Ian D. Sharp, and Jose A. Garrido — Walter Schottky Institut, Technische Universität München, Am Coulombwall 4, 85748 Garching, Germany

In bioelectronic hybrids, composed of photoreactive proteins on inorganic electrodes, the electron transfer between protein and electrode will largely determine the efficiency of the energy transfer. Electron transfer processes depend on a large variety of parameters, such as substrate density of states, protein orientation, electrode-protein distance, etc. It is thus desirable to develop advanced spectroscopic techniques which can provide spatially and energetically resolved information about electron transfer across the electrode/protein interface. We report on the characterization of functional carbon-based surfaces using standard electrochemical techniques as well as ambient and electrochemical scanning tunnelling microscopy and spectroscopy (STM/STS). We will present our work on the modification and functionalization of both diamond and graphene substrates, reporting on novel protocols to obtain an effective grafting of proteins on these carbon surfaces. We have investigated the electron transfer in these protein/ carbon hybrid structures. Using standard electrochemical spectroscopy and STS, we have been able to study the electron transfer between conductive diamond electrodes and covalently immobilized proteins. In addition, we will study how graphene modifies these interfacial phenomena on graphene/diamond hybrid electrodes.

HL 4.5 Mon 11:15 POT 251

Entwicklung und Simulation von SiC-Thyristoren mit integrierter Amplifying-Gate-Struktur — •Korbinian Kaltenecker und Jens-Peter Konrath — Dt.-Frz. Forschungsinstitut Saint-

Louis, 5 rue du General Cassagnou, F-68301 Saint-Louis, France

Siliziumcarbid (SiC) hat als Halbleitermaterial bezüglich seiner elektrischen und physikalischen Eigenschaften viele Vorteile gegenüber Silizium. Aufgrund des höheren Bandabstands, der hohen Durchbruchfeldstärke und der guten Wärmeleitfähigkeit werden SiC-Bauteile besonders im Bereich der Leistungsanwednungen entwickelt. Ein typisches Bauteil aus SiC, an dessen Umsetzung in diesem Gebiet gearbeit wird, ist der Thyristor. Zur Zeit sind Thyristoren mit einer Sperrspannung von bis 6 kV kommerziell verfügbar. Bauteile mit bis zu 12 kV Sperrspannung, die mit Pulsströmen größer 10 kA und Pulsweiten von bis zu mehreren Mikrosekunden betrieben werden können, sind Gegenstand der Forschung. Hinsichtlich der Verbesserung der Qualität und Größe der SiC-Wafer, ist nun die Entwicklung großflächiger Thyristoren möglich geworden. Die Integration einer Amplifying-Gate-Struktur in den Thyristor (AGT) ist für großflächige, auf Silizium basierenden Thyristoren ein standartmäßiges Verfahren, um den notwendigen Gate-Strom zum Anschalten des Bauteils klein zuhalten, die Zündgeschwindigkeit zu erhöhen und eine homogene Zündausbreitung zu erreichen. Dieses Verfahren soll nun auf SiC-Bauteile übertragen werden. Wir stellen hier die Realisierung von AGTs, erste experimentelle Resultate, sowie Ergebnisse der Simulation eines solchen Bauteils vor.

HL 4.6 Mon 11:30 POT 251

Dielectrophoretic assembly of field-effect transistors using sorted semiconducting carbon nanotubes — •Juliane Posseckardt[1], Yann Battie[2], Romain Fleurier[2], and Michael Mertig[1] — [1]TU Dresden, Professur für Physikalische Chemie, Mess- und Sensortechnik, 01062 Dresden, Germany — [2]LEM UMR 104 Onera-CNRS 92322 Châtillon, France

We report on the direct assembly of single-walled carbon nanotube field-effect transistors (SWCNT-FETs) by dielectrophoresis using highly enriched semiconducting carbon nanotubes.

The SWCNTs have been sorted using an improved separation technique by density gradient ultracentrifugation made in two steps. The sorted SWCNTs have been characterized by Raman and UV-vis-IR spectroscopy.

The out-of-solution guided assembly from sorted semiconducting fraction is superior in comparison to conventional assembly from unsorted fractions because of the missing necessity to break down purely metallic current bridges. By this, transistors with a high ON/OFF ratio can be produced in one step.

15 min. break

HL 4.7 Mon 12:00 POT 251

Time-resolved picosecond photocurrents in contacted carbon nanotubes — •Leonhard Prechtel[1], Li Song[2], Stephan Manus[2], Dieter Schuh[3], Werner Wegscheider[4], Nadine Erhard[1], and Alex W. Holleitner[1] — [1]Walter Schottky Institut and Physik-Department, TU München — [2]Fakultät für Physik and Center for NanoScience (CeNS), LMU, München — [3]Institut für Experimentelle und Angewandte Physik, Universität Regensburg — [4]Laboratorium für Festkörperphysik, ETH Zürich

We introduce coplanar stripline circuits to resolve the ultrafast photocurrent dynamics of freely suspended carbon nanotubes (CNTs) in the time-domain. By applying an on-chip pump-probe laser spectroscopy we demonstrate that CNTs, contacted by metal electrodes, exhibit a picosecond photocurrent response. We find a combination of an optically induced ultrafast displacement current, transport of photo-generated charge-carriers at the Fermi velocity to the electrodes, and interband charge-carrier recombination processes to dominate the ultrafast photocurrent of the CNTs.

HL 4.8 Mon 12:15 POT 251

Localized defects in single carbon nanotubes imaged with high-resolution tip-enhanced Raman spectroscopy — •Carsten Georgi and Achim Hartschuh — Department Chemie & CeNS, Ludwig-Maximilians-Universität München, Germany

Raman spectroscopy is a powerful tool to study defects in sp^2 carbon materials including carbon nanotubes, graphite and graphene [1]. Defects in the crystalline structure of these materials activate scattering by large momentum phonons giving rise to the characteristic D-band Raman signal. We imaged the D-band scattering in metallic single-walled carbon nanotubes with a spatial resolution of 15 nm using tip-enhanced Raman spectroscopy (TERS). The spatial extension of the D-band signal in the vicinity of localized defect sites was visualized and found to be about 2 nm. Furthermore, localized defects were intentionally photo-generated using the strong optical near-fields at the tip while simultaneously recording the temporal evolution of the local Raman spectrum. From these experiments, the relation between defect density and Raman D-band intensity could be derived for the investigated nanotubes. This relation is highly relevant for the characterization of carbon nanotubes via Raman spectroscopy [2].

[1] A. C. Ferrari *et al.*, Phil. Trans. R. Soc. Lond. A **362**, 2477 (2004)

[2] C. Georgi, A. Hartschuh, Appl. Phys. Lett. **97**, 143117 (2010)

HL 4.9 Mon 12:30 POT 251

Optical Absorption of Free-standing Monolayer and Bilayer Graphene in the Ultraviolet Regime — •Tobias Utikal[1,2], Dong-Hun Chae[1], Siegfried Weisenburger[1,2], Harald Giessen[2], Markus Lippitz[1,2], and Jurgen Smet[1] — [1]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany — [2]4th Physics Institute, University of Stuttgart, 70550 Stuttgart, Germany

We present direct measurements of the optical absorption of free-standing graphene and Bernal-stacked bilayer graphene from the infrared to the ultraviolet regime. In the visible part of the spectrum our data show a slowly rising absorption towards the blue spectral region. The absolute values clearly reproduce previous findings and can be attributed to a renormalized fine structure constant [1].

However, in the ultraviolet regime, the spectra show a strong increase of the absorption. Broad peaks appear at 4.55 eV and 4.52 eV for monolayer and bilayer graphene, respectively. Using a simple model we can reproduce the experimental data in the ultraviolet as well as in the infrared regime with nearly perfect agreement. From our findings we conclude that the shape of the absorption spectra is a direct consequence of the unique band structure of graphene and its bilayer.

[1] Nair et al., Science 320, 1308 (2008)

HL 4.10 Mon 12:45 POT 251

Excited state spectroscopy on a bilayer graphene double quantum dot — •Christian Volk[1,2], Stefan Fringes[1], Bernat Terres[1,2], Jan Dauber[1], Stephan Engels[1], Stefan Trellenkamp[2], Uwe Wichmann[1], and Christoph Stampfer[1,2] — [1]JARA-FIT and II. Institute of Physics B, RWTH Aachen, 52074 Aachen, Germany — [2]Institute for Bio- and Nanosystems, Forschungszentrum Jülich, 52425 Jülich, Germany

Graphene double quantum dots are promising candidates for future spin-based quantum information applications. Here, we present tunneling spectroscopy experiments on a bilayer graphene double quantum dot device which can be tuned by five all-graphene lateral gates. The device has been prepared by exfoliation of natural bulk graphite, electron beam lithography and reactive ion etching. The diameter of the quantum dots are roughly 60 nm and the constrictions acting as tunneling barriers are 30 nm in width. Low noise charge stability measurements have been carried out in order to determine the gate lever arms and the addition energies of the two coupled quantum dots. Periodically ordered triple points of high conductance are present on a wide energy range as well as faint co-tunneling lines and excited states inside the triple points. We obtain addition energies of 18 and 23 meV respectively for the two dots. High resolution measurements on individual triple points allow us to resolve the energy spectra of excited states (level spacing 1.8 meV) and the interdot coupling energy (on the order of 2-4 meV).

HL 4.11 Mon 13:00 POT 251

Disorder induced energy gaps in graphene nanoribbons — •Jan Dauber[1], Bernat Terrés[1,2], Christian Volk[1,2], Stefan Trellenkamp[2], Uwe Wichmann[1], and Christoph Stampfer[1,2] — [1]JARA-FIT and II. Institute of Physics, RWTH Aachen University, 52074 Aachen, Germany — [2]Institute of Bio and Nanosystems, Forschungszentrum Jülich, 52425 Jülich, Germany

Graphene with its unique electronic properties is one of the most promising materials for future nanoelectronic applications. However, the missing band gap in graphene makes it difficult to transfer state-of-the-art electronic device concepts to a graphene-based technology. By tailoring graphene into narrow ribbons a transport and effective energy gap can be opened, which is crucial for semiconductor related applications. We show that these effective energy gaps scale inversely with the nanoribbon width and are roughly constant as function of length. The origin of these effective energy gaps and the local resonances are

assumed to be related with the disorder potential arising from the substrate and the edge roughness. We present transport measurements on lithographically defined and etched graphene nanoribbons with focus on studying the influence of the disorder potential on the transport gaps. Treatments with hydrofluoric (HF) acid are used to change the disorder potential and result in different transport characteristics. With a short HF dip the disorder potential is significantly reduced and a complete HF release, which removes the underlying silicon oxide, leads to fully suspended graphene nanostructures with only edge roughness induced disorder and no substrate interaction.

HL 4.12 Mon 13:15 POT 251

Nonlinear elasticity of graphene and other hexagonal carbon allotropes — •Pasquale Pavone[1,2], Rostam Golesorkhtabar[1,2], Jürgen Spitaler[1,2], and Claudia Ambrosch-Draxl[1] — [1]Atomistic Modelling and Design of Materials, University of Leoben, Austria — [2]Materials Center Leoben, Forschung Gmbh, Leoben, Austria

In this work, we present a first-principles study of the linear and nonlinear elastic properties of diamond, graphene monolayers, as well as simple-hexagonal, hexagonal, and rhombohedral graphite. Calculations are performed using the pseudo-potential density-functional-theory code Quantum ESPRESSO (QE) and both the local-density and generalized-gradient approximations for the exchange-correlation energy. For each system, the Lagrangian stress tensor is calculated for distorted structures defined by given values of the Lagrangian strain. The investigation of the stress vs. strain curves allows the determination of second and higher-order elastic constants. The results we have obtained for elastic constants at different orders are discussed in comparison with experiment and previous calculations, and with results achieved using the full-potential LAPW codes WIEN2k and `exciting`. In particular, we consider the issue of numerical accuracy in the ab-initio calculation of higher-order elastic constants. Furthermore, we investigate the role of van-der-Waals interlayer interactions by using the vdW-DF extension to the QE software package.

HL 5: Innovative Systems and Devices

Time: Monday 10:15–12:30 Location: POT 06

HL 5.1 Mon 10:15 POT 06

Memristive switching in vanadium dioxide thin films — Danilo Bürger, Varun John, György Kovács, Ilona Skorupa, Manfred Helm, and •Heidemarie Schmidt — Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01314 Dresden

Memristive devices [1] exhibit an improved performance at ultra-small scales. The microscopic model for memristive behavior in oxide nanostructures often depends on the distribution of oxygen vacancies and is determined by the cation species. In 2008 HP presented the first bipolar TiO2-based memristor for resistive applications, where the drift of oxygen vacancies causes a change in the resistance of ultrathin TiO2 films [2] which can be locally modified by ion implantation [3]. We prepared vanadium dioxide (VO2) thin films with the reversible metal-insulator phase transition at the thermochromic switching temperature of around 340 K by pulsed laser deposition on (0001)-sapphire substrates and analyzed the electric-pulse-induced thermochromic switching in the VO2 gap region at room temperature due to local heating. As a result, we find the typical pinched hysteresis loop of a memristor, a repeatable switching behavior for billions of voltage pulses and switching times shorter than 50 ns in VO2 thin films.

[1] L. Chua, IEEE Transactions on Circuits Theory 18, 507 (1971). [2] D. B. Strukov, G. S. Snider, D. R. Stewart, and R. S. Williams, Nature 453, 80 (2008). [3] S. Zhou, E. Čižmár, K. Potzger, M. Krause, G. Talut, M. Helm, J. Fassbender, S. A. Zvyagin, J. Wosnitza, and H. Schmidt, Phys. Rev. B 79, 113201 (2009)

HL 5.2 Mon 10:30 POT 06

Disorder induced localization in crystalline phase-change materials — •Peter Jost[1], Theo Siegrist[1,2], Hanno Volker[1], Michael Woda[1], Philipp Merkelbach[1], Carl Schlockermann[1], and Matthias Wuttig[1] — [1]I. Physikalisches Institut (IA), RWTH Aachen University, 52056 Aachen, Germany — [2]Department of Chemical and Biomedical Engineering, Florida State University, Tallahassee, FL 32310

Phase-change materials (PCMs) are ideally suited for data storage devices employing the amorphous to crystalline phase transition. In this work[1] we report on a metal insulator transition (MIT) in the crystalline state of the pseudo-binary alloys between GeTe and Sb_2Te_3. The insulating state results from a degree of disorder which is untypically high for crystalline solids. The change of disorder upon annealing leads to the MIT. Moreover, we will demonstrate that this MIT is accompanied by a universal minimum metallic conductivity for all alloys under investigation. While MITs have been discussed as consequences of disorder induced localization (Anderson) and electron correlation effects (Mott) at the same time, the latter (Mott type) is often dominant. We will, however, show that disorder induced localization must be prevalent here. Thus, the crystalline phase of PCMs constitutes a very uncommon state of matter being equally interesting for technical applications and fundamental research on localization physics.

[1] Siegrist, T. et al. Accepted for publication in Nature Mater.

HL 5.3 Mon 10:45 POT 06

Electronic Transport Properties of Nb/InAs-Nanowire/Nb Josephson Junctions — •H. Yusuf Günel[1], Igor E. Batov[2], Hilde Hardtdegen[1], Kamil Sladek[1], Andreas Penz[1], Gregor Panaitov[3], Detlev Grützmacher[1], and Thomas Schäpers[1] — [1]Institute of Bio- and Nanosystems (IBN-1) and JARA-Fundamentals of Future Information Technology, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka, Moscow district, Institutskaya 2, 142432 Russia — [3]Institute of Bio- and Nanosystems (IBN-2) and JARA-Fundamentals of Future Information Technology, Forschungszentrum Jülich, 52425 Jülich, Germany

We experimentally studied the electronic transport properties of Nb/InAs-Nanowire/Nb Josephson junctions. Highly doped InAs nanowires were used as a weak link between two superconducting electrodes, in order to form a Josephson junction (JJs). At temperatures below the critical temperature of Nb (Tc~7K) a clear supercurrent was observed in the current-voltage characteristics. In addition, we analyzed the temperature and magnetic field dependence of the Josephson supercurrent. A complete suppression of the supercurrent was observed at a temperature of around 7K and a magnetic field of 0.5T, respectively. In detailed magnetic field dependent measurements clear oscillations were observed in the differential resistance. Furthermore, at zero magnetic field the differential resistance revealed characteristic features of multiple Andreev reflections.

HL 5.4 Mon 11:00 POT 06

low-k dielectric and amorphous SiO2 - a comparative TEM/EELS analysis — •Pradeep Singh[1], Sven Zimmerman[2], Steffen Schulz[1], Stefan Schulze[2], and Michael Hietschold[1] — [1]Chemnitz University of Technology, Institute of Physics, Chemnitz, Germany — [2]Fraunhofer ENAS, Department Back-End of Line, Chemnitz, Germany

The use of low dielectric constant materials (k<3) as a replacement of SiO2 (k=3.9) in the Back End of Line (BEOL) reduces interconnect delay, power dissipation and crosstalk noise. Current low-k dielectrics (SiCOH) prepared by the doping of methyl group in the SiO2 networks; have been studied very little from the structural point of view. In this study, we choose porous SiCOH as a low k dielectric material with dielectric constant k = 2.4 to investigate its structural, optical and electronic properties. The radial distribution function (rdf) derived from the Selected Area Electron Diffraction (SAED) allows to identify the atomic arrangement in the matrix. This gives the opportunity to investigate the structural difference between amorphous SiO2 and low-k dielectrics. Careful investigation of electron energy-loss spectroscopy (EELS) combined with TEM, provides information about the elemental composition, chemical bonding, band structure, dielectric functions, valence, and conduction electron densities. The rdf curve of porous SiCOH indicates a significant difference in density and structural arrangement as compared to amorphous SiO2.

15 min. break

HL 5.5 Mon 11:30 POT 06

Quantitative Characterization of Dielectric and Electronic Properties on the Nanometer Scale — •Matthias Fenner[1], Ferry Kienberger[1], Hassan Tanbakuchi[1], Hans-Peter Huber[2], and Markus Hochleitner[2] — [1]Agilent Technologies Inc., — [2]Christian-Doppler-Laboratory, Johannes Kepler University Linz, Austria

We report recent advances in calibrating methods for Scanning Microwave Microscopy (SMM). This combines Atomic Force Microscopy (AFM) and a Vector Network Analyzer using microwave tip sample interaction to characterize dielectric and electronic material properties on the nanometer scale. It features quantitative measurements of

1.Calibrated capacitance with attofarad sensitivity

2.Calibrated semiconductor dopant density in the range from 10^14 atoms/cm^3 to 10^20 atoms/cm^3

For capacitance calibration, a standard sample of stepped dielectric with differently sized conductive gold pads is used. Depending on the size of the various gold pads and the dielectric step height, the corresponding capacitance values ranged from 0.1 fF to 22 fF at a noise level of ~1 aF. The electrical footprint of the AFM-tip was measured on the stepped dielectric when the tip is placed on the dielectric only, resulting in an effective tip diameter of ~50 nm and tip-sample capacitance of ~5 aF. The dopant density calibration is performed by imaging the cross section of a standard sample with differently doped layers (dopant stair case) from 10^14 atoms/cm^3 to 10^20 atoms/cm^3. We present the methods for calibration as well as applications of SMM.

HL 5.6 Mon 11:45 POT 06

Si-InAs heterojunction Esaki tunnel diodes with high current densities — •Cedric Bessire, Mikael Björk, Heinz Schmid, Kirsten Moselund, Hesham Ghoneim, Siegfried Karg, and Heike Riel — IBM Research Zurich, Säumerstrasse 4, 8803 Rüschlikon, Switzerland

The tunnel field effect transistor (TFET) is considered to be one of the most promising candidates for low power operation because its turn-on characteristics can be steeper than that of conventional FETs, which could allow drastic scaling of the supply voltage. However, to date TFET implementations show poor performance of the drive current compared to conventional CMOS devices due to low tunneling probability. For high currents in TFETs degenerated semiconductors and abrupt interfaces are needed. This can be evaluated by Esaki tunnel diodes that indicate the limits of the drive current.

We report on Si-InAs heterojunctions with high tunnel current densities and negative differential resistance region in low forward bias. The p-n diodes were fabricated by growing InAs nanowires in oxide mask openings on silicon substrates. At substrate doping concentrations of 1e16 and 1e19 cm-3, conventional diode characteristics were obtained, from which a valence band offset between Si and InAs of 130 meV was extracted. For a substrate doping of 4e19 cm-3, heterojunction tunnel diode characteristics were obtained showing current densities in the range of 50 kA/cm2 at 0.5 V reverse bias. In addition, in situ doping of the InAs wires was performed using disilane to further boost the tunnel currents up to 100 kA/cm2 at 0.5 V reverse bias.

HL 5.7 Mon 12:00 POT 06

Evaluation of measurement techniques for characterization of charge trapping materials for memory applications — •Ekaterina Yurchuk, Thomas Melde, and Thomas Mikolajick — NaMLab gGmbH, Nöthnitzer Str. 64, 01187 Dresden, Germany

The charge trapping memories are based on the charge storage in isolated trap states within the gate dielectric of the field effect transistor. The trap parameters can be extracted from the charge loss dynamics, as retention measurements. The aim of the present work was to identify the most suitable measuring technique for subsequent evaluation of the trap density distribution within the memory layer.

Two methods for experimental determination of retention characteristics on SONOS (silicon-oxide-nitride-oxide-polysilicon) capacitor structures were studied. The most common approach for measuring the threshold voltage shift is the application of zero gate voltage during the wait time. On the contrary, the constant capacitance method applies a regulated gate voltage to maintain the flatband condition. The effect of temperature, program state and programming conditions on the charge loss for both measuring techniques are analyzed. The constant capacitance method allows the predefinition of the field conditions in bottom oxide and thus must be more appropriate for the extraction of trap density distribution. However, the carried out experiments and simulations of the discharging process could only partially confirm this assumption.

HL 5.8 Mon 12:15 POT 06

Silicon to nickel-silicide axial nanowire heterostructures as Bio-FETs — •Sebastian Pregl[1], Walter Weber[2], and Gianaurelio Cuniberti[1] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, 01062 Dresden, Germany — [2]NaMLab GmbH, D-01187 Dresden, Germany

Silicon Nanowire based field effect transistors (FETs) have shown to be capable of label-free and real-time detection of biomolecules in fluidic media. Antagonist binding events lead to a gating effect and therefore a change in source-drain current. Next generations of biosensor FETs have to become more sensitive and strategies have to be developed to handle sample related screening and parasitic pH effects. Our research is focused on utilization of bottom-up synthesised Schottky barrier FETs (SB-FETs) for this new kind of sensors. Silicon nanowires grown with catalytic chemical vapor deposition (CVD) are contacted to Nickel pads which form source and drain. Annealing leads to axial nickel-silicidation resulting in an atomic sharp metal-semiconductor interface and therefore a defined Schottky barrier. So build SB-FETs show inverse subthreshold slopes as low as 110 mV/dec and a high on/off current ratio. This indicates the possibility of manipulating the barrier height by applied electrical fields in a very efficient way. Using this SB-FET as a detector for biological species promises therefore a very high sensitivity. Current investigations on the nature of the sensing effect on protein adsorption are running. The effect on the sensing regions (Schottky junctions vs. channel) will be assessed.

HL 6: SKM Symposium: Elementary Processes in Organic Photovoltaics (SYOP)

Time: Monday 10:30–13:00 Location: TRE Ma

Invited Talk HL 6.1 Mon 10:30 TRE Ma

Charge separation in organic solar cells and the principle of detailed balance — •Uwe Rau[1] and Thomas Kirchartz[2] — [1]IEK5-Photovoltaics, Forschungszentrum Jülich, Germany — [2]Experimental Solid State Physics, Blackett Laboratory of Physics, Imperial College London, UK

The invention of the solar cell as an electro-optical power device dates back to the year 1954. In 1961, Shockley and Queisser derived the maximum conversion efficiency of an ideal pn-junction solar cell by applying the principle of detailed balance. This principle, known since the years 1924/25, is strictly valid only close to thermal equilibrium. Despite of this restriction, application of this principle to solar cells under illumination, i.e. in a non-equilibrium situation, is commonly accepted and successfully used even for the analysis of non-ideal solar cells. During the last two decades, new photovoltaic technologies like dye sensitized or organic solar cells have emerged from laboratories. The large difference of organic semiconductors to their inorganic counterparts challenges our general understanding of solar cells. The present contribution will start from the fundamentals of photovoltaic energy conversion and discuss the principles that are common to all these devices. In a next step, a general approach based on the principle of detailed balance is introduced that allows us to describe organic and inorganic solar cells and to highlight their different working principles. These differences have immediate consequences on the limitations, the practical design and the technical realization of the various types of devices.

Invited Talk HL 6.2 Mon 11:00 TRE Ma

Three-Dimensional Nanoscale Organization of Bulk Heterojunction Polymer Solar Cells — •Joachim Loos — University of Glasgow, School of Physics and Astronomy, Glasgow, Scotland, UK

Polymer and hybrid solar cells have the potential to become one of

the leading technology of the 21st century in conversion of sun light to electrical energy because their ease processing from solution producing printable devices in a roll-to-roll fashion with high speed and low cost. The performance of such devices critically depends on the nanoscale organization of the photoactive layer, which is composed of at least two functional materials, the electron donor and the electron acceptor forming a so-called bulk heterojunction; however, control of its volume morphology still is a challenge. In this context, advanced analytical tools are required that are able to provide information on the local volume morphology of the photoactive layer with nanometer resolution. In this contribution we introduce electron tomography as the technique being able to explore the 3D morphology or polymer and hybrid solar cells and critically discuss first results achieved.

Invited Talk HL 6.3 Mon 11:30 TRE Ma
Reliable prediction of charge transfer excitations using optimally tuned range-separated hybrid functionals — •Leeor Kronik — Weizmann Institute of Science, Rehovoth, Israel

Charge transfer excitations are an essential concept in organic photovoltaics. Typically, electron excitations are well-described from first principles using time-dependent density functional theory (DFT). However, this is not the case for charge transfer excitations, which are very poorly described by all widely used approximations within time-dependent DFT.

Here, we overcome this difficulty by presenting a broadly-applicable, non-empirical first-principles approach based on using a range-separated hybrid functional within the generalized Kohn-Sham approach to time-dependent DFT. Its key element is the optimal choice of a range-separation parameter such that Koopmans' theorem is obeyed as closely as possible. We explain the physics behind this approach and demonstrate its validity, accuracy, and advantages for determining charge transfer excitation energies. Additionally, we show that the same approach can be used for predicting fundamental gaps of finite objects directly from generalized Kohn-Sham DFT eigenvalues.

* Work performed in collaboration with T. Stein and R. Baer, Hebrew University, Jerusalem

Invited Talk HL 6.4 Mon 12:00 TRE Ma
Charge separation and recombination in organic solar cells — •James Durrant — Imperial College London

My lecture will focus on charge separation and recombination in polymer / fullerene solar cells. The talk will be based around transient optical and optoelectronic studies of yields and lifetimes of charge carriers in blend films and solar cells. Comparative studies will be presented of different materials systems, including over 20 different polymers. On the basis of these data, I will address the parameters which influencing charge separation and recombination, including the roles of interfacial energetics, interface structure and blend nanomorphology and macroscopic electric fields and how these processes impact upon device performance.

Invited Talk HL 6.5 Mon 12:30 TRE Ma
Efficient and stable organic vacuum deposited p-i-n-type tandem solar cells — •Martin Pfeiffer — Heliatek GmbH, Dresden, Germany

We report on latest progress in the field of p-i-n type tandem solar cells. An efficiency of 8.3% on an active area of 1cm* has been confirmed by Fraunhofer ISE for a tandem cell where both photoactive layers are based on bulk-heterojunctions comprising a donor-type oligomer co-deposited with fullerene C60. We discuss the remaining loss factors in the present system and the way towards further optimization. Moreover, we show that p-i-n type tandem solar cells can be extremely stable: Extrapolated lifetimes corresponding to more than twenty years of illumination have been achieved for cells with an initial efficiency of 6%. Moreover, we report on efficient modules with integrated series interconnection. Finally, we show that high efficiencies (above 6% on 1cm^2) and lifetimes (several thousand hours both in a light-soaking test and when stored at 85°C) can be achieved for p-i-n tandem cells prepared on PET foil.

HL 7: Single Photon Sources and Qbits

Time: Monday 11:00–12:30 Location: FOE Anorg

HL 7.1 Mon 11:00 FOE Anorg
Hyperfine interaction in electron spin qubits in quantum dots coupled via an optical cavity — •Julia Hildmann and Guido Burkard — Fachbereich Physik, Universitaet Konstanz, D-78457 Konstanz, Deutschland

Electron spin states in semiconductor structures represent good candidates for implementing quantum bits (qubits) [1]. Logical gates between distant qubits can be realized using a high finesse cavity and an adjustable laser field [2]. Virtual Raman transitions between an electron in the conduction band and a heavy hole in the valence band provide a controllable mechanism for single and two qubit operations. However there are several processes in semiconductor quantum dots leading to decoherence. In the time scale for the optical control of the qubit states the main source of the decoherence is due to Fermi contact hyperfine interaction with the surrounding nuclear spins (e.g. Overhauser shift of the Zeeman frequency) [3]. Here we calculate the fidelities of the two qubit operations in the presence of the nuclear spins. [1] D. Loss and D. P. DiVincenzo, Phys Rev. A 57, 120 (1998). [2] A. Imamoglu et al, Phys. Rev. Lett. 83, 4204 (1999). [3] W. A. Coish and J. Baugh, Phys. Stat. Solidi (b) 149, 1443 (2009).

HL 7.2 Mon 11:15 FOE Anorg
Single Photon Emission from a Quantum Dot in a Photonic Crystal Waveguide — •Simon Pütz, Arne Laucht, Thomas Günthner, Norman Hauke, Max Bichler, Michael Kaniber, and Jonathan J. Finley — Walter Schottky Institut, Technische Universität München, Am Coulombwall 4, D-85748 Garching, Germany

We experimentally investigate a single self-assembled InGaAs quantum dot embedded in a GaAs photonic crystal W1 waveguide as a source of single photons. We locate the position of the quantum dot by performing spatially-resolved photoluminescence experiments. Low temperature measurements performed with detection perpendicular to the surface and with detection at the cleaved end of the waveguide allow us to qualitatively compare the emission properties of the same quantum dot for the different geometries. While the relative emission intensity depends on the coupling strength of the quantum dot to the waveguide, power-dependent and time-resolved measurements show similar characteristics. Most importantly, autocorrelation measurements prove the single photon character of emission, making such a system an ideal candidate for on-chip photonic applications.

HL 7.3 Mon 11:30 FOE Anorg
Single photon emission from ultralow density InP/GaInP quantum dots — •Stefan Kremling[1], Asli Ugur[2], Sven Höfling[1], Lukas Worschech[1], Fariba Hatami[2], Ted Masselink[2], and Alfred Forchel[1] — [1]Technische Physik, Wilhelm Conrad Röntgen Research Center for Complex Material Systems, Physikalisches Institut, Universität Würzburg, Am Hubland, D-97074 Würzburg — [2]Department of Physics, Humbold Universität zu Berlin, Newtonstrasse 15, D-12489 Berlin

We have investigated ultralow-density InP quantum dots (QDs) in $In_{0,48}Ga_{0,52}P$. The QDs were grown using gas-source molecular-beam epitaxy (GSMBE) with ultralow growth rate. InP QDs emitting in the visible red spectral range and therefore they are ideal candidates for free space single photon applications, as Si avalanche photodiodes (APD) have their maximum efficiency in this spectral region.

Autocorrelation measurements under cw excitation were performed with a single QD and a pronounced antibunching dip was observed. Furthermore we investigated the electronic structure and magneto-optical properties. In-plane anisotropy will reduce the point group symmetry and therefore annihilate the spin degeneration and the bright exciton doublet splits into two linearly combined states, separated by a fine structure splitting. At zero magnetic field, the quantum dots show a large perpendicular linearly polarized fine structure splitting up to $320\mu eV$. Magneto-optical measurements in Faraday geometry exhibit a diamagnetic shift of $4\mu eV/T^2$ and Zeeman splitting with an effective exciton g-factor of ≈ 1.

HL 7.4 Mon 11:45 FOE Anorg

Excitation pulse width dependence of triggered single–photon emission from InP/(Al,Ga)InP quantum dots — •Christian Kessler[1], Matthias Reischle[1], Wolfgang-Michael Schulz[1], Marcus Eichfelder[1], Robert Rossbach[1], Michael Jetter[1], Paul Gartner[2], Matthias Florian[2], Christopher Gies[2], Frank Jahnke[2], and Peter Michler[1] — [1]Institut für Halbleiteroptik und Funktionelle Grenzflächen, Universität Stuttgart, Allmandring 3, 70569 Stuttgart — [2]Institut für Theoretische Physik, Universität Bremen, Postfach 330 440, 28334 Bremen

Compact and efficient single–photon sources are a key component for future applications such as quantum cryptography and quantum communication. Electrically excited semiconductor quantum dots (QDs) are a promising approach and cover a wide emission wavelength range, depending on the material system. Recently, it was demonstrated, that InP QDs, which emit in the technologically important red spectral range, show triggered single photon emission ($g^{(2)}(0) = 0.24$) up to 200 MHz excitation rate [1]. However, the nonzero $g^{(2)}(0)$–value could not fully be assigned due to background emission.

Here we demonstrate the influence of the finite excitation pulse width on the second–order correlation function and thereby the quality of the single–photon emission. We propose that a second exciton is captured if recombination occurs prior the end of the excitation pulse and thus leading to emission of a second photon. This mechanism is compared to a theoretical model and a good agreement is found.

[1] M. Reischle et al., APL 97, 143513 (2010)

HL 7.5 Mon 12:00 FOE Anorg

Spectroscopy of electrically controlled intentionally positioned and shape engineered single InAs quantum dots — Minisha Mehta[1], Dirk Reuter[2], Andreas D. Wieck[2], Stefan Michaelis de Vasconcellos[1], Artur Zrenner[1], and •Cedrik Meier[1] — [1]Physics Department ,Paderborn, Germany — [2]Applied Solid State Physics, Ruhr-University of Bochum, Bochum, Germany

Precise control of position and electronic/excitonic states of self-assembled quantum dots (QDs) might open exciting options towards single QD devices. We report the realization of an electrically driven single photon source by integrating an epitaxial InAs QD within a micron sized GaAs based p-i-n junction device. Two different growth techniques were employed: QD position control was achieved using site-selective growth of InAs QDs on focused ion beam (FIB) patterned GaAs surfaces. Engineering of electronic/excitonic states was achieved utilizing the growth of flushed InAs QDs on smooth GaAs surface via MBE. After the complete growth of p-i-n diode-like structure, FIB patterning and etching was used to fabricate LEDs having active area of 2×2 μm^2. Then, carrier injection and subsequent radiative recombination from site-selective and flushed InAs QDs was investigated individually. Few or single dots are expected to be electrically addressed in these devices. The result from micro-electroluminescence (EL) shows single dot characteristics from both devices. The EL spectra consist of sharp emission lines and their dependence on injection current is presented. Thus, these results suggest a promising pathway for quantum devices [1]. [1] M. Mehta et al., Appl. Phys. Lett. 97, 143101 (2010).

HL 7.6 Mon 12:15 FOE Anorg

SiGe-quantum dot arrays for Single Photon Detection — •Jürgen Moers[1,2], Natalia P. Stepina[3], Julian Gerharz[1,2], Anatoly V. Dvurechenskii[3], and Detlev Grützmacher[1,2] — [1]Institute of Bio- and Nanosystems, Forschungszentrum Jülich, D 52425 Jülich, Germany — [2]Jülich Aachen Research Alliance — [3]Institute of Semiconductor Physics, Russian Academy of Science, 630090 Novosibirsk, Russia

Emission and detection of single photons is required for a broad range of future device applications. In this work a Si based single photon detector employing hopping transport in densely packed Ge quantum dot (Ge-QD) arrays is proposed. The hopping transport through a high-density Ge-QDs array crucially depends on the average occupation of the Ge-QD array. Changing the charge state of one QD by illumination causes a change in the conductance of the whole array. Thus, step-like variations of the conductance due to the absorption of single photons and hence carrier generation in one single dot is noticeable. Time resolved 4-point measurements of the conductance of the device at 4.2K were performed. A fiber coupled laser with 1.55 μm wavelength and initial laser power of 1 mW was used for illumination. To get extremely low light intensity the initial laser power was attenuated up to 60 dB. The conductance traces of the device show step like changes due to single Ge-QD charging and discharging. It could be shown, that the number of these events depends linearly on the light intensity, which is a prerequisite for single photon detection.

HL 8: Joint Focussed Session: Thin Film Chalcogenide Photovoltaics I

Time: Monday 11:00–13:00 Location: GER 37

Topical Talk HL 8.1 Mon 11:00 GER 37

Cu(In,Ga)Se$_2$ solar cells: the importance of lateral variations of the absorber quality — •Susanne Siebentritt — University of Luxembourg, Laboratory for Photovoltaics, Belvaux, Luxembourg

Thin film solar cells are considered the second generation of photovoltaic technologies, because of their considerable cost reduction based on the small amounts of material and energy used in production. Among these technologies solar cells based on Cu(In,Ga)Se$_2$ show the highest efficiencies in the lab as well as in industry. Record efficiencies above 20 % have been reached with these polycrystalline solar cells.

It becomes more and more evident that lateral inhomogeneities, most prominently grain boundaries, limit the efficiency. Electrostatic band bending at grain boundaries appear a major obstacle for higher open circuit voltages. Fluctuations of the band gap and the quasi-Fermi level splitting have been determined by laterally resolved photoluminescence. Some of these variations can be related to lateral changes of the Cu supply during growth - with far reaching consequences for the design of preparation processes.

Topical Talk HL 8.2 Mon 11:30 GER 37

Efficient Photovoltaic Devices using Multinary Chalcogenide Semiconductors — •Hans-Werner Schock and Thomas Unold — Helmholtz Zentrum Berlin für Materialien und Energie, Hahn-Meitner Platz 1, 14109 Berlin, Germany

Multinary compounds like Cu(In,Ga)S,Se$_2$ are very promising materials for thin film solar cells currently reaching photoconversion efficiencies beyond 20 % for small device areas. The tolerance of chalcopyrite semiconductors regarding grain structure and defects allows to fabricate Cu(In,Ga)Se$_2$ thin films with a variety of deposition technologies and significant differences in the growth parameters and composition. In the long term, modifications of materials and devices are needed in order to overcome limitations by the use of rare elements e.g replacing indium by the combination of a group II and a group IV element to form the kesterite compound Cu_2ZnSnS_4. Advanced methods for film characterisation facilitate the analysis of such new materials, also in-situ during film growth. The combination of analytical methods based on x-ray methods, electron beams and optical and electrical spectroscopy give insights in the microstructure and related electronic properties of the absorber films. Due to the large degrees of freedom in multinary materials, analysis and control of structural and electronic inhomogeneities is essential to reach efficient photoconversion.

Topical Talk HL 8.3 Mon 12:00 GER 37

From Micro Meter to Mega Watt: Pentanary Chalcopyrite Thin film Solar Cells — Joerg Palm, Alejandro Avellan, •Thomas Dalibor, Stefan Jost, Helmut Vogt, Thomas Niesen, Paul Mogensen, and Franz Karg — AVANCIS GmbH & Co KG, Otto-Hahn Ring 6, 81739 München

CIS based thin film solar cells and modules are currently entering the phase of mass production with hundreds of megawatts capacity per year. This presentation illustrates how materials and device research in cooperation between industrial R&D and university groups significantly support the development of highly efficient solar cells. The pentanary chalcopyrite absorber film based on Cu, In, Ga, Se and S is preferably formed in a two stage process by chalcogenization of metal precursor films. The understanding of the reaction paths from metals via binaries to the pentanary phase has been deepened by X-ray diffraction studies. The chalcopyrite/II-VI hetero-junction is a com-

plex interface between absorber surface region, buffer layers and the transparent conducting oxide. Several heterojunction partners are being investigated in terms of device efficiency, band alignment and interface structure. The physical processes involved in layer removal for monolithic interconnection completely change while going from mechanical patterning via nanosecond pulsed laser to ultrashort laser pulses. Device simulation helps identifying loss mechanisms in the solar cell structure. In the AVANCIS pilotline modules of size 30cm x30cm are processed with a record efficiency well above 15%. We finally present the realization of a mass production process at AVANCIS.

Topical Talk HL 8.4 Mon 12:30 GER 37

Electrical Characterization of Cu(In,Ga)(Se,S)$_2$ -Based Solar Cells at Low Temperatures — •Udo Reislöhner — Friedrich-Schiller-Universität Jena, Physikalisch-Astronomische Fakultät, Institut für Festkörperphysik, Max-Wien-Platz 1, D-07743 Jena, Germany

Thin-film solar cells based on Cu(In,Ga)(Se,S)$_2$-absorbers are industrially produced as mass product on a high level of quality. Due to rising production capacities and promising non-vacuum processes like chemical deposition or printing techniques a further cost reduction is expected. But contrary to the great success in production is the peculiar lack of comprehension concerning basic electrical spectroscopy of band-gap levels in this material system. A prominent example is the so called N1-defect observed by capacitance based methods like thermal admittance spectroscopy (TAS) and DLTS. It has unusual properties, e.g. a continuous shift of its band-gap level after moderate annealing, and has been controversially discussed for longer than a decade. However, these measurements extend to temperatures well below 200K and thereby overlap with the temperature domain where charge carrier transport by hopping is expected in the absorber. By consequently considering the impact of hopping transport on the capacitance measurement a hitherto undiscovered reason for a TAS-signal is found and the N1-signal is shown not to be correlated with a defect. Instead, this signal is generated by the freezing-out of carrier mobility with decreasing temperature when hopping conduction prevails. The consequence of this finding on electrical measurements and defect spectroscopy at Cu(In,Ga)(Se,S)$_2$-based solar cells will be discussed.

HL 9: Joint Focussed Session: Transparent Conductive Oxides I

Time: Monday 11:15–13:00 Location: WIL A317

Topical Talk HL 9.1 Mon 11:15 WIL A317

Surface and Bulk Properties of Post-Transition Metal Oxide Semiconductors — Philip D.C. King, Sepehr Vasheghani Farahani, Tim D. Veal, and •Chris F. McConville — Department of Physics, University of Warwick, Coventry, CV4 7AL UK

Oxide semiconductors have become of great interest lately with enormous opportunities for new uses that will potentially improve existing materials and device applications. The fact that some of these materials, such indium tin oxide, in a relatively low quality form, have seen significant industrial use as transparent conductors has perhaps contributed to the belated recognition of the possibilities as semiconductors in their purer form. Here, the surface and bulk electronic properties of epitaxially grown high-quality oxide semiconductors (In_2O_3, CdO, and ZnO) will be discussed. Optical, electronic and structural properties of these semiconducting oxide films will be presented. The valence band density of states and the surface electronic properties of these oxide semiconductors have been studied using high-resolution photoemission spectroscopy and compared with theoretical band structure calculations. A common property of these oxide semiconductors is found to be the presence of a surface electron accumulation layer, in marked contrast to the electron depletion generally observed at the surfaces of conventional semiconductors. Additionally, hydrogen is found to be a donor and any native defects have a propensity to be donors in already n-type material. The origin of these phenomena will be discussed in terms of the band structure and intrinsic properties of these materials.

Topical Talk HL 9.2 Mon 11:45 WIL A317

***Ab-initio* calculation of electronic and optical properties of transparent conductive oxides** — •André Schleife[1,3], Claudia Rödl[1], Frank Fuchs[1], Jürgen Furthmüller[1], Benjamin Höffling[1], Karsten Hannewald[1], Patrick Rinke[2], Joel Varley[3], Anderson Janotti[3], Chris G. Van de Walle[3], and Friedhelm Bechstedt[1] — [1]IFTO and ETSF, FSU Jena, Germany — [2]FHI and ETSF, Berlin, Germany — [3]Materials Department, UC Santa Barbara, USA

Parameter-free calculations are a modern and sophisticated complement to advanced experimental techniques when exploring the properties of materials. Due to the rapidly increasing computing power they promise a deep understanding of the underlying physics also for more complex transparent conductive oxides.

We take the excitation aspect of photoemission processes into account by calculating the quasiparticle electronic structure using the modern HSE03+G_0W_0 framework. Solving a Bethe-Salpeter equation for the optical polarization function allows us to account for excitonic and local-field effects that govern the optical absorption.

After an introduction into these recent theoretical-spectroscopy techniques we apply them to ZnO, SnO_2, In_2O_3, and Ga_2O_3. We present results for the electronic band structure (including spin-orbit coupling), the band alignment, dielectric functions, exciton binding energies, and optical oscillator strengths. The influence of a degenerate electron gas, which occurs in these typically n-type materials, is investigated. Our findings are discussed with respect to available experimental results.

Topical Talk HL 9.3 Mon 12:15 WIL A317

Bulk semiconducting oxides: crystal growth and physical properties — •Roberto Fornari — Leibniz Institute for Crystal Growth, IKZ, Max-Born-Str. 2, 12489 Berlin

Semiconducting oxides have attracted considerable interest in the last few years. In addition to the widely studied ZnO, much attention has recently been devoted to Ga2O3, In2O3 and SnO2. The epitaxial growth has already been achieved on different hetero-substrates; however due to the relatively poor crystallographic quality of the obtained layers it was not possible to get devices or even reliably measure their physical properties so far. It is thus urgent to provide homo-substrates which may allow the deposition of high-quality epilayers with low residual carrier density and fewer extended defects. IKZ has recently undertaken an effort to grow large single crystals of these oxide compounds. In this presentation the growth of transparent semiconducting Ga2O3 single crystals will be reviewed. Single crystals with diameter of 18 mm diameter and 50-60 mm length were grown along the b-axis from an Iridium crucible under a dynamic protective atmosphere. The transmission in IR-region was directly correlated with the free carrier concentration and was found to depend on the growth atmosphere and/or post growth annealing. Typical electrical properties at room temperature are: resistivity = 0.12 Ohmcm, electron concentration = 2-5E17 cm-3 and mobility = 110 cm2/Vs; these results seem to derive from a donor level with activation energy of about 32 meV. Results of thermodynamic calculations, dislocation density studies, ICP-OMS, DTA, EPR and High Resolution TEM are also presented.

HL 9.4 Mon 12:45 WIL A317

The electronic properties of β -Ga_2O_3 — •Mansour Mohamed[1], Christoph Janowitz[1], Isaak Unger[1], Zbigniew Galazka[2], Justin R. Weber[3], and Recardo Manzke[1] — [1]Humboldt-Universität zu Berlin, Institut für Physik, Newtonstr. 15, 12489 Berlin, Germany — [2]Leibniz-Institut für Kristallzüchtung, Max-Born-Str. 2, 12489 Berlin, Germany — [3]Materials Department, University of California, Santa Barbara, California 93106-5050, USA

Ga_2O_3 belongs to the group of transparent conducting oxides (TCOs) with a wide band gap. It exhibits the largest band gap with E_g = 4.9 eV [1] and thus a unique transparency from the visible into the UV region. The n-type high-quality β -Ga_2O_3 single crystals were grown by the Czochralski method [2]. The crystals were characterized by different techniques (LEED, STM). The experimental valence band structure of β-Ga_2O_3 was determined by high-resolution angle-resolved photoelectron spectroscopy (ARPES) utilizing synchrotron radiation. The calculated band structure was determined using advanced density functional theory (DFT) calculations employing hybrid functionals and projector augmented wave (PAW) potentials. From theory, we obtained a direct band gap of 4.87 eV and a slightly smaller indirect band gap of 4.83 eV, with the valence-band maximum (VBM) located

slightly away from the M symmetry point. The experimental band structure of β-Ga_2O_3 is compared and discussed with the theoretical calculations. The effect of changing the temperature from 300K to 20K on the experimental band structure β-Ga_2O_3 was studied.

HL 10: Joint Focussed Session: Theory and Computation of Electronic Structure: New Frontiers I

Time: Monday 11:15–13:00 Location: TRE Phy

Topical Talk HL 10.1 Mon 11:15 TRE Phy

Range separation: success, doubts and perspectives — •Andreas Savin — CNRS and UPMC Univ Paris 6, Laboratoire de Chimie Theorique, F-75252 Paris, France

The difficulty of finding simple approximations for density functionals can be alleviated by passing some of the exchange and correlation description to a wave function. A way to produce such hybrids is to consider that for short-range inter-electronic separations exchange and correlation effects are transferable and thus able to be captured by simple models.

Range-separated hybrids can be applied to different levels of density functional approximation (LDA, GGA, ...) and wave function approximation (single determinant, second order perturbation theory, RPA, coupled cluster, ...).

The methods do not bring significant improvement in most fields of application where density functional approximations have been successful. However, they improve accuracy when usual approximations fail, such as van der Waals interactions [1], or where self-interaction becomes an important issue. The computational effort is smaller than for the corresponding wave function method, mainly because smaller basis sets can be used.

Finally, some unexplored path / open questions will be discussed, such as the choice of the interaction operator, improving the density functional approximation, or the role of mixed "short-range/long-range terms".

[1] W. Zhu, et al, J. Chem. Phys., 132, 244108 (2010).

HL 10.2 Mon 11:45 TRE Phy

Van der Waals interactions in semiconductor solids — •Guo-Xu Zhang, Alexandre Tkatchenko, Joachim Paier, Heiko Appel, and Matthias Scheffler — Fritz-Haber-Institut der MPG, Berlin, Germany

The binding in semiconductor solids arises mainly from the covalent hybridization of atomic orbitals. Hence, it is typically assumed that van der Waals (vdW) interactions play a minor role for their cohesion. In order to probe this conventional wisdom we develop a method to calculate accurate long-range vdW coefficients for ions and atoms in crystals. We first assess the validity of the Clausius-Mossotti relation between the polarizability and dielectric function for bulk semiconductors by comparing periodic TDDFT calculations to direct extrapolation of the frequency-dependent TDDFT polarizability for finite clusters. We find a good agreement between these two approaches for computing vdW $C_6(V)$ coefficients for a broad variation in the unit cell volume V for diamond, Si, and Ge crystals. When using TDDFT@HSE with the Nanoquanta kernel, the volume-dependent dielectric constant of Si and Ge is in excellent agreement with experimental data. The crystal-field screening reduces the vdW coefficients by a factor of two compared to corresponding free-atom and effective hybridized $C_6[n(r)]$ values [1]. The use of accurate $C_6(V)$ coefficients in the PBE+vdW method [1] improves cohesive properties of Si and Ge in comparison to experimental data. [1] A. Tkatchenko and M. Scheffler, Phys. Rev. Lett., **102**, 073005 (2009).

HL 10.3 Mon 12:00 TRE Phy

Van der Waals interactions in complex materials: Beyond the pairwise approximation — •Alexandre Tkatchenko[1], Robert A. DiStasio Jr.[2], Roberto Car[2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany — [2]Princeton University, NJ, USA

Despite the well-known fact that van der Waals (vdW) interactions are many-body in nature and the polarizability is a non-local function, popular vdW-DF [1] and DFT+vdW [2] methods are based on (semi)-local approximations for the polarizability and only model the pairwise part of vdW interactions. Here we show how to go beyond the pairwise (semi)-local approximation to vdW interactions by coupling the recently developed TS scheme [2] with the Fluctuating-Coupled-Dipole Model (CFDM) [3]. The TS scheme provides parameter-free input atomic polarizability distributions and the CFDM allows to model both polarizing and depolarizing local fields, and captures the many-body nature of vdW interactions. Results are presented for small and medium-size molecules, as well as solids. We find that the many-body screening plays a major role in modifying the polarizability of large systems. Our results for vdW coefficients in semiconductor clusters and solids are in excellent agreement with TDDFT calculations. [1] M. Dion *et al.*, Phys. Rev. Lett., **92**, 246401 (2004); [2] A. Tkatchenko and M. Scheffler, Phys. Rev. Lett., **102**, 073005 (2009); [3] M. W. Cole *et al.*, Mol. Simul. **35**, 849 (2009).

HL 10.4 Mon 12:15 TRE Phy

The random phase approximation and beyond: an assessment for molecular binding energies and reaction barrier heights — •Xinguo Ren[1], Joachim Paier[2], Patrick Rinke[1], Andreas Grüneis[3], Georg Kresse[3], Gustavo E. Scuseria[4], and Matthias Scheffler[1] — [1]Fritz Haber Institute (Berlin) — [2]Humboldt University (Berlin) — [3]University of Vienna (Vienna) — [4]Rice University (Houston)

The random phase approximation (RPA) for the correlation energy has become a promising approach for describing electronic systems in various bonding situations. Recent efforts have focused mainly on correcting the general tendency of RPA to underestimate bond strengths e.g. by adding corrections from second-order screened exchange (SOSEX) [1,2] or single excitations (SE) [3]. In this work, we systematically assess the influence of SOSEX, SE and their combinations on the atomization energies of the G2-I molecular set, as well as the chemical reaction barrier heights of the HTBH38/04 and NHTBH38/04 benchmark sets [4]. We find that RPA+SOSEX+SE applied as a perturbation to the PBE exchange-correlation functional gives the most balanced description. However, for reaction barrier heights RPA based on PBE turns out to be better and is surprisingly accurate. The underlying mechanism governing the performance of RPA and its variants in different circumstances will be analysed. [1] A. Grüneis *et al.*, J. Chem. Phys. **131**, 154115 (2009). [2] J. Paier *et al.* J. Chem. Phys. **132**, 094103 (2010). [3] X. Ren *et al.*, arXiv:cond-mat/1011.2724. [4] Y. Zhao *et al.* J. Phys. Chem. A **109**, 2012 (2005)

HL 10.5 Mon 12:30 TRE Phy

Au_N clusters (N=1-6) supported on MgO(100) surfaces: the effect of exact exchange and dispersion interactions on adhesion energies. — •Lauro Oliver Paz-Borbón[1], Giovanni Barcaro[2], Alessandro Fortunelli[2], Sergey Levchenko[1], and Matthias Scheffler[1] — [1]Fritz Haber Institut der Max Planck Gesellschaft, Berlin. — [2]Istituto per i Processi Chimico-Fisici del Consiglio Nazionale delle Ricerche, Pisa.

Understanding the interaction between a metal nanoparticle and an oxide surface is a prerequisite for further development of nanocatalysts displaying tailor-made properties. In this work, we study the interaction of an Au adatom and Au_N clusters (N=2-6) supported on pristine and defected MgO(100) surfaces, using a DFT all-electron full-potential approach [1], under a hierarchy of exchange-correlation (XC) functional approximations: ranging from the generalized gradient approximation (PBE and RPBE) to hybrid functionals (PBE0, HSE06) and exact exchange (EX) plus correlation in the random phase approximation (EX-cRPA/cRPA+). Our results for the Au adatom at the oxygen site show that, by reducing the *self-interaction error* (SIE) through the inclusion of EX, smaller adhesion energies values are found when compared to those calculated using hybrid and semi-local functionals; concurrently, the diffusion energy barrier increases. Dispersion interactions [2] are found to play a crucial role in determining the energetics of Au_N clusters. [1] Blum, V. *et al.*, *Computer Physics Communications* 2009, 2175, 180. [2] Tkatchenko, A., Scheffler, M., *Phys.*

Rev. Lett. 2009, 102, 073005.

HL 10.6 Mon 12:45 TRE Phy

One dimensional model systems in time-dependent density functional theory — •Nicole Helbig[1], Johanna I. Fuks[1], Ilya V. Tokatly[1,2], and Angel Rubio[1,3] — [1]ETSF Scientific Development Centre and Universidad del País Vasco, San Sebastián, Spain — [2]IKERBASQUE, Basque Foundation for Science, Bilbao, Spain — [3]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

We present a local density approximation (LDA) for one-dimensional (1D) systems interacting via the soft-Coulomb interaction based on quantum Monte-Carlo calculations. Results for the ground-state energies and ionization potentials of finite 1D systems show excellent agreement with exact calculations, obtained by exploiting the mapping of an N-electron system in d dimensions, onto a single electron in $N \times d$ dimensions properly symmetrized by the Young diagrams. We conclude that 1D LDA is of the same quality as its three-dimensional (3D) counterpart, and we infer conclusions about 3D LDA. The linear and non-linear time-dependent responses of 1D model systems using LDA, exact exchange, and the exact solution are investigated and show very good agreement in both cases, except for the well known problem of missing double excitations. Consequently, the 3D LDA is expected to be of good quality beyond linear response. We employ the 1D LDA and exact exchange functionals to investigate the description of Rabi oscillations in time-dependent density functional theory and show that adiabatic approximations to the exchange-correlation potential lead to detuned Rabi oscillations.

HL 11: Transport: mainly Theory

Time: Monday 12:00–13:15 Location: POT 51

HL 11.1 Mon 12:00 POT 51

Two-dimensional correlation spectroscopy as new tool in noise spectroscopy — •Sebastian Starosielec, Jörg Rudolph, and Daniel Hägele — AG Spektroskopie der kondensierten Materie, Ruhr-Universität Bochum

The measurement of fluctuations, e.g. spin fluctuations via Spin Noise Spectroscopy reveals intrinsic properties of physical systems even in thermal equilibrium. However, the frequency-resolved power spectra do not represent all the system's dynamical properties. For example, an inhomogeneously broadened spectral feature cannot be distinguished from a purely homogeneously broadened signal by the usually measured noise power spectrum. In 2010, Liu et.al. showed in a theoretical example that the homogeneous linewidth of a single spin in a semiconductor quantum dot can be determined from third-order correlations of the measured time-dependent Faraday-signal even in the presence of inhomogeneous broadening [1].

We have implemented a spectrum analyzer for two-dimensional correlation spectroscopy measuring $S^{\mathrm{corr}}(\omega,\omega') = \langle I_\omega I_{\omega'}\rangle - \langle I_\omega\rangle\langle I_{\omega'}\rangle$ up to 90 MHz, with I_ω being the frequency dependent intensity of the time dependent signal [2]. S^{corr} allows to distinguish between the homogenous and inhomogenous broadening. We discuss a broad range of application for S^{corr} including the detection of critical dynamics at second order phase transitions and the detection of coherent signals on a large background of noise.

[1] R.B. Liu et al., New J. Phys. 12, 013018 (2010)
[2] S. Starosielec et al., Rev.Sci.Instrum. 81, (to appear Dec. 2010).

HL 11.2 Mon 12:15 POT 51

Direction Dependence of Spin Relaxation in Confined 2D Systems — •Paul Wenk[1] and Stefan Kettemann[1,2] — [1]School of Engineering and Science, Jacobs University Bremen, Bremen 28759 — [2]Asia Pacific Center for Theoretical Physics and Division of Advanced Materials Science Pohang University of Science and Technology (POSTECH) San31, Hyoja-dong, Nam-gu, Pohang 790-784, South Korea

Spin dynamics in semiconductors have been studied for decades, but still the prime condition for building spintronic devices, namely the understanding of spin relaxation, is not satisfactorily fulfilled. In this talk we present the dependence of spin relaxation on the direction of the quantum wire under Rashba and Dresselhaus (linear and cubic) spin orbit coupling. Comprising the dimensional reduction of the wire in the diffusive regime, the lowest spin relaxation and dephasing rates for (001) and (110) systems are found. The analysis of spin relaxation reduction is then extended to non-diffusive wires and we show that, in contrast to the theory of dimensional crossover from weak localization to weak antilocalization in diffusive wires (PRL98.176808, PRB81.125309), the relaxation due to cubic Dresselhaus spin orbit coupling is reduced and the linear part shifted with the number of transverse channels.

HL 11.3 Mon 12:30 POT 51

Anomalous Cherenkov spin-orbit sound — •Sergey Smirnov — Institut für Theoretische Physik, Universität Regensburg

The Cherenkov effect is a well known phenomenon in the electrodynamics of fast charged particles passing through transparent media. If the particle is faster than the light in a given medium, the medium emits a forward light cone. This beautiful phenomenon has an acoustic counterpart where the role of photons is played by phonons and the role of the speed of light is played by the sound velocity. In this case the medium emits a forward sound cone. Here, we show that in a system with spin-orbit interactions in addition to this normal Cherenkov sound there appears an anomalous Cherenkov sound with forward and backward sound propagation [1]. Furthermore, we demonstrate that the transition from the normal to anomalous Cherenkov sound happens in a singular way at the Cherenkov cone angle. The detection of this acoustic singularities therefore represents an alternative experimental tool for the measurement of the spin-orbit coupling strength.

[1] S. Smirnov, arXiv:1010.4002 (2010)

HL 11.4 Mon 12:45 POT 51

Stochastic resonance in nanoelectronic devices — •Fabian Hartmann[1], David Hartmann[1], Peter Kowalzik[1], Alfred Forchel[1], Luca Gammaitoni[2], and Lukas Worschech[1] — [1]Technische Physik, Physikalisches Institut, Universität Würzburg and Wilhelm Conrad Röntgen Research Center for Complex Material Systems, Am Hubland, D-97074 Würzburg, Germany — [2]NiPS Laboratory, Dipartimento di Fisica, Universita di Perugia, I-06123 Perugia, Italy, and Istituto Nazionale di Fisica Nucleare, Sezione di Perugia, I-06123 Perugia, Italy

Noise degrades the performance of any device. This simple statement is not true if principle associated with Stochastic Resonance (SR) comes into play. Here the output exhibits a maximum signal-to-noise ratio (SNR) for noise floors unequal to zero. The authors have fabricated submicron-sized nanoelectronic devices and tested the noise activated response in these bistable devices under weak periodic modulation. We demonstrate that the weak periodic input can be synchronized with an optimum amount of noise and thus the operation condition of SR is fulfilled.

HL 11.5 Mon 13:00 POT 51

Random-telegraph-signal noises due to defects in ballistic nanotube transistors — •Neng-Ping Wang[1] and Stefan Heinze[2] — [1]Physics Department, Ningbo University, Fenghua Road 818, Ningbo 315211, P.R. China — [2]Institute of Theoretical Physics and Astrophysics, Christian-Albrechts-Universitaet zu Kiel, Leibnizstr. 15, D-24098 Kiel, Germany

Recently, there has been remarkable progress in carbon nanotube field-effect transistors (CNFETs). High performance and even ballistic transport have been demonstrated, and there is increasing focus on integrating such transistors into operational device circuits. However, all materials exhibit some low-frequency electrical noise which appears as 1/f noise and random telegraph signals (RTSs). The low-frequency noise increases inversely with the system size, so it is important to understand microscopic aspect of RTS noise in nanotubes.

Here we report calculations of the RTS noises due to single trapped charges in CNFETs using the non-equilibrium Greens function method in a tight-binding approximation. We find that the RTS noise amplitude depends on the nanotube-direction position of the charge. When a trapped charge is farther from the source (or drain) lead and closer to the middle of the channel, the RTS noise in the turn-on regime increases, while the RTS noise in the "on" regime decreases. We calculate

the electron potential along nanotube and explain such dependence of the RTS noise. We examine also how the RTS noise depends on both the thickness and dielectric constant of the gate dielectric, suggesting routes to reduce electrical noise.

HL 12: Quantum Dots and Wires: Arsenides

Time: Monday 12:00–13:30 Location: POT 151

HL 12.1 Mon 12:00 POT 151

Calculation of the Diameter dependent Polytypism in GaAs Nanowires — •Volker Pankoke, Peter Kratzer, and Sung Sakong — Fakultät für Physik Universität Duisburg-Essen, Lotharstr. 1,47048 Duisburg, Germany

The formation energies of GaAs nanowires (NWs) have been calculated from a structural motif approach, supporteed by first-principles data of small diameter wires. The calculated nanowires are cut from the bulk material in [111] direction and [0001] direction for zinc blende (ZB) and wurtzite (WZ) structure, respectively. Afterwards the hydrogen free surfaces were completely relaxed. GaAs bulk material has ZB structure,but the ground state of nanowires also depends on surfaces and edges.We considered wires with hexagonal cross sections with {11-20} and {10-10} facets in case of wurtzite structure, and {10-1} and {11-2} for zinc blende structure.

We performed both density functional calculations and structural motif expansion for several of these different wires and found, that the wurtzite formation energy of small nanowires with diameters less than 80 Å is lower than the zinc blende one, due to the lower surface energy of wurtzite. This still holds if edges are negligible. The influence of additional dangling bonds at the edges and its effect on the WZ ZB transition is discussed.

HL 12.2 Mon 12:15 POT 151

Spatially resolved photocurrent spectroscopy on a single pn-doped GaAs nanowire — •Daniel Sager[1], Christoph Gutsche[2], Andrey Lysov[2], Matthias Offer[3], Ingo Regolin[2], Werner Prost[2], Franz-Josef Tegude[2], Axel Lorke[3], and Gerd Bacher[1] — [1]Werkstoffe der Elektrotechnik & CeNIDE, Universität Duisburg-Essen, Bismarckstr. 81, 47057 Duisburg, Germany — [2]Halbleitertechnologie & CeNIDE, Universität Duisburg-Essen, Lotharstr. 55, 47048 Duisburg, Germany — [3]Experimentalphysik & CeNIDE, Universität Duisburg-Essen, Lotharstr. 55, 47048 Duisburg, Germany

Due to their geometry, nanowires based on direct bandgap semiconductors are seen as ideal candidates for photovoltaic applications. Therefore, a detailed knowledge of the light to charge conversion process is essential for the future device design of solar cells. This can be accessed by spatially and temporally resolved photocurrent spectroscopy.

Single GaAs nanowires grown by metal-organic vapour phase epitaxy have been doped with Zn and Sn for p- and n-type doping, respectively, to create a doping transition in axial direction [1]. With spatially resolved photocurrent spectroscopy electron-hole pairs are photo-generated and the resulting current is measured as a function of the laser spot position. A photocurrent, which is proportional to the light illumination is found. We demonstrate maximum photocurrent generation directly at the pn-junction, which is strongly decreasing if the laser spot is placed outside the junction.

[1] I.Regolin, et al., J. Cryst. Growth (2010), doi:10.1016/j.jcrysgro.2010.08.028

HL 12.3 Mon 12:30 POT 151

Dynamic and directional modulation of the optical emission of individual GaAs nanowires using surface acoustic waves — •Jörg B. Kinzel[1], Daniel Rudolph[2], Gerhard Abstreiter[2], Jonathan J. Finley[2], Gregor Koblmüller[2], Achim Wixforth[1], and Hubert J. Krenner[1] — [1]Lehrstuhl für Experimentalphysik 1, Universität Augsburg, Germany — [2]Walter Schottky Institut, Technische Universität München, Germany

The influence of surface acoustic waves (SAW) on the optical emission of individual GaAs nanowires (NW) is investigated by micro photoluminescence (μ-PL) spectroscopy at low temperatures. In time-integrated experiments we observe a pronounced quenching of the NW emission as the amplitude of the SAW is increased. This quenching is maximum for SAW propagation along the NW axis and minimum in a perpendicular arrangement. This observation can be readily understood by a SAW-induced break-up of electron-hole pairs which is suppressed for the perpendicular configuration since the NW diameter $\sim 50-100$ nm is significantly smaller the SAW wavelength ~ 5 μm By introducing a tunable phase relation between the exciting laser pulse and the radio frequency signal exciting the SAW we observe a clear oscillation of the PL signal. In addition, time-correlated single photon counting (TCSPC) spectroscopy proves that this effect arises from a dynamic modulation of the NW emission with the frequency of the SAW.

HL 12.4 Mon 12:45 POT 151

Impact of growth conditions on morphology, structure and electrical properties of MOVPE grown InAs nanowires — •A. Penz[1,3], M. von der Ahe[1,3], K. Sladek[1,3], S. Wirths[1,3], K. Weis[1,3], C. Blömers[1,3], C. Volk[1,3], F. Dorn[2,3], T. Weirich[2,3], T. Schäpers[1,3], H. Hardtdegen[1,3], and D. Grützmacher[1,3] — [1]Institute of Bio- and Nanosystems (IBN-1), Forschungszentrum Jülich, 52428 Jülich, Germany — [2]GFE, Gemeinschaftslabor für Elektronenmikroskopie — [3]JARA - Fundamentals of Future Information Technology

The bottom-up assembly of semiconductor nanowires holds promise for future nanoelectronic devices. The high room temperature carrier mobility and the narrow direct bandgap make InAs an eligible material for this application. However, as recently reported, the conductivity of InAs nanowires could be influenced detrimentally by crystal defects such as twin planes and stacking faults. In this contribution, we report on different strategies to affect the nanowire crystallographic structure. Growth is performed by selective area MOVPE on partially masked substrates. The influence of growth rate, substrate orientation and Si doping on morphological, structural and electrical properties was investigated by scanning and transmission electron microscopy and two-and four-terminal measurements. It is found that especially the growth rate reduces the stacking fault density. Furthermore we observe an increase of conductivity and a decrease of nanowire aspect ratio with higher doping concentration. A correlation between doping, growth rate and electrical characteristics will be presented.

HL 12.5 Mon 13:00 POT 151

Strain-tuning of the excitonic fine structure splitting in semiconductor quantum dots — •Johannes D. Plumhof[1], Vlastimil Krapek[2], Fei Ding[1], Klaus D. Jöns[3], Robert Hafenbrak[3], Petr Klenovsky[2], Andreas Herklotz[1], Kathrin Dörr[1], Armando Rastelli[1], Peter Michler[3], and Oliver G. Schmidt[1] — [1]IFW Dresden, Helmholtzstr. 20, D-01069 Dresden — [2]Institute of Condensed Matter Physics, Masaryk University, Kotlářská 2, 61137 Brno, Czech Republic — [3]Institut für Halbleiteroptik und Funktionelle Grenzflächen, University of Stuttgart, Allmandring 3, 70569 Stuttgart

For the creation of polarization entangled photon pairs from semiconductor quantum dots (QDs) it is important to decrease the fine structure splitting (FSS) of the neutral exciton to energies comparable to the emission linewidth. We employ a piezoelectric actuator (PMN-PT) to manipulate the excitonic emission of GaAs/AlGaAs as well as InGaAs/GaAs QDs embedded in ≈200 nm thick (Al)GaAs membranes. By attaching the membranes on the PMN-PT we can apply anisotropic strain to the nanostructures. Polarization resolved μ-photoluminescence spectroscopy is used to estimate the excitonic FSS as well as the orientation of the linear polarization of the emitted light. The strain makes it possible to manipulate the FSS in a range of 70 μeV. We also observe rotations of up to 70° of the linear polarization of the light emitted by neutral excitons. These effects can be explained as an strain-induced anticrossing of the bright excitonic states.

HL 12.6 Mon 13:15 POT 151

Fabrication and optical properties of GaAs quantum dots by filling of self-assembled nanoholes — •David Sonnenberg, Andreas Graf, Christian Heyn, and Wolfgang Hansen — Institut

für Angewandte Physik, Universität Hamburg, 20355 Hamburg, Germany

We study a novel type of GaAs quantum dots (QDs), which are formed by filling of self-assembled nanoholes in semiconductor surfaces during molecular beam epitaxy. Here, we report on the fabrication and optical properties of these QDs. In our case, the local droplet etching (LDE) process is started with the generation of Al droplets on the AlAs surface. Using appropriate process temperatures, nanoholes are drilled beneath the liquid droplets into the substrates. After drilling, the holes were partially filled with GaAs in order to create strain-free GaAs QDs. The only partial filling results in highly uniform QDs with size precisely controlled by the filling level [1]. The generation of very homogeneous QD ensembles is demonsrated by photoluminescence (PL) linewiths of less than 10 meV. Micro-PL measurements of single QDs show sharp excitonic lines and linewiths combarable to the established InAs QDs [2]. We discuss here PL measurements on single and ensembles of LDE GaAs QDs as function of the QD size.

[1] Heyn et al., Appl. Phys. Let. 94, 183113 (2009)
[2] Heyn et al., Nanoscale Res. Lett. (2010) 5:1633-1636

HL 13: Invited Talk: Bernd Kästner

Time: Monday 12:45–13:15 Location: FOE Anorg

Invited Talk HL 13.1 Mon 12:45 FOE Anorg

Semiconductor quantized current and voltage standard — •Bernd Kaestner — Physikalisch-Technische Bundesanstalt (PTB), Bundesallee 100, 38116 Braunschweig

From the groundbreaking work of Josephson it became clear that superconducting solid state devices allow to generate a quantized voltage only defined by an applied excitation frequency f and two fundamental constants, namely the electron charge e and Planck constant h. The Josephson effect has been successfully applied in the field of electrical quantum metrology as voltage standard. Though superconductors show many other astonishing properties semiconductors have been the most relevant class of material for microelectronics. The generation of a quantized voltage by an all semiconductor device has not been possible yet. Here we report on the realization of a semiconductor quantized voltage source allowing to generate voltages V = f *(h/e) upon input of an AC voltage with frequency f. The design of the device can be regarded as a semiconductor integrated quantized circuit. It consists of a non-adiabatic single-electron pump [1] being able to drive quantized currents through high impedance loads. The pumping mechanisms and potential accuracy are discussed with respect to applications as a quantum current standard. When operating such a pump at frequency f and monolithically integrating it with a Quantum Hall device in series the functionality of quantized voltage generation can be implemented. The device shows robust operation up to frequencies of a few GHz.

[1] M. D. Blumenthal, B. Kaestner, L. Li, et al., Nature Physics 3, 343 - 347 (2007).

HL 14: Invited Talk: Karl W. Böer

Time: Monday 13:00–13:30 Location: POT 06

Invited Talk HL 14.1 Mon 13:00 POT 06

Why does a thin Layer of CdS on top of CdTe, and other thin-film solar cells improve their efficiency dramatically — •Karl W. Boer — Physics and Astronomy, Newark DE 19716

Karl W. Boer, University of Delaware When changing the bias from forward to Voc , the field at the CdS side of the CdS/CdTe junction increases. When it reaches the threshold of field-quenching the hole density increases while the electron density decreases, and the electron conductivity in CdS decreases with further shifting bias, i.e. with the increasing field. For reasons of the minimum entropy principle, a high-field domain must appear and absorbs the additional voltage drop. This limits the field at the junction interface to * 50 kV/cm, that is below the tunneling field. It thereby reduces junction leaking. With field quenching, the Fermi level moves further away from the conduction band, and this band must disconnect at the interface from the conduction band of the CdTe. This requires a change in the electron affinity as a function of bias. A similar change of the work function from a blocking contact of CdS as function of the conductivity has been observed, supporting this assumption. In forward bias the two conduction bands seem to be connected, easing the electron flux from CdS into CdTe. With reduced leakage Voc and FF is increased, explaining the observed improvement of the efficiency of the CdS/CdTe solar cell.

HL 15: Joint Session: Organic Semiconductors I: Solar Cells A

Time: Monday 14:00–17:30 Location: ZEU 222

Topical Talk HL 15.1 Mon 14:00 ZEU 222

Light harvesting in single polymer chains and inorganic nanostructures — •John M. Lupton — Institut für Experimentelle und Angewandte Physik, Universität Regensburg — Department of Physics and Astronomy, University of Utah, Salt Lake City

Optimization of materials for energy conversion applications requires an understanding of intermolecular heterogeneity to ultimately formulate synthetic approaches to maximizing the fraction of a particular subensemble. Single molecule spectroscopy can offer such insight as an exquisitely sensitive tool to unravel the underlying complexity of organic semiconductors. In the context of solar cells, for example, the technique can help to identify purely intramolecular exciton migration and charge separation processes.

Recently, we have explored the migration of excitons in single molecules as a function of the initial excitation energy, thus offering information on thermalization processes within the polymer chain. The approach allows a direct spectroscopic identification of the absorption of individual chromophores on the chain, whereas mere emission tends to provide information only on the lowest-energy unit in the intramolecular excitonic cascade [1].

The heterogeneity in light-harvesting characteristics is particularly pronounced in semiconductor nanostructures, where particle morphology directly influences the heterojunction band structure and the excitonic spectrum [2].

[1]Walter et al., Phys. Rev. Lett. 103, 167401 (2009).
[2]Borys et al., Science (in press).

HL 15.2 Mon 14:30 ZEU 222

Highly efficient vacuum processed BHJ solar cell based on merocyanines — •Vera Steinmann[1], Hannah Bürckstümmer[2], Nils M. Kronenberg[1], Martin R. Lenze[1], Dirk Hertel[1], Frank Würthner[2], and Klaus Meerholz[1] — [1]Department für Chemie, Universität Köln, Germany — [2]Institut für Organische Chemie and Röntgen Research Center for Complex Material Systems Universität Würzburg, Germany

Bulk heterojunction (BHJ) organic solar cells have attracted considerable interest due to their potential for large-scale, cost-effective and environmentally friendly power generation. Small molecules have been successfully introduced in solution- (SOL) as well as vacuum- (VAC) processed devices, reporting efficiencies (PCE) up to 4.4% and 5.7%

respectively. For simple layer stack devices (2-3 layers) based on CuPc as electron donor and C60 as electron acceptor PCEs up to 5.0% have been achieved.

Recently, we presented a direct comparison of highly efficient SOL and VAC BHJ cells based on merocyanine dyes (MC) with a similarly simple layer stack as reported in the literature. Our most efficient devices exhibited PCEs up to 4.9%. Further optimizations on the VAC processed cells led to high PCEs exceeding 6% while keeping the same simple layer stack. In addition, these cells have demonstrated exceptional performance even at lower light intensities.

Due to the simple chemical variability of MC dyes, they are ideally suited for tandem solar cells. We will present first attempts in this direction.

HL 15.3 Mon 14:45 ZEU 222

Efficiency-Limiting Processes in Bulk Heterojunction Organic Solar Cells — Ian Howard, Ralf Mauer, Fabian Etzold, Valentin Kamm, Michael Meister, Hannah Mangold, and •Frédéric Laquai — Max Planck Research Group for Organic Optoelectronics, MPI for Polymer Research, Mainz, Germany

Despite significant study, the efficiency-limiting processes that govern the efficiency of bulk heterojunction photovoltaic devices still remain ambiguous. In particular the role of interfacial charge-transfer (CT) states as potential intermediates of free charge carriers is diversely debated. In this contribution we directly observe charge generation and recombination processes in state-of-the-art polymer:methanofullerene photovoltaic blends by transient absorption spectroscopy and compare polythiophene (P3HT) of varying regioregularity and low-bandgap polymers as electron donor materials. We observe a common feature of these blends is ultrafast ($<$ 100 fs) exciton dissociation at the donor-acceptor interface. However, a certain fraction of excitons create CT states that predominantly recombine geminately within a few nanoseconds. On the other hand the fraction of free charge carriers recombines bimolecularly on a time scale competing with charge extraction and can thus be swept out of the device as photocurrent. The results demonstrate the importance of ultrafast free carrier generation and suppression of interfacial CT state formation to achieve high power conversion efficiencies in various material systems. [1] I.A. Howard, R. Mauer, M. Meister, F. Laquai, J. Am. Chem. Soc. 2010, 132, 14866. [2] I.A. Howard, F. Laquai, Macromol. Chem. Phys. 2010, 211, 2063.

HL 15.4 Mon 15:00 ZEU 222

Bias-Dependent Transient Absorption on Organic Solar Cells; Connection to Device Performance? — •Ian Howard, Ralf Mauer, Valentin Kam, Michael Meister, and Frédéric Laquai — Max Planck Forschungsgruppe für Organische Optoelektronik, Max-Planck-Institut für Polymerforschung, Mainz, Deutschland

We directly observe the bias dependence of charge-transfer state separation in organic bulk heterojunctions using in-situ transient absorption on operating organic solar cells. The effect of bias on charge-transfer state lifetime ($<$ 2ns) is found to be minimal, however suppression of nongeminate recombination with bias on later timescales ($>$10 ns) is observed and explains the bias dependence of the photocurrent. The bias independence of charge-transfer state separation is directly applicable to interpreting organic solar cell performance under standard AM1.5 illumination. However, due to the differences in charge densities and dynamic versus steady-state behavior between pulsed measurements and standard operating conditions, the effects of bias on the suppression of nongeminate recombination are not simplistically transferable. We consider to what extent pulsed transient absorbtion techniques on devices can be used to reveal nongeminate recombination mechanisms in devices operating under standard illumination conditions.

HL 15.5 Mon 15:15 ZEU 222

Degradation effects related to the hole transport layer in organic solar cells — •Bernhard Ecker[1], Jairo Nolasco[2], Josep Pallarés[2], Lluis Marsal[2], Jörg Posdorfer[3], Jürgen Parisi[1], and Elizabeth von Hauff[1] — [1]Energy and Semiconductor Research Laboratory, Institute of Physics, Carl von Ossietzky University, 26111 Oldenburg (Germany) — [2]Departament d'Enginyeria Electrònica Elèctrica i Automàtica, Universitat Rovira i Virgili, Avda. Països Catalans 26, 43007 Tarragona (Spain) — [3]Enthone Nano Science Centre, Ormecon GmbH, Ferdinand-Harten-Str. 7, 22949, Ammersbek (Germany)

We discuss the influence of the hole transport layer on the device stability in organic bulk-heterojunction solar cells. Two water based hole transport layers, poly(3,4-ethylenedioxythiophene) : poly(styrene sulfonate) (PEDOT:PSS) and polyaniline : poly(styrene sulfonate) (PANI:PSS), and one isopropyl alcohol based PANI:PSS transport layer were investigated. Solar cells were prepared with the three different hole transport layers and degraded under illumination. Current-voltage, capacitance-voltage, and capacitance-frequency data were collected at varying light intensities over a period of 7 hours. Solar cell performance and stability were compared between non encapsulated and encapsulated samples to obtain understanding about degradation effects related to oxygen and water as well as degradation mechanisms related to the intrinsic instability of the solar cell materials and interfaces. We show that the properties of the hole transport layer can have a significant impact on the stability of organic solar cells.

15 min. break

HL 15.6 Mon 15:45 ZEU 222

Characterization of trap states in small-molecule organic solar cells by using Impedance Spectrocopy. — •Lorenzo Burtone, Debdutta Ray, Karl Leo, and Moritz Riede — Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden Germany

In this work, we focus on the characterization of trap levels in the electronic gap of organic semiconductors used in solar cells. These states can modify the electric field inside the device, considerably affecting charge generation and transport and consequently the solar cell efficiency. A method to characterize traps by using impedance spectroscopy is presented. We propose a new equivalent circuit based on previously reported theoretical models and we apply it in the fitting procedure of the measured data. In particular, we measure the impedance spectra of two flat heterojunction small molecule solar cells, where one of them has doped electron and hole transport layers. We observe the contribution of trap states at low frequencies in the capacitance spectra for the devices with doped transport layers. The experimental results can be understood with the equivalent circuit proposed and the trap state contribution can be evaluated. From a fitting procedure, we estimate the density of trap states to be around $1x10^{17}cm^{-3}eV^{-1}$. Moreover we observe from the impedance analysis the presence of dopants in the intrisic layer with an estimated effective concentration of about $8.4x10^{17}cm^{-3}$. This value is in agreement with very low doping concentration and suggests the formation of a non-abrupt junction between intrinsic and doped layers.

HL 15.7 Mon 16:00 ZEU 222

The effect of energetic disorder on open-circuit voltage in organic photovoltaics — •James C Blakesley, Ilja Lange, and Dieter Neher — University of Potsdam, Germany

Open-circuit voltage (VOC) is one of the most important figures of merit describing the quality of organic photovoltaics (OPVs). Usually it is assumed that VOC depends on the energy difference between the highest occupied molecular orbital (HOMO) of the donor and the lowest unoccupied molecular orbital (LUMO) of the acceptor, but large deviations from this trend are often found. In reality, there is a distribution of energy levels within the components, and this should also be taken into account.

We simulate bulk heterojunction OPVs using a simulation that includes the effects of energetic disorder [1].We find that VOC depends on: 1) the nominal donor-HOMO to acceptor-LUMO energy gap; 2) the charge-carrier generation and recombination rates; 3) the electrodes; and 4) the amount of energetic disorder. While the first three of these points have been much discussed previously, the effect of the fourth has not been conclusively demonstrated. An increase in the amount of energetic disorder leads to a reduction in the VOC due to relaxation of the carriers into the lowest lying energy levels. We find an analytical expression that predicts well the modelled VOC, and suggest the use of an effective donor-acceptor energy gap that takes energetic disorder into account. Measurements of Fermi-level pinning might be useful for determining this effective energy gap. [1] J. C. Blakesley and N. C. Greenham, J. Appl. Phys. 106, 034507 (2009)

HL 15.8 Mon 16:15 ZEU 222

Modelling Temperature-Dependent Current-Voltage Curves of Organic Photovoltaic Devices — •Simon Züfle, Martin T. Neukom, Benjamin Perucco, Nils A. Reinke, and Beat Ruhstaller — ICP, ZHAW, Winterthur, Schweiz

Current-voltage curves allow to determine both fill-factor and effi-

ciency of organic photovoltaic devices and are therefore a commonly used characterisation technique. Since analytical models for current-voltage curves fail in describing the fundamental processes of photogenerated current, more complex numerical calculations are mandatory for obtaining insight into the device physics. The analysis of multiple current-voltage curves at different temperatures calls for CPU-efficient algorithms combining state-of-the-art physical models and high calculation speed.

In order to model current-voltage curves simple drift-diffusion calculations with constant mobilities and thermionic emission as injection model are frequently used. In this study we investigate current-voltage curves measured at different temperatures with the help of a nonlinear least-square fitting algorithm in combination with a comprehensive physical model for charge carrier transport and injection. We evaluate the performance of different models for charge carrier transport, including the Gaussian Disorder Model, by simultaneously fitting multiple curves and discussing the mathematical quality of the fit. We employ an efficient algorithm for extracting material-specific parameters that allows modelling of measured current-voltage curves on a minute time-frame with a desktop PC.

HL 15.9 Mon 16:30 ZEU 222

Role of drift and diffusion in organic solar cells measured by transient photocurrents — •Wolfgang Tress, Karl Leo, and Moritz Riede — Institut für Angewandte Photophysik, TU Dresden, Dresden, Germany

The role of the electric field and the contribution of diffusion to photocurrents are controversially discussed in the case of organic solar cells. We investigate flat heterojunction organic solar cells with systematically varied barriers at the contacts that are created by a HOMO offset between donor and hole transport layer. These barriers lead to S-kinks in the IV curve and to strong imbalanced and even reversed forces on charge carriers resulting from the field on the one hand and the concentration gradient on the other hand. By applying a rectangular illumination signal with varied light intensities, we observe in the photocurrent transients a pile-up of charge carriers at an extraction barrier. If an injection barrier is present, there exists a region in the IV curve where charges are extracted against the electric field by a strong diffusion gradient. These findings are based on the analysis of transient current data in the μs regime using electrical simulations based on a drift-diffusion model. The simulations show that observed overshoots in the photocurrent transients result from these imbalance effects and give new insights into the working principle of organic solar cells.

HL 15.10 Mon 16:45 ZEU 222

Charge extraction with linearly increasing voltage: A numerical model for parameter extraction — •Martin Neukom, Simon Züfle, Nils Reinke, and Beat Ruhstaller — Institute of Computational Physics, Technikumstr 9, 8401 Winterthur, Switzerland

Device characterisation is an essential part in the process of improving the performance and lifetime of organic solar cells. Most of the device and material parameters are not accessible by measurements therefore sophisticated measurement techniques in combination with numerical simulations are needed to extract these parameters. A frequently used method to determine material parameters like charge carrier mobilities and the recombination coefficient is the CELIV technique (charge extraction by linearly increasing voltage). In this technique a voltage ramp is applied to the device in order to extract free charge carriers inside the bulk. With a simple analytical formula the mobility is commonly estimated on the basis of the temporal position of the current peak. We simulate the CELIV experiment, transient and steady-state measurement techniques with a fully-coupled opto-electronic model. On the one hand we investigate the limitations of the analytical formulas for mobility determination. On the other hand we use our model to fit several experimental datasets simultaneously to obtain elementary material parameters like the electron and hole mobility, recombination coefficient, photon to charge conversion efficiency and injection barriers in both printed and spin-coated bulk heterojunction solar cells. We deduce the influence of these material parameters on the overall device performance.

HL 15.11 Mon 17:00 ZEU 222

Simulating electron transfer reactions in organic solar cell components — •Harald Oberhofer[1] and Jochen Blumberger[2] — [1]Department of Chemistry, University of Cambridge, UK — [2]Department of Physics and Astronomy, University College London, UK

Organic solar cells are envisaged as a promising alternative to silicon based solar cells. They are cheap and easy to produce, light and flexible, and easily deployed on walls or roofs. Unfortunately, these advantages currently come at the price of small photo-electric conversion efficiencies. To help overcome this deficiency we use advanced density functional theory (DFT) based methods to investigate the electron-conducting properties of modified Fullerene crystals which are commonly used as electron-conducting component in organic solar cells.

In our contribution we will briefly discuss the techniques used to estimate electron transfer rates from computer simulations. Then we present our calculations on modified Fullerene crystals. We studied $C_{61}H_2$—a commonly used test system—and [6,6]-phenyl-C61-butyricacid-methyl-ester (PCBM) for 3 different crystal lattices which are commonly found in experiments. In the crystal we estimated electron transfer rates between next- and next-nearest neighbours with and without the application of an external electric field. These results where then used to estimate the electron mobility for the different lattice types. These results can represent a starting point for the optimisation of electron conduction in next-generation organic solar cells.

HL 15.12 Mon 17:15 ZEU 222

Time resolved microwave conductivity reveals charge carrier dynamics in organic semiconductors — •Johannes Erben[1], Andreas Sperlich[1], Hannes Kraus[1], Tom J. Savenije[1,3], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius-Maximilians-University of Würzburg, D-97074 Würzburg — [2]ZAE Bayern, D-97074 Würzburg — [3]Department of Chemical Engineering, Delft University of Technology, NL-2628 BL Delft, The Netherlands

Understanding of the light induced charge carrier dynamics in organic semiconductors is essential to improve material properties and processing parameters, and, at long sight, device performance. Time Resolved Microwave Conductivity (TRMC) gives direct access to the microscopic transport properties, as the high frequency alternating electric field limits the drift of the charge carriers. After laser pulse excitation TRMC signal decays in P3HT:PCBM blends with varying PCBM content have been observed exhibiting a power law time dependence. The influence of morphology and temperature on the charge carrier recombination and mobility on a microscopic scale can thus be investigated.

HL 16: Microcavities

Time: Monday 14:30–17:15 Location: FOE Anorg

HL 16.1 Mon 14:30 FOE Anorg

Interdependence of first- and second-order coherence for quantum-dot micropillar lasers — •Jean-Sebastian Tempel[1], Ilya Akimov[1], Marc Assmann[1], Christian Schneider[2], Sven Höfling[2], Caroline Kistner[2], Stephan Reitzenstein[2], Lukas Worschech[2], Alfred Forchel[2], and Manfred Bayer[1] — [1]Experimentelle Physik 2, Technische Universität Dortmund, 44221 Dortmund — [2]Technische Physik, Physikalisches Institut, Universität Würzburg, 97074 Würzburg

We present investigations on the coherence of the emission from the fundamental mode of a quantum-dot microcavity laser. We measured the first-order field-correlation function $g^{(1)}(\tau)$ with a Michelson interferometer, from which we directly determine the coherence time. To fully characterize the coherence properties of the cavity emission, we apply a model that connects first- and second-order coherence. Hereby it is possible to overcome the limited sensitivity of the streak camera used for photon correlation measurements, and thus to extend the accessible excitation power range for $g^{(2)}(\tau)$ down to the thermal regime.

HL 16.2 Mon 14:45 FOE Anorg

Emission characteristics of a highly correlated system of a

quantum dot coupled to two distinct micropillar cavity modes — •Stefanie Weiler[1], Ata Ulhaq[1], Sven Marcus Ulrich[1], Stephan Reitzenstein[2], Andreas Löffler[2], Alfred Forchel[2], and Peter Michler[1] — [1]Universität Stuttgart, Allmandring 3, 70569 Stuttgart — [2]Universität Würzburg, Am Hubland, 97074 Würzburg

Quantum dots (QDs) are promising candidates for quantum information technology. Even though they are referred to as artificial atoms, the interaction of QDs with the surrounding solid state medium has to be considered to explain the recently discovered and yet not fully theoretically explained effect of nonresonant dot-cavity coupling. In our work [S. Weiler et al., PRB 82, 205326 (2010)] we have investigated the emission characteristics of a system of one QD coupled to two distinct modes of a surrounding micropillar cavity. We have verified the anti-correlation among the QD and the two modes via auto- and cross-correlation measurements, revealing a highly correlated system. Systematic lifetime and coherence time measurements (p-shell excitation) gave important insight in the emission dynamics and coherence of the system. QD and modes show the lifetime behavior expected by Purcell enhancement, when controllably varying the emitter-mode detuning. The mode emission coherence stays at a constant low level for all detunings. When exciting the QD resonantly, we could demonstrate nonresonant coupling to the nearby mode and with increasing power also to the far detuned fundamental mode of the system.

HL 16.3 Mon 15:00 FOE Anorg

Spin mediated magneto-optical cavity quantum electrodynamics effects in quantum dot micropillar systems — •Peter Gold[1], Stephan Reitzenstein[1], Steffen Münch[1], Philipp Franeck[1], Andreas Löffler[1], Sven Höfling[1], Lukas Worschech[1], Alfred Forchel[1], Ilya Ponomarev[2], and Tom Reinecke[2] — [1]Technische Physik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Naval Research Laboratory, Washington, D.C. 20735, USA

We report on magneto-optical studies of strongly coupled quantum dot - micropillar cavity systems. Laterally extended $In_{0.3}Ga_{0.7}As$ quantum dots (QDs) in the active layer of a micropillar cavity facilitate the observation of strong coupling. These QDs are characterized by large oscillator strength and they exhibit a large diamagnetic response, which is exploited to demonstrate magneto-optical resonance tuning. In addition, the coherent interaction between spin resolved states of the QDs and microcavity photon modes is studied. We access the spin degree of freedom by applying a non-zero magnetic field in Faraday configuration, so that the spin degeneracy of the QD exciton is lifted, while the resonance tuning of the Zeeman split exciton lines is achieved by temperature variation. A detailed oscillator model is used to extract coupling parameters of the individual spin and cavity modes. Our results demonstrate an effective coupling between photon modes that is mediated by the exciton spin states [1]. We further show simulations of the photon-photon coupling in dependence of the coupling parameters.

[1] S. Reitzenstein et al., Phys. Rev. B 82, 121306 (R) (2010)

HL 16.4 Mon 15:15 FOE Anorg

Site-controlled quantum dots in an electrically driven single-sided micropillar cavity — •Sebastian Maier, Christian Schneider, Alexander Huggenberger, Tobias Heindel, Stefan Heckelmann, Stephan Reitzenstein, Sven Höfling, Lukas Worschech, Martin Kamp, and Alfred Forchel — Technische Physik and Wilhelm Conrad Röntgen Research Center for Complex Material Systems, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

Spatial control over the position of a single quantum dot is important for the realization of quantum optical and quantum electronic devices. We integrated site-controlled InAs quantum dots (SCQDs) in an electrically driven p-i-n diode by performing molecular beam epitaxial (MBE) growth on a pre-patterned substrate. The SCQDs are grown on a line of nanoholes fabricated with electron beam lithography and wet etching. We employed a low quality factor single-sided micropillar cavity design with diameters smaller than 2 μm that allows for directed and highly efficient light emission. The bottom (top) distributed Bragg reflector (DBR) consist of 24 p-doped (5 n-doped) pairs of quarter-wavelength thick layers of AlAs and GaAs. The SCQDs are centered in the intrinsic GaAs λ-cavity. Microelectroluminescence measurements of electrically driven SCQDs reveal emission from single SCQDs with narrow linewidths down to 170 μeV.

HL 16.5 Mon 15:30 FOE Anorg

Whispering gallery mode lasing in electrically driven quantum dot micropillars — •Ferdinand Albert, Tristan Braun, Tobias Heindel, Christian Schneider, Stephan Reitzenstein, Sven Höfling, Lukas Worschech, and Alfred Forchel — Technische Physik and Wilhelm Conrad Röntgen Research Center for Complex Materials, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

High quality factor and low mode volume nanophotonic devices featuring pronounced cavity quantum electrodynamics (cQED) effects are attracting considerable scientific attention with respect to efficient light sources. For instance they allow for the realization of efficient and compact microlasers. In this respect electrically driven quantum dot based micropillar lasers are of particular interest because of a straightforward current injection by a ring-shaped top contact. While standard micropillar lasers are characterized by a highly directional emission normal to the samples surface, we report on in-plane lasing emission under electrical pumping from whispering gallery modes (WGMs) confined in the central cavity layer of the micropillars. We present WGM lasing with Q-factors up to 40.000 and laser threshold currents below 10 μA. Our devices provide a significantly better heat sinking compared to standard WGM lasers based on microdisks and, thus, a better control of the emission wavelength. The latter is of particular importance for the realization of THz radiation from micropillar WGM lasers by means of difference frequency generation.

15 min. break

HL 16.6 Mon 16:00 FOE Anorg

In-plane manipulation of quantum dots by electric fields — •Johannes Beetz, Caroline Kistner, Stephan Reitzenstein, Christian Schneider, Sven Höfling, Martin Kamp, and Alfred Forchel — Universität Würzburg, Technische Physik, Am Hubland, 97074 Würzburg

Devices for applying vertical electric fields to quantum dots (QDs) are usually fabricated by conventional measures of lithography — e.g. electron beam lithography — using a pn-type heterostructure. The creation of lateral electrodes is even much more challenging, especially if they need to be applied to the active region of microcavites. This is of special interest since it is impossible to influence the in-plane electronic structure of self-assembled QDs with a vertical electric field. To generate the field inside the cavity layer of a micropillar, its sidewalls have to be provided with two diametrically opposed electric connections on the level of the cavity. In order to achieve this, we exploited focused ion beam induced deposition to define contacts on the micropillar's steep sidewalls. We optimized deposition parameters and contact architecture to preserve the cavity's Q-factor while achieving an effective coupling of the electric field into the cavity for minimized leakage currents. To evaluate the effect of the lateral field we examined the spectral emission of QDs located inside the cavity. We demonstrate the manipulation of the emission energy by the quantum confined Stark-effect with tuning ranges up to 0.1 meV. Moreover, first studies show a reduction of the exciton fine structure splitting, which is interesting for the generation of entangled photons.

HL 16.7 Mon 16:15 FOE Anorg

Optical properties of monolithic InGaN quantum dot pillar microcavities — •Kathrin Sebald, Moritz Seyfried, Joachim Kalden, Heiko Dartsch, Christian Tessarek, Stephan Figge, Carsten Kruse, Detlef Hommel, and Jürgen Gutowski — Institute of Solid State Physics, University of Bremen, Germany

The realization of monolithic microcavities (MCs) with InGaN quantum dots (QDs) as active region can improve the performance of VCSELs as well as the single-mode emission of pillar structured MCs. In this contribution, we will present the successful implementation of InGaN QDs into fully epitaxial monolithic MCs showing discrete resonator modes for pillar structured samples and emission lines of single QDs. The complete structure, consisting of two DBRs surrounding the GaN λ cavity, was grown by MOVPE. A layer of InGaN QDs was embedded in the cavity at the antinode position of the electric field. Pillar shaped MCs with various diameters were prepared from the planar samples by FIB etching. Their three-dimensional optical confinement results in the clear occurrence of a transversal mode structure. Quality factors of up to 300 have been achieved. Furthermore, micro-photoluminescence spectra reveal distinct spectrally sharp emission lines around 2.73eV which can be attributed to the emission of single InGaN QDs. Their markedly enhanced intensities when com-

pared to QD lines off resonance give clear evidence of these QDs to efficiently couple to the modes. Single emission lines can be traced up to 120K. These finding are very encouraging, and further optimization gives the opportunity for an efficient utilization of InGaN QD-based devices.

HL 16.8 Mon 16:30 FOE Anorg

Experimental realization of high-Q AlAs/GaAs micropillar cavities with submicrometer diameters — •Florian Dunzer[1], Matthias Lermer[1], Niels Gregersen[2], Jesper Mørk[2], Stephan Reitzenstein[1], Sven Höfling[1], Martin Kamp[1], and Alfred Forchel[1] — [1]Technische Physik and Wilhelm Conrad Röntgen Research Center for Complex Material Systems, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]DTU Fotonik, Department of Photonics Engineering, Technical University of Denmark, Building 343, DK-2800 Kongens Lyngby, Denmark

Quantum Dots (QDs) integrated in micropillar cavities with both high quality factors (Q) and small mode volumes (Vmode) constitute a promising class of solid-state quantum light sources. For instance, pronounced cavity quantum electrodynamics effects in the weak and strong QD-cavity coupling regime can be observed in these systems. A figure of merit for the observation of pronounced effects in the two regimes are the ratios Q/Vmode and Q/(sqrt(Vmode)), respectively. Q factors as high as 165,000 have been demonstrated for micropillars with large mode volume (Vmode>50(λ/n)) [1]. To reduce Vmode one might simply decrease the diameter (dc) of the pillars, yet resulting in a significant reduction of Q due to side wall scattering losses and mode mismatch. These effects limit Q to about 2,000 for dc<1 micrometer [2]. To overcome this problem, we have designed and implemented a novel AlAs/GaAs cavity design showing Q factors higher than 10,000 for micropillars with submicron diameters (Vmode<3.5(λ/n)).

HL 16.9 Mon 16:45 FOE Anorg

Polarization properties of the exciton-polariton occupation in ZnO-based microresonators — •Chris Sturm, Helena Hilmer, Steve Linke, Rüdiger Schmidt-Grund, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Linnéstraße 5, 04103 Leipzig

The possibility of the realization of a high temperature Bose-Einstein condensate (BEC), ultra-low threshold lasers and polariton based LEDs makes exciton-polaritons very interesting. Of special interest are ZnO-based microresonators since the formation of exciton-polaritons was observed up to 410 K and the predicted temperature for the formation of a BEC is 610 K [1,2]. Here we report on the influence of the polarization of cavity-photons, which are involved in the exciton-photon coupling, on the occupation of the lower polariton branch in ZnO-based microresonators. From photoluminescence spectra we deduce that scattering of the exciton-polaritons into the states at the bottleneck region is the largest contribution. At negative detuning, the scattering rates are larger for the TM-polarization than for the TE-polarization. This is caused by the TE-TM splitting of the involved cavity-photons. With increasing detuning the difference vanishes and the scattering into the ground state is enhanced (compared to that one into the bottleneck region). Furthermore, we obtained at $T = 10$ K a superlinear dependence of the exciton-polariton occupation on the excitation density for an intermediate detuning regime ($|\Delta| \leq 20$ meV).
[1] C. Sturm *et al.*, New. J. Phys. **11**, 073044 (2009).
[2] S.F. Chichibu *et al.*, Semicond. Sci. Technol. **20**, S67 (2005).

HL 16.10 Mon 17:00 FOE Anorg

ZnO mesa-structures in planar microcavities — •Helena Hilmer, Chris Sturm, Steve Linke, Rüdiger Schmidt-Grund, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Linnéstr. 5, 04103 Leipzig

The realization of Bose-Einstein Condensation (BEC) above room temperature in ZnO-based microresonators is still a topic of dedicated research. These systems offer both interesting physics as well as desirable applications. Until now we have observed our microresonators to be in the strong coupling regime up to 410 K [1].

Our microresonators have been grown on c-sapphire substrates by means of pulsed laser deposition. They consist of a ZnO-cavity as active medium, with an optical thickness of half a medium wavelength, that is sandwiched between two all-oxide Bragg reflectors (BR). Yttria stabilised zirconia and Al_2O_3 have been chosen as BR materials. In contrast to former samples, the cavity layer was structured with circular mesas of diameters ranging from 10...100 μm with a depth of only a few nanometers by photolithography and subsequent etching in highly diluted phosphoric acid. This leads to a blueshift of the uncoupled cavity-photon mode energy of about 20 meV in the etched area surrounding the mesa and therefore also to a shift of the lower polariton branch. The impact of such mesa as trap for polaritons and the effect on the polariton population is investigated.
[1] C. Sturm *et al.*, New. J. Phys. **11**, 073044 (2009).

HL 17: Nitrides: Growth and Characterization

Time: Monday 14:30–16:45 Location: POT 51

HL 17.1 Mon 14:30 POT 51

Epitaxial GaN around ZnO nanopillars — •Mohamed Fikry[1], Manfred Madel[2], Ingo Tischer[2], Klaus Thonke[2], and Ferdinand Scholz[1] — [1]Institut für Optoelektronik, Universität Ulm, Albert-Einstein-Allee 45, 89081 Ulm — [2]Institut für Quantenmaterie ,Universität Ulm, Albert-Einstein-Allee 45, 89081 Ulm

We report on an investigation of the epitaxial quality of GaN layers overgrown coaxially around ZnO nanopillars. In a first step, regularly arranged ZnO nanopillars were grown using pre-patterning by e-beam lithography or self-organized hexagonal polystyrene sphere masks. Alternatively, ZnO pillars were also successfully grown on top of GaN pyramids. In a second step, GaN layers were grwon around the ZnO pillars by Metal Organic Vapor Phase Epitaxy. At growth temperatures above 800 °C, the ZnO pillars are dissolved by the hydrogen carrier gas leaving hollow GaN nanotubes. Characterization involved photoluminescence (PL), scanning electron microscopy and cathodoluminescence. The fair quality of the deposited GaN layers is confirmed by a sharp low temperature PL peak at 3.48 eV attributed to the donor bound exciton emission. Further peaks at 3.42 eV and 3.29 eV show the possible existence of basal plane and prismatic stacking faults.

HL 17.2 Mon 14:45 POT 51

Optical properties of inversion domain boundaries in GaN — •Thomas Kure[1], Ronny Kirste[1], Ramon Collazo[2,3], Gordon Callsen[1], Juan Sebastián Reparaz[1], Anthony Rice[2], Seji Mita[3], Jinqiao Xie[3], Zlatko Sitar[2,3], and Axel Hoffmann[1] — [1]Technische Universität Berlin, Berlin, Germany — [2]North Carolina State University, Raleigh, North Carolina, USA — [3]HexaTech Inc., Raleigh, North Carolina, USA

Influenced by the growth method and growth parameters the polarity of epitaxial grown GaN films can be manipulated to form pure N- or Ga-polarity or states of mixed polarity. GaN grown on heterosubstrates can even form spatially adjacent areas of different polarities differentiated by an inversion domain boundary (IDB). Besides their structural differences each of the areas has unique optical properties, likewise the IDB itself. Furthermore, due to a polar selective doping behaviour, it is possible to fabricate a lateral p/n junction.

Using spatially-resolved photoluminescence spectroscopy (μ-PL) we revealed a temperature dependant enhancement of the luminescence by one order of magnitude at the IDB. Thereby, we confirmed an earlier published model [1]. Samples intentionally doped with Mg, which led to a p/n-junction, revealed an unexpected difference of the enhancement compared to the undoped samples. In addition, we used spatially-resolved electroluminescence spectroscopy (μ-EL) to investigate the influence of an external electric field. [1] V. Fiorentini, Applied Physics Letters 82, 1182 (2003)

HL 17.3 Mon 15:00 POT 51

Raman spectroscopic investigations on epitaxial grown GaN on sapphire — •Christian Röder[1], Cameliu Himcinschi[1], Jens Kortus[1], Frank Habel[2], and Gunnar Leibiger[2] — [1]TU Bergakademie Freiberg, Institute for Theoretical Physics, Leipziger Str. 23, D-09596 Freiberg — [2]Freiberger Compound Materials GmbH, Am Junger-Löwe-Schacht 5, D-09599 Freiberg

One of the biggest challenges of GaN layer preparation is the lack of

cost-efficient and high-quality substrates for homoepitaxy. In order to optimize the growth conditions and to understand relaxation mechanisms we investigated a series of heteroepitaxial grown GaN layers on sapphire differing in their layer thickness. By means of confocal Raman spectroscopy we obtained depth spatial information. Analyzing the position of the E2(high) phonon mode we found a wavenumber shift within all layers. This indicates a stress relaxation from the interface to the top of the layer. Furthermore we observed a decreasing compressive stress with increasing layer thickness. Assuming a planar stress state the determined shifts were converted to stress values. These results were compared with simulations using a model of wafer curvature. Additionally the shift of the E2(high) mode was correlated with results of photoluminescence (PL) measurements performed at 293 K. The changes of the band gap derived from the PL data were in excellent agreement compared with the strain dependent band structure at the Γ point. The authors would like to thank the European Union (EFRE) as well as the Free State of Saxony for financial support within the ADDE project.

HL 17.4 Mon 15:15 POT 51

Growth and microstructure of GaN:Cu - a possible spinaligner for nitride-based spintronic — •Philipp R. Ganz[1,2], Gerda Fischer[3], Christoph Sürgers[1,3], Huang Teng Hsing[4], Liuwen Chang[4], and Daniel M. Schaadt[1,2] — [1]DFG-Center for Functional Nanostructures, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [2]Institut für Angewandte Physik, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [3]Physikalisches Institut, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [4]Department of Materials and Optoelectronic Science / Center for Nanoscience and Nanotechnology, National Sun Yat-Sen University, Kaohsiung 80424, Taiwan, R. O. C.

Group-III nitride semiconductors are attractive for spintronic device applications due to the long and temperature independent spin-lifetime in InN quantum dots. For spin-injection into these quantum dots, spin-aligner which yields at room-temperature ferromagnetism and a high spin-polarization is essential. A possible candidate for a nitride-based spin-aligner is GaN:Cu, which exhibit ferromagnetic behavior far above room-temperature, although Cu is an intrinsic non-magnetic material. However, questions regarding the incorporation of Cu in GaN and the origin of the ferromagnetic behavior are still open. Bulk GaN:Cu samples were grown by plasma assisted MBE. We carried out a detailed study on the structural and magnetic properties from nitrogen- to Ga-rich conditions. Under Ga-rich conditions, the formation of Cu-Ga-islands on the surface was observed. The properties of these islands and the bulk material were studied by transmission electron microscopy.

15 min. break

HL 17.5 Mon 15:45 POT 51

Defect Characterisation of GaN Based High Electron Mobility Transistors — •Sebastian Rönsch[1], Michael Krieger[1], Heiko Weber[1], Giorgio Schweeger[2], and Markus Sickmöller[2] — [1]Lehrstuhl für Angewandte Physik, Universität Erlangen-Nürnberg — [2]AZZURRO Semiconductors AG, Magdeburg

GaN and related III-V semiconductors are promising materials for the application in high-power electronics. In particular, epitaxially grown AlGaN/GaN heterojunctions are excellent suited for the development of high-power transistors. The intrinsic material properties of AlGaN and GaN induce a two dimensional electron gas with high electron mobility at the interface of the heterojunction. For further improvement of the overall device performance, the heterojunction and its two dimensional electron gas was characterized by different measurement techniques. Hall measurements were performed to investigate the charge carrier concentration and the mobility of the two dimensional electron gas. The mobility of the charge carriers is limited due to electrically active defects within the band gap of GaN. In order to achieve a profound understanding of the defect mechanisms Deep Level Transient Spectroscopy (DLTS) was applied resulting in the defect parameters: activation energy, capture cross section and concentration. Additional Capacitance-Voltage (CV) measurements were carried out to verify the charge carrier concentration determined by the Hall measurements.

HL 17.6 Mon 16:00 POT 51

Band offsets in cubic GaN/AlN superlattices - Theory and Experiment — •Marc Landmann, Christian Mietze, Eva Rauls, Klaus Lischka, Donat J. As, and Wolf Gero Schmidt — Universität Paderborn, Germany

The presently unknown band offset in non-polar cubic GaN/AlN superlattices has been investigated by intersubband and interband spectroscopy as well as ab-initio calculations [1]. On the one hand, the conduction band offset has been determined from the comparison of the measured transition energies with model calculations within the effective mass approximation. On the other hand, the valence and conduction band offset has been accurately simulated by calculating many body corrections within the GW approximation on top of hybrid-functional density functional theory (DFT) calculations. A conduction band offset of (1.4±0.1) eV and a valence band offset of (0.5±0.1) eV has been thus obtained as a result of both approaches.

[1] C. Mietze, M. Landmann, E. Rauls, M. Tchernycheva, F.H. Julien, W. G. Schmidt, K. Lischka and D. J. As (submitted to Phys. Rev. B, 2010).

HL 17.7 Mon 16:15 POT 51

Second- and third-harmonic generation in periodically polarity-inverted GaN wave guides — •Stefan Krischok[1], Sindy Hauguth-Frank[1], Pierre Lorenz[1], Vadim Lebedev[2], Oliver Ambacher[2], Rüdiger Goldhahn[3], Björn Braunschweig[4], Gerhard Lilienkamp[4], and Winfried Daum[4] — [1]Inst. für Mikro- und Nanotechnologien, TU Ilmenau — [2]Fraunhofer IAF, Freiburg — [3]Inst. für Exp. Physik, OvG Universität Magdeburg — [4]Inst. für Energieforschung und Phys. Technologien, TU Clausthal

Quasi-phase matching has proven as promising technique for efficient second- and third-harmonic generation (SHG and THG). For hexagonal GaN the spatial modulation of the nonlinear coefficients can be achieved by a periodic polarity inversion, which was realized by etching periodic stripes into an AlN nucleation layer on sapphire substrates followed by GaN overgrowth by molecular beam epitaxy leading to either Ga- or N-face films with sharp inversion domain boundaries. The nonlinear frequency conversion was studied by an amplified Ti:sapphire laser system pumping an optical parametric amplifier to provide continuous tuning of the fundamental wave length between 1000 and 1600 nm. For a structure with 5.36 μm periodicity, quasi-phase-matched SHG was observed at 1070 nm which is consistent with expectation based on the ordinary and extraordinary refractive indices obtained by ellipsometry. In addition, quasi-phase-matched THG is detected at 1217, 1313, and 1452 nm. A detailed interpretation of these data as well as results of the structural and optical characterization of the N- and Ga-face layers will be presented.

HL 17.8 Mon 16:30 POT 51

Quantum-Confined Stark Effect Observed in (In,Ga)N/GaN Nanowire Heterostructures — •J. Lähnemann, C. Pfüller, O. Brandt, U. Jahn, E. Luna, T. Flissikowski, L. Schrottke, M. Knelangen, A. Trampert, and H. T. Grahn — Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5–7, 10117 Berlin

Light emitting diodes for the visible spectral region based on planar (In,Ga)N/GaN heterostructures suffer from a high dislocation density and lack of suitable substrates. An alternative is the integration of these heterostructures into nanowires (NWs) grown on Si by molecular beam epitaxy. Indications for the absence of the quantum-confined Stark effect (QCSE) have been reported in the literature, when the piezoelectric polarization is reduced due to an efficient strain relaxation in the NW geometry. In order to elucidate the origin of the observed luminescence centered at 2.4 eV, we combine transmission electron microscopy, cathodoluminescence and micro-photoluminescence (μ-PL) spectroscopy on single NWs. The μ-PL spectra contain a combination of two types of transitions: (i) several sharp lines from localization centers, which are not affected by the excitation power and (ii) a broader band that blueshifts with higher excitation powers. The former are probably related to composition fluctuations in the (In,Ga)N, while the latter is attributed to an inter-well transition between the two 11 nm thick (In,Ga)N insertions separated by an only 2 to 3 nm thick barrier layer. The blueshift under high excitation evidences a screening of the polarization field. Thus, the QCSE appears to be present in these NW heterostructures in contrast to previous reports.

HL 18: Quantum Hall Effect

Time: Monday 14:30–15:30 Location: POT 151

HL 18.1 Mon 14:30 POT 151

Huge Magnetoresistance in a High Mobility Two-Dimensional Electron Gas — •Lina Bockhorn[1], Patrick Barthold[1], Dieter Schuh[2], Werner Wegscheider[3], and Rolf J. Haug[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover — [2]Institut für Experimentelle und Angewandte Physik, Universität Regensburg — [3]ETH Zürich, Switzerland

We study the fractional Quantum-Hall effect in high mobility two-dimensional electron gas (2DEG). Hall geometries are created by photolithography on a GaAs/GaAlAs quantum well containing a 2DEG. The 2DEG have an electron density of n_e=3.1*10^{11}cm^{-2} and a mobility of μ_e=11.9*10^6cm^2/Vs at a temperature of 1.5 K.
We observe a strong negative magnetoresistance at zero magnetic field. In lowering the electron density the magnetoresistance gets more pronounced and reaches values of more than 300%. We observe that the huge magnetoresistance vanishes for increasing the temperature. An additional density dependent factor is introduced to be able to fit the parabolic magnetoresistance to the electron-electron interaction correction.
A discrepancy between theory and experiment is observed. A possible origin could be that the influence of the density fluctuation for high mobility 2DEG is not correctly described by theory. In our high mobility samples a very small, but finite density variation across the sample induces an additional long range potential, up to now not treated in theory.
arXiv:1012.0168

HL 18.2 Mon 14:45 POT 151

THz photoresponse of quantum Hall edge channels — •Christian Notthoff[1,2], Kevin Rachor[3], Detlfe Heitmann[3], Dirk Reuter[4], Andreas Wieck[4], and Axel Lorke[2] — [1]Nanoparticle Process Technology, Universität Duisburg-Essen, Lotharstr.1, D-47048 Duisburg — [2]Fachbereich Physik, Universität Duisburg-Essen, Lotharstr.1, D-47048 Duisburg — [3]Institut für Angewandte Physik, Universität Hamburg, Jungiusstr. 11,D-20355 Hamburg — [4]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, Universitätsstraße 150, D-44780 Bochum

We present THz photoresponse measurements on quasi-Corbino-shaped GaAs/AlGaAs heterostructures in the quantum Hall regime. A Fourier spectrometer is used as a broad band, black-body source with a very low spectral intensity compared to THz-Lasers used in other experiments. At filling factors $\nu > 2$, we find two independent contributions to the photoresponse-signal. One contribution clearly results from bolometric heating inside the bulk and the other one is caused by a non-bolometric mechanism. Furthermore, combining the quasi-Corbino shape with a cross-gate technique allows us to directly investigate the THz-induced transport between adjacent edge states, thus avoiding bulk effects. In the absence of bulk effects a pronounced photo voltage at zero applied bias is revealed. The photo voltage and its dependence on the bias current can be described using the model of an illuminated photodiode, resulting from the reconstruction of the Landau bands of the sample edge. Moreover, the photodiode model is also applicable to the samples where the bulk effects are present.

HL 18.3 Mon 15:00 POT 151

Probing electron-electron interactions in quantum Hall systems by scanning tunneling spectroscopy — •Marcus Liebmann[1], Stefan Becker[1], Christoph Karrasch[2], Torge Mashoff[1], Marco Pratzer[1], Volker Meden[2], and Markus Morgenstern[1] — [1]II. Physikalisches Institut B and JARA-FIT, RWTH Aachen University, 52074 Aachen — [2]Institut für Theorie der Statistischen Physik and JARA-FIT, RWTH Aachen University, 52074 Aachen

Some of the most intriguing quantum Hall phases, e.g., the fractional quantum Hall phase, are driven by electron-electron (e-e) interaction. A central challenge towards a microscopic investigation of quantum Hall physics dominated by e-e interaction is to provide a sufficiently clean and electrically decoupled system, which can be probed down to the relevant length scales, most notably the magnetic length $l_B = \sqrt{\hbar/(eB)} \approx 10$ nm (6 T). Using low-temperature scanning tunneling spectroscopy applied to the Cs-induced two dimensional electron system (2DES) on p-type InSb(110), we probe e-e interaction effects in the quantum Hall regime. The 2DES is decoupled from the p-doped bulk of the sample exhibiting spreading resistance within the insulating quantum Hall phases. In quantitative agreement with calculations we find an exchange enhancement of the spin splitting at odd fillings. We observe that both the spatially averaged as well as the local density of states feature a characteristic Coulomb gap at the Fermi level. These results show that e-e interaction effects can be probed down to a resolution below all relevant length scales.

HL 18.4 Mon 15:15 POT 151

Theory of the microwave induced zero resistance states in two-dimensional electron systems — •Sergey Mikhailov — Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany

The microwave induced zero resistance states [1] and microwave induced resistance oscillations [2] were discovered in the very-high-electron-mobility GaAs/AlGaAs quantum-well systems about ten years ago but have not been understood so far. We show [3] that this phenomenon is explained by the influence of the nonlinear ponderomotive forces which arise in the near-contact regions of the two-dimensional electron gas under the action of microwaves. The theory [3] agrees with all accumulated experimental facts and provides a simple and natural explanation of the frequency, polarization, magnetic field, mobility, power and temperature dependencies of the observed effects.

[1] R. G. Mani et al., Nature 420, 646 (2002); M. A. Zudov et al., Phys. Rev. Lett. 90, 046807 (2003)

[2] M. A. Zudov et al., Phys. Rev. B. 64, 201311 (2001); P. D. Ye et al., Appl. Phys. Lett. 79, 2193 (2001)

[3] S. A. Mikhailov, arXiv:1011.1094v1 (4 Nov 2010)

HL 19: Silicon and Germanium

Time: Monday 14:30–18:00 Location: POT 251

HL 19.1 Mon 14:30 POT 251

Phase Separation and Size Controlled Nanocrystal Formation in GeO — •Christoph Sahle[1], Christian Sternemann[1], Alexander Nyrow[1], Alexander Schwamberger[1], Florian Wieland[1], Manuel Zschintzsch[2], Johannes Borany[2], Achim Hohl[3], and Metin Tolan[1] — [1]Fakultät Physik/DELTA Technische Universität Dortmund, Otto-Hahn-Straße 4, 44227 Dortmund, Germany. — [2]Institute of Ion Beam Physics and Materials Research, Forschungszentrum Dresden-Rossendorf e.V., P.O. Box 510119, 01314 Dresden, Germany. — [3]Institute for Materials Science, Darmstadt University of Technology, 64287 Darmstadt, Germany.

Semiconducting group IV nanocrystals (NC), such as Ge- and Si-NC, have drawn a lot of attention in recent years because of their potential use in new generations of light emitting diodes, fast and stable non-volatile flash memories or highly efficient solar cells. Although intensive research has been conducted regarding the photoluminescence and charge storage properties of readily produced oxide embedded NCs little is known about the phase separation and NC formation process. Here, we present *in* and *ex situ* X-ray absorption near edge structure (XANES) spectroscopy data of the temperature induced disproportionation, i.e phase separation of GeO_x ($x \approx 1$) into Ge and GeO_2, which leads to the formation of Ge NCs embedded in a Ge oxide matrix. The formation of size controlled Ge NCs is achieved using a GeO_x–SiO_2 superlattice approach. The influence of reducing hydrogen in the annealing ambient on the phase separation process and resulting NC density is discussed.

HL 19.2 Mon 14:45 POT 251

Structural modifications of low energy heavy ion irradiated Ge — •Tobias Steinbach, Jan Wernecke, and Werner Wesch — Institute of Solid State Physics, Friedrich Schiller University Jena

During LEI irradiation of germanium extreme structural changes can be observed. To study the effects and the mechanism of porous layer formation in Ge in more detail samples were irradiated with different ion species, ion energy and angle of incidence. In order to increase the penetration depth, irradiations were performed with ion energies in the range of several MeV. We present ion induced morphological changes in Ge over a wide range of ion fluence N_I, beginning with the amorphization process of c-Ge followed by the formation of voids in the amorphous phase and its transformation into a porous structure at high N_I. Depending on N_I different regimes of porous layer formation are observed (SEM and TEM investigations) and we could demonstrate that the rate of the volume expansion depends only on nuclear energy deposition ϵ_n. However, the formation depth of the voids as well as the shape and the dimension of the porous structure depend on the ion species (chemical properties of the irradiated ions) and irradiation temperature, respectively. In addition, for all perpendicular ion irradiations a formation of a microstructure at the surface occurs whereas for non-perpendicular ion irradiation a plastic deformation, i.e. a surface shift, without a microstructure formation was observed. The effect of plastic deformation will be discussed in detail and provides an explanation for the different surface structures observed for different ion incidence.

HL 19.3 Mon 15:00 POT 251

Structure characterization on selective Ge CVD-heteroepitaxy on free standing Si (001) nanopatterns — •Grzegorz Kozlowski, Peter Zaumseil, Yuji Yamamoto, Joachim Bauer, Bernd Tillack, and Thomas Schroeder — IHP, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany

Ge is attracting increasing interest to build up future photonic technologies. The main reasons for choosing Ge is given by its superior optoelectronic properties with respect to Si and its compatibility with Si CMOS processing in contrast to III-V materials. The major stumble block for the integration of high quality Ge films on Si is however given by the 4.2% lattice mismatch which causes misfit and threading dislocations (TD). It is known that Ge deposited in smaller window tends to show lower TD density. We focus our work on the growth studies of selective Ge heteroepitaxy on nanopatterned Si (001) wafers with SiO_2 mask. Synchrotron-based grazing incidence X-ray diffraction is applied to study the structure, defect and strain characteristics with high resolution and sensitivity in a non-destructive way. In addition, special focus is devoted by Raman, transmission electron microscopy (TEM) and finite element method (FEM) simulation to determine the influence of SiO_2 growth masks on the quality of a) patterned Si substrates and b) the overgrowing Ge epilayers.

HL 19.4 Mon 15:15 POT 251

Surfactant-mediated epitaxy of germanium layers on vicinal silicon substrates — •Jasper Ruhkopf[1], Tobias F. Wietler[1], Eddy P. Rugeramigabo[1], Dominic Tetzlaff[1], Jan Krügener[2], and Eberhard Bugiel[1] — [1]Institute of Electronic Materials and Devices, Leibniz Universität Hannover, Schneiderberg 32, 30167 Hannover — [2]Information Technology Laboratory, Leibniz Universität Hannover, Schneiderberg 32, 30167 Hannover

Ge layers on vicinal Si wafers can be used as virtual substrates for GaAs growth. This provides the opportunity to combine the benefits of GaAs, needed for example for high-efficiency photovoltaic cells, with the advantages of silicon technology. The necessary strain relaxation of the Ge layers can be achieved by surfactant-mediated epitaxy (SME) employing Sb as surfactant. Ge layers were grown by SME on vicinal Si(001) substrates with different miscut angles. The surface reconstruction and step arrangement were analyzed in situ with electron diffraction methods. The dislocation pit density was examined by atomic force microscopy. The crystalline quality and the degree of strain relaxation were studied by high resolution X-ray diffraction (HRXRD). A small tensile strain was found which conformed well to calculations of the thermal stress induced in the cooling process.

HL 19.5 Mon 15:30 POT 251

Enhanced luminescence of self-assembled germanium islands in silicon photonic crystal nanocavities — •Stefan Lichtmannecker[1], Norman Hauke[1], Thomas Zabel[1], Fabrice Laussy[1], Dominique Bougeard[2], Gerhard Abstreiter[1], Yasuhiko Arakawa[3], and Jonathan Finley[1] — [1]Walter Schottky Institut, Garching — [2]Universität Regensburg — [3]University of Tokyo, Japan

We present optical investigations of two dimensional silicon photonic crystal defect nanocavities with high density ($10^9\,cm^{-2}$) germanium islands acting as an internal light source. Power and time dependent micro photoluminescence (μ–PL) spectroscopy at a lattice temperature of 25K reveals an enhancement of the photoluminescence signal recorded from the cavity modes by a factor of 350x compared to the unprocessed regions of the device. This enhancement is not fully accounted for spatial redistribution of the emission profile through the cavity mode. Quantitative analysis of power dependent μ–PL measurements and comparison with time resolved measurements suggest that the observed enhancement of the cavity mode emission is due to an enhanced internal quantum efficiency via the Purcell effect.

By systematically investigating the dependence of the emission intensity on the cavity Q-factor we observe a clear trend that lower Q-cavities produce the most intense emission. These observations are supported by simulations of our system using a dissipative master equation approach. Supported financially by the DFG via NIM, TUM IGSSE and TUM IAS.

HL 19.6 Mon 15:45 POT 251

Extrinsic doping in silicon revisited — •Udo Schwingenschlögl[1], Alexander Chroneos[2], Cosima Schuster[3], and Robin Grimes[2] — [1]PSE Division, KAUST, Thuwal 23955-6900, Kingdom of Saudi Arabia — [2]Department of Materials, Imperial College London, London SW7 2BP, United Kingdom — [3]Institut für Physik, Universität Augsburg, 86135 Augsburg, Germany

Both n-type and p-type doping of silicon is at odds with the charge transfer predicted by Pauling electronegativities and can only be reconciled if we no longer regard dopant species as isolated atoms but rather consider them as clusters consisting of the dopant and its four nearest neighbor silicon atoms. The process that gives rise to n-type and p-type effects is the charge redistribution that occurs between the dopant and its neighbors, as we illustrate here using electronic structure calculations. This view point is able to explain why conventional substitutional n-type doping of carbon has been so difficult.

Reference: Appl. Phys. Lett. 96, 242107 (2010)

HL 19.7 Mon 16:00 POT 251

In-situ incorporation and distribution of boron dopants in silicon nanowires — •Pratyush Das Kanungo[1], Xin Ou[2], Reinhard Koegler[2], Alexander Tonkikh[1], Wolfgang Skorupa[2], and Peter Werner[1] — [1]Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle, Germnay — [2]Forschungszentrum Dresden - Rossendorf, FWIM, 01314 Dresden, Germany

Silicon nanowires (Si NWs) are promising candidates for future nanoelectronic devices and circuits. However, controlled doping and measurement of doping profiles are two of the biggest challenges that need to be addressed before using them as building blocks for functional devices. By measuring the current-voltage characteristics of a molecular beam epitaxy-grown and heavily in-situ boron-doped Si NW of diameter around 100 nm, and separately measuring the local spreading resistance across the cross-section of a NW of the same doping level, we have analyzed the incorporation, distribution and deactivation of boron atoms. It was observed that the incorporated and active boron atoms form a multi-shell structure. The area very near (around 5 nm) to the outer surface is fully depleted of active dopants because of the surface states existing at the outer surface of the NW. Underneath this depleted shell, two heavily doped cores are formed. The first one is relatively thinner (around 30 nm), but it contains relatively higher active boron concentration than the thicker (around 70 nm) inner core. We further establish that this nonuniformity in active boron concentration is related to the in-situ doping process itself which can offer two different pathways for incorporation of boron.

15 min. break

HL 19.8 Mon 16:30 POT 251

Kelvin probe force microscopy on doped semiconductor nanostructures with local, carrier-depleted space charge regions — •Christine Baumgart[1], Anne-Dorothea Müller[2], Falk Müller[2], Manfred Helm[1], and Heidemarie Schmidt[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Institut für Ionenstrahlphysik und Materialforschung, P.O. Box 510119, 01314 Dresden — [2]Anfatec Instruments AG, Melanchthonstr. 28, 08606 Oelsnitz

Failure analysis and optimization of semiconducting devices require knowledge of their electrical properties. Kelvin probe force microscopy (KPFM) is the most promising non-contact electrical nanometrology technique to meet the demands of today's semiconductor industry. We present its applicability to locally doped silicon structures. Quantitative dopant profiling by means of KPFM measurements is successfully demonstrated on a conventional static random access memory (SRAM) cell and on cross-sectionally prepared Si epilayers by applying a recently introduced new explanation of the measured KPFM signal [1]. Additionally, the influence of local, carrier-depleted space charge regions and of the electric fields across them is discussed. It is explained how drift and diffusion of injected charge carriers in intrinsic electric fields influence the surface region of the investigated semiconductor and thus may disturb the detected KPFM bias.

[1] C. Baumgart, M. Helm, H. Schmidt, Phys. Rev. B 80, 085305 (2009).

HL 19.9 Mon 16:45 POT 251

New luminescence line at 1.09 eV in two stage deformed silicon — •Matthias Allardt, Sabine Kolodinski, Ellen Hieckmann, and Jörg Weber — Technische Universität Dresden, 01062 Dresden, Germany

This work focuses on photoluminescence (PL) and cathodoluminescence (CL) in Fz silicon, deformed in a two stage process: a low-stress uniaxial predeformation at 8 MPa @ 800 °C and a subsequent high-stress deformation at 300 MPa @ 420 °C. Slip lines on the sample surface show that two glide systems have been activated during the deformation process. A new spectral line at 1.09 eV could be observed both in the PL and CL investigations. A line shape analysis at different temperatures give evidence that this line originates from a free-to-bound transition with a trap binding energy of 80 meV. The nature of the luminescence center will be discussed. The work was funded under the SAB Project-Nr. 14255/2423.

HL 19.10 Mon 17:00 POT 251

Raman scattering study of ro-vibrational modes of interstitial H_2 in crystalline Si — •Sandro Koch, Edward Lavrov, and Jörg Weber — Technische Universität Dresden, 01062 Dresden, Germany

Raman scattering studies of Si samples hydrogenated in a rf plasma have been performed. Ro-vibrational $Q(J)$ transitions for rotational quantum number $J = 0, 1, 2$, and 3 have been investigated in the temperature range from 90 to 388 K. We demonstrate that the $Q(2)$ transition appears in the Raman spectra above 200 K as suggested by Hiller et al. [PRB 74, 235214 (2006)]. Additionally, the $Q(3)$ transition is detected at 388 K. From the temperature dependence of the phonon spectrum of the Si host, we can show that the coupling between rotational states of H_2 depends on the temperature.

HL 19.11 Mon 17:15 POT 251

Thermally stimulated current in solid phase crystallized poly-Si thin films — •Markus Moser, Lars-Peter Scheller, and Norbert Nickel — Helmholtz-Zentrum Berlin für Materialien und Energie, Kekuléstr. 5, 12489 Berlin, Germany

Polycrystalline silicon (poly-Si) is an attractive material for many thin film electronic devices due to its improved carrier mobility and long term stability compared to amorphous silicon (a-Si). Furthermore it can be deposited on large areas of cheap substrates such as glass or plastic. However, the use of such low cost substrates limits process temperatures to values below 600°C which strongly influences the electrical and structural properties of the material. In particular, the performance of electronic devices containing poly-Si is affected by grain boundaries, impurities and lattice defects that cause localized states in the band gap. These defect states can trap charge carriers and can act as efficient recombination centers limiting the performance of thin-film transistors and solar cells. Thermally stimulated current measurements (TSC) are a helpful tool to detect these states. In this work, TSC is applied to poly-Si films on Corning glass which are produced by electron beam evaporation and subsequent solid phase crystallization. The measurements reveal a superposition of contributions from different gap states. A thermal cleaning procedure is used to resolve the individual components. Six states with activation energies ranging from 116 meV to 543 meV are obtained. The results are discussed in terms of possible intrinsic and extrinsic defects.

HL 19.12 Mon 17:30 POT 251

Contact materials for sulphur hyperdoped black silicon — •Thomas Gimpel[1], Kay-Michael Günther[1], Anna Lena Baumann[2], Augustinas Ruibys[2], Stefan Kontermann[2], and Wolfgang Schade[1,2] — [1]Clausthal University of Technology, EFZN, EnergieCampus, Am Stollen 19, 38640 Goslar — [2]Fraunhofer Heinrich Hertz Institute, EnergieCampus, Am Stollen 19, 38640 Goslar

Irradiating a plane silicon surface with a train of intense femtosecond-laser pulses in a sulphur-containing atmosphere leads to a structured surface with enhanced absorption properties in the visible and near infrared spectral range, even at wavelengths below the bandgap. Because the resulting layer system shows photovoltaic activity it is proposed to turn this absorption into an efficient charge carrier generation for photovoltaic applications. Extracting those charge carriers is difficult, because of a structured, nanocrystalline covering surface layer with thickness of d<1μm and a sulphur content of about 1 at.% which influences the mechanical adhesion and contact resistances. Deposition techniques like screenprinting, sputtering, pulsed laser deposition and thermal evaporation are compared. We use different metal layer systems like silver, titanium/palladium/silver, chromium/gold and transparent contacts like indium tin oxide. By means of impedance spectroscopy we evaluate the contact behaviour finding the appropriate contact material.

HL 19.13 Mon 17:45 POT 251

Determination of the complex refractive index in the infrared region for femtosecond-laser-formed silicon surfaces using ray-tracing — •Augustinas Ruibys[1], Christian Lehmann[2], Thomas Gimpel[3], Anna Lena Baumann[1], Stefan Kontermann[1], and Wolfgang Schade[1,3] — [1]Fraunhofer Heinrich Hertz Institute, Energie-Campus, Am Stollen 19, 38640 Goslar — [2]FU Berlin, Fachbereich für Experimentalphysik, Arnimallee 14, 14195 Berlin — [3]Clausthal University of Technology, EFZN, Energie-Campus, Am Stollen 19, 38640 Goslar

The femtosecond-laser processing of silicon surface in the SF6 gas creates cone-shaped structures, which have a thin 0.1 - 1 μm layer of multi-crystalline substance with approximately 0.5 at.% of sulphur. This layer is known to be photovoltaically active in the visible wavelengths as well as in the infrared and has the potential for cost effective solar cells. However, not much is known about the fundamental properties of this multi-crystalline layer. Measuring the optical properties in the infrared and simulating ray-traces in the coned surface, allows calculating the complex refractive index and the associated absorption coefficient. The simulated refractive index spectra are presented for samples processed in SF6 gas and vacuum in the wavelength range 1100 nm - 2500 nm. The obtained absorption coefficient spectra for samples processed in SF6 are of the order of 10^4 cm-1. This high absorption in the infrared is discussed from the point of view of the introduced sub-band-gap energy levels on the one hand and high free carrier absorption on the other hand.

HL 20: Innovative Materials

Time: Monday 14:30–15:45 Location: POT 06

HL 20.1 Mon 14:30 POT 06

Synthesis of functional nano-micro structural materials by a simple flame transport approach — •Yogendra Kumar Mishra, Sören Kaps, Xin Jin, Dawit Gedamu, Ingo Paulowicz, Arnim Schuchardt, Sebastian Wille, and Rainer Adelung — Functional Nanomaterials, Institute for Materials Science, Faculty of Engineering, Christian-Albrechts-University, Kaiserstrasse 2, 24143 Kiel, Germany

Recent studies on the growth of semiconductor and ceramic nanostructures ranging from 1D arrays to 3D networks, have attracted immense research motivation due to their multi-functional properties which offer a huge amount of applications like nanoelectronics, sensors and mainly biological engineering. However mass scale synthesis of nanos-

tructures or synthesis of hyperbranched interconnected extremely large networked nanostructures is still an open challenge. The vapour liquid solid (VLS) process is the most used technique but according to the recent demands in nanotechnology the VLS process needed further simplification or development of new techniques. The present work demonstrates a very simple flame transport synthesis (FTS) approach which offers synthesis of desired semiconductor and ceramic nanostructures. A complete overview of the family of ZnO nano-micro structures along with the glimpses of SnO2, Fe2O3, Bi2O3 and Al2O3 nanostructures synthesized by FTS approach will be presented and the role of different growth parameters will be discussed. Preliminary results of the corresponding current-voltage response, elastic modulus as well as possible applications in biomedical engineering will be presented.

HL 20.2 Mon 14:45 POT 06

Self assembly of 1D-nanoparticles at interfaces using external fields — •Anindya Majumder[1,3], Oliver Jost[2], Jörg Opitz[3,4], Gianaurelio Cuniberti[3], and Eckhard Beyer[1,2] — [1]Institute of Surface and Manufacturing Technology, Dresden University of Technology, 01062 Dresden, Germany — [2]Fraunhofer IWS, Winterbergstraße 28, 01277 Dresden, Germany — [3]Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, 01062 Dresden, Germany — [4]Fraunhofer IZFP, Maria-Reiche-Str. 2, 01219 Dresden, Germany

Self-assembly of nanoparticles has promising technological applications since it provides efficient building blocks for physical, chemical, and biological systems. Localization of nanoparticles at liquid-liquid interfaces by manipulating the particle surface energy is an upcoming area with great potential for applied and fundamental research. Apart from regular technological applications, such tailor made assembly opens a window to fabricate self assembled interfacial structured hybrid materials with unique properties. Carbon nanotubes (CNTs) represent an anisotropic and perfectly one-dimensional class of nanoparticles with extraordinary properties. CNTs were functionalized by various surfactants to prevent its agglomeration due to van-der-Waals forces. This dispersion was added to an immiscible solvent and CNTs were self assembled with the aid of electric field via dielectrophoresis between pre-fabricated inter-digitated electrodes on silicon substrates. A potential drop across the interface may provide sufficiently deep potential wells for self assembly at the interface.

HL 20.3 Mon 15:00 POT 06

Properties of annealed RF-sputtered Cu_2O thin films — •Daniel Reppin, Andreas Laufer, Angelika Polity, Detlev M. Hofmann, and Bruno K. Meyer — I. Physikalisches Institut, Justus-Liebig-Universität Giessen, Heinrich-Buff-Ring 16, 35392 Giessen

Cuprous oxide is a p-type semiconductor with a band gap in the visible spectral range, it is sustainable, non-toxic and cheap in production and therefore an interesting material for photovoltaic applications.

Cu_2O thin films were sputtered from a copper and a Cu_2O composite target in a RF sputtering chamber under different oxygen flows. Afterwards the films were annealed under nitrogen flow in the range of 400 to 930 °C for ten minutes. The effect of the annealing time was also investigated. Subsequently the optical and electrical properties of the annealed films were compared to the 'as-deposited' films. After the annealing procedure the films sputtered from the Cu-target show a reduced carrier concentration by a factor of 100 ($2.5 \cdot 10^{17}$ -> $2.5 \cdot 10^{15}$ cm^{-3}) while the mobility increases from 0.37 to 35 cm^2/Vs. The band gap of the films changed from 2.10 to 2.53 eV. These effects are related to a better crystalline quality and therefore a reduction of defects in the crystal structure of the Cu_2O. The results using the Cu_2O-target will be discussed at the conference.

HL 20.4 Mon 15:15 POT 06

Rb_4O_6: strongly correlated 2p shell system under pressure — •shahab naghavi, stanislav chadov, gerhard h. fecher, and claudia felser — institut für anorganische chemie und analytische chemie, Johannes gutenberg universtität mainz

the strongly correlated 2p open-shell of Rb_4O_6 exhibits a variety of interesting physical phenomena at high pressures. In this compound, there are two different kinds of anionic oxygen molecules in the solid simultaneously, hyperoxide and peroxide. By mean of the first-principle electronic structure calculation, we study the Rb_4O_6 system under pressure. Its peculiar feature is the strongly correlated p electrons of the hyperoxide molecules (O_2^{2-}). Around 75 GPa a transition from an insulating antiferromagnetic phase to a half-metallic ferromagnetic phase takes place. At pressures higher than 75 GPa, all anionic oxygen molecules (peroxide and hyperoxide) carry magnetic moments. Finally, above 160 GPa a metallic phase appears, where all oxygen molecules show the same bond lengths without magnetic moment.

HL 20.5 Mon 15:30 POT 06

Molecular beam epitaxy of Heusler alloys on InAs heterostructures — •Boris Landgraf, Sascha Bohse, Christian Heyn, and Wolfgang Hansen — Institut für Angewandte Physik, Universität Hamburg, 20355 Hamburg, Germany

The injection of highly spin-polarized electrons from ferromagnets into low-dimensional semiconductor systems is important for spintronic applications. The main problem encountered when building such spintronic devices is that spin-polarization of electrons gets lost at the metal/semiconductor interface. We investigate epitaxial growth as well as structural, magnetical, and electrical properties of Heusler/semiconductor hybrid systems. In particular, we focus on Ni_2MnIn Heusler grown on InAs(001) as well as on modulation-doped InGaAs/InAs/InGaAs heterostructures. One previous finding [1] with this hybrid system reveals that As diffuses from InAs into the Heusler film and forms a significant intermixing layer. We pursue two possibilities to overcome this problem. One is the growth of a MgO diffusion-barrier to avoid intermixing at the interface. Corresponding data will be discussed. Another solution is the use of other Heusler candidates. For that reason, we run a new metal molecular beam epitaxy (MBE) chamber in our laboratory, which is connected with a commercial III/V semiconductor MBE via an in-vacuo transfer system. This MBE chamber enables the growth of MgO as well as of different Heusler alloys.

[1] A. Zolotaryov et al., *J. Cryst. Growth* 2397–2404, 311 (2009)

HL 21: Symposium: Artificial Optical Materials (SYOM)

Time: Monday 14:30–17:15 Location: HSZ 01

Invited Talk HL 21.1 Mon 14:30 HSZ 01

Photonic Metamaterials and Transformation Optics: Recent Progress — •Martin Wegener — Karlsruhe Institute of Technology (KIT), DFG-Center for Functional Nanostructures (CFN), 76128 Karlsruhe, Germany

Metamaterials are artificial materials composed of sub-wavelength building blocks that are densely packed into an effective material. This concept allows for achieving effective optical properties that are not accessible in natural substance. In 2007, negative-index metamaterials have reached visible operation frequencies. Today, taking advantage of progress in three-dimensional nanofabrication, photonic metamaterials have even become truly three-dimensional. However, the reduction of metal losses still poses a major challenge. In this talk, I will start with a brief overview and then emphasize recent results of our group such as, e.g., (i) adding semiconductor quantum well gain and (ii) designing/fabricating/characterizing three-dimensional invisibility cloaking structures operating at visible frequencies. The latter has only become possible by using diffraction-unlimited optical lithography in three dimensions - the counterpart of STED fluorescence microscopy.

Invited Talk HL 21.2 Mon 15:00 HSZ 01

Keeping a tight focus on matter — •Philip St. J. Russell — Max-Planck Institute for the Science of Light, Guenther-Scharowsky Strasse 1/24, 91058 Erlangen, Germany

Photonic crystal fibres uniquely permit laser light to be kept tightly focused in a hollow micron-sized channel over propagation lengths of hundreds of metres. Recent experiments show how this can be used to enhance nonlinear light-matter interactions in gases and to trap and propel small particles using light.

Invited Talk HL 21.3 Mon 15:30 HSZ 01

The Physics of Photonic Crystals LEDs — •Claude Weisbuch[1,2] and Elison Matioli[1] — [1]Laboratoire de Physique de

la Matière Condensée, CNRS, Ecole Polytechnique, Palaiseau, France — [2]Materials Department, UCSB, Santa Barbara, CA, USA

Photonic crystal (PhC) based Light Emitting Diodes (LEDs) display a rare blend of fundamental and applied concepts in solid state and semiconductor physics. Their remarkable properties rely on a mix of intrinsic materials properties and of electromagnetic properties of the PhC. Detailed understanding of PhC LED concepts can be obtained from studies of physics in and of devices.

Coffee Break

Invited Talk HL 21.4 Mon 16:15 HSZ 01
Using nanophotonic structures to overcome conventional limits in solar energy conversion — •Shanhui Fan — Ginzton Laboratory, Department of Electrical Engineering, Stanford University, Stanford, California 94305, U.S.A.

The use of nanophotonic structures drastically alter the nature of light-matter interactions, and opens new opportunities for overcoming some of the conventional limits in solar energy conversion. In this talk, we show that broad-band nanoscale modal confinement can be used to achieve light trapping efficiencies that are far beyond the Yablonovitch limit. We also discuss some of our recent works on solar bandwidth compression, with the ultimate aim of overcoming the Shockley-Queisser limit using only single-junction solar cells.

Invited Talk HL 21.5 Mon 16:45 HSZ 01
Plasmonic nanocavities: New design concepts and determination of the complete mode spectrum using electron-beam spectroscopies — •Stefan A. Maier — The Blackett Laboratory, Department of Physics, Imperial College London, London SW7 2AZ, United Kingdom

New design concepts such as the exploitation of dark modes, Fano resonances, and transformation optics allow for the design of plasmonic nanocavities with fascinating spectral properties, such as broadband superfocusing and invisibility dips, while at the same time retaining the deep sub-wavelength mode volume. A variety of cavity designs will be discussed, for applications ranging from optical sensing to photovoltaics. Furthermore, it will be shown that electron energy loss spectroscopy is an ideal tool for the determination and imaging of the mode spectrum of complex plasmonic cavities, including the elusive dark modes.

HL 22: SKM Symposium: Spin Caloric Transport (SYST)

Time: Monday 14:30–17:00 Location: TRE Ma

Invited Talk HL 22.1 Mon 14:30 TRE Ma
On the theory of the spin wave Seebeck effect — •Gerrit Bauer — Kavli Institute of NanoScience, TU Delft, Netherlands

The spin Seebeck effect, discovered by Uchida et al. [1], has been observed in various ferromagnets, such as the metal Py [1], insulating Yttrium Iron Garnet (YIG) [2], the semiconductor GaAlMn [3] and the Heusler compound Co2MnSi [4]. Possibly, the effect is caused by the non-equilibrium spin wave dynamics induced by a thermal gradient, which leads to a net spin current injected by the ferromagnet into a normal metal contact [5,6]. This mechanism appears to explain experiments on the spin Seebeck effect in YIG [2]. This talk will address new theoretical developments to understand the spin (wave) Seebeck effect.

The reported results have been obtained in collaboration with J. Xiao, K. Xia, K. Uchida, E. Saitoh, and S. Maekawa and has been support by the Dutch FOM foundation.

[1] K. Uchida et al., Nature 445, 778-781 (2008).
[2] K. Uchida et al., Nature Mater. 9, 894 (2010).
[3] C.M. Jaworski et al., Nature Mater. 9 , 898 (2010).
[4] S. Bosu et al., unpublished.
[5] J. Xiao et al., Phys. Rev. B 81, 214418 (2010).
[6] H. Adachi et al., arXiv:1010.2325.

Invited Talk HL 22.2 Mon 15:00 TRE Ma
Spin Seebeck effect in metals and insulators — •Ken-ichi Uchida and Eiji Saitoh — Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan

Recent studies on spintronics and spin caloritronics have revealed that a spin current, a flow of spin angular momentum, is strongly coupled with a heat current in various magnetic systems. From both basic science and applied engineering points of view, the interplay of these two currents is of crucial importance. The spin-Seebeck effect (SSE) [1-6] is a phenomenon enabling the conversion of heat currents into spin voltage, a potential for driving nonequilibrium spin currents, in ferromagnets.

In this paper, we report the experimental observation of the SSE in ferromagnetic metals [1] and insulators [3,5]. The SSE drives a spin current flowing across an interface between a ferromagnet and an attached Pt film and the spin current is converted into electric voltage by the inverse spin-Hall effect [7] in the Pt film.

This work was supported by a Grant-in-Aid for Scientific research in Priority Area "Creation and Control of Spin Current" and Scientific Research A from MEXT, Japan.

[1] K. Uchida et al., Nature 455, 778 (2008). [2] J. Xiao et al., Phys. Rev. B 81, 214418 (2010). [3] K. Uchida et al., Nature Mater. 9, 894 (2010). [4] C. M. Jaworski et al., Nature Mater. 9, 898 (2010). [5] K. Uchida et al., Appl. Phys. Lett. 97, 172505 (2010). [6] H. Adachi et al., arXiv:1010.2325 (2010). [7] E. Saitoh et al., Appl. Phys. Lett. 88, 182509 (2006).

Invited Talk HL 22.3 Mon 15:30 TRE Ma
Spin-Seebeck effect: Local nature of thermally induced spin currents in GaMnAs — •Roberto Myers — Department of Materials Science and Engineering, The Ohio State University, Columbus, Ohio, U.S.A.

The spin-Seebeck effect refers to a spatial distribution of spins in a ferromagnetic material induced by a thermal gradient. This macroscopic spatial distribution of spins is several orders of magnitude larger than the spin diffusion length. Here we describe measurements of the spin-Seebeck effect in the ferromagnetic semiconductor, GaMnAs, and a related ferromagnetic metal MnAs. The thermally induced spatial distribution of spins is inferred from the sign and magnitude of the inverse spin Hall voltage generated from local spin currents in platinum bars that are in electrical contact with the ferromagnetic material. From an experimental point of view, GaMnAs provides unique measurement geometries since the magnetic easy axes can be engineered in different directions and the low Curie temperature makes it convenient to perform spin-Seebeck measurements across the magnetic phase transition. Using different experimental configurations we measure either the isolated spin-Seebeck signal, the planar and transverse Nernst effect, or a combination of the spin-Seebeck and Nernst effects. One of the most intriguing aspects of the spin-Seebeck effect is the observation that the spatial distribution of spins is maintained across electrical breaks revealing that the effect does not arise from a longitudinal spin current of charge carriers.

Invited Talk HL 22.4 Mon 16:00 TRE Ma
Heat conduction of low-dimensional quantum magnets — •Christian Hess[1], Nikolai Hlubek[1], Patrick Ribeiro[1], Bernd Büchner[1], Surjeet Singh[2], Romuald Saint-Martin[2], and Alexandre Revcolevschi[2] — [1]Leibniz-Institute for Solid State and Materials Research, IFW Dresden, Institute for Solid State Research, 01171 Dresden, Germany — [2]Laboratoire de Physico-Chimie de L'Etat Solide, ICMMO, UMR8182, Université Paris-Sud, 91405 Orsay, France

Some years ago, a new, magnetic mode of heat transport which occurs in low-dimensional $S = 1/2$ quantum magnets has been discovered and is intensely studied since then. The magnetic heat conductivity κ_{mag} of such quantum magnet materials can be exceptionally large (even at room temperature), dwarfs the phonon heat conduction and thereby leads to an overall magnitude of the heat conductivity which is comparable to that of metals. The analysis of κ_{mag} yields detailed information about the scattering processes which govern the magnon transport, such as scattering involving defects, phonons and magnons in the materials. After reviewing the main experimental findings, this talk focuses on recent experimental results on one-dimensional $S = 1/2$ Heisenberg chain materials. Evidence for ballistic magnetic transport

and magnetic mean free paths of more than one micrometer is found in these materials, i.e. at the length scale of typical spin diffusion lengths in spintronic experiments. In our experiments we carefully study the effect of various disorder types (viz. bond disorder, magnetic and non-magnetic site disorder) on this transport phenomenon.

Invited Talk HL 22.5 Mon 16:30 TRE Ma
Evidence of spin polarized heat current acting on magnetization — •Jean-Philippe Ansermet — EPFL, station 3, CH-1015 Lausanne, Switzerland

Nanomagnets of controlled geometry can be formed and contacted electrically by the method of electrodeposition in nanopores. The talk will focus on recent results, where Joule heating was used as a source of heating on a nanoscale. Evidence for thermal spin transfer torque was demonstrated (Haiming Yu, S. Granville, D. P. Yu, J.-Ph. Ansermet, Phys. Rev. Lett. 104, 146601 (2010)). Heat currents crossing the free layer of an asymmetric spin valve are shown to change its switching field. The data are accounted for with a thermodynamic model for the spin current accompanying heat transport.

HL 23: Joint Focussed Session: Thin Film Chalcogenide Photovoltaics II

Time: Monday 14:45–15:45 Location: GER 37

Topical Talk HL 23.1 Mon 14:45 GER 37
Dünnschicht-Chalkogenid-Solarzellen: Überblick und Forschungsfelder — •Michael Powalla — Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg

Unter allen Dünnschichtsolarzellenkonzepten bietet die sogenannte CIGS-Technologie (Copper, Indium, Gallium, Selenium, Sulfur) das höchste Kostenreduktionspotenzial in der industriellen Fertigung. Dies ist begründet in dem im Labor nachgewiesenen hohen Wirkungsgradpotenzial, welches vergleichbar mit Solarzellen aus polykristallinem Silizium ist.

Der Vortrag gibt einen Überblick über den Stand der Entwicklung der CIGS-Solarzellen und -module in der Industrie und der Forschung. Ein Fokus liegt dabei auf der Licht absorbierenden, p-halbleitenden CIGS-Schicht, der Grenzfläche und dem n-leitenden Heterokontaktpartner. Die CIGS-Schicht wird mittels thermischer Koverdampfung oder in einem sequentiellen Verfahren hergestellt. Für den n-leitenden Frontkontakt werden unterschiedliche II/VI-Materialien verwendet, die sowohl im chemischen Bad als auch von der Gasphase abgeschieden werden können.

Am ZSW wird eine Kleinzellenlinie sowie eine Modullinie (Glassubstrate bis 30 cm x 30 cm) zur Herstellung von CIGS-Solarzellen betrieben. Speziell für flexible Substratträger (Polyimid, Metallfolien) werden Beschichtungen auf einer Rolle-zu-Rolle-Beschichtungsanlage durchgeführt. Aktuelle Forschungsergebnisse wie z. B. die Erreichung des weltbesten Wirkungsgrades für Dünnschichtsolarzellen von 20,3 % mit einer CIGS/CdS-Diode werden präsentiert.

HL 23.2 Mon 15:15 GER 37
Thin film solar cells based on the ternary compound Cu_2SnS_3 — •Dominik M. Berg, Phillip J. Dale, and Susanne Siebentritt — University of Luxembourg, Laboratory for Photovoltaics, 41 rue du Brill, L-4422 Belvaux, Luxembourg

Thin films of kesterite ($Cu_2ZnSn(S/Se)_4$) semiconductors are considered promising absorber layer materials for low cost thin film photovoltaic devices. Experimental and theoretical investigations show, however, that the existence region of a single phase kesterite is relatively small making it difficult to grow single phase absorbers. The semiconducting compound Cu_2SnS_3 is a common secondary phase that forms in Cu and Sn rich kesterite thin films during growth. Its appearance in a kesterite device would limit the V_{OC} due to its smaller band gap. However, the band gap of about 1 eV, reported hole concentrations of 10^{18} cm^{-3}, and an absorption coefficient in the visible region of 10^5 cm^{-1} make the Cu_2SnS_3 compound itself a promising candidate for low cost photovoltaic applications.

In this report we demonstrate the successful fabrication of a thin film solar cell based on Cu_2SnS_3 via a precursor annealing process. The precursor is prepared by low cost electrodeposition. A maximum external quantum efficiency of about 60% at 800 nm and a band gap of 1.0 eV could be measured. To the best of our knowledge, there have been no other reports on the fabrication of Cu_2SnS_3 based solar cell devices so far. Loss mechanisms and ways to increase efficiency will be discussed.

HL 23.3 Mon 15:30 GER 37
Investigation of lattice defects and compositional gradients in Cu(In,Ga)Se_2 thin films for solar cells — •Jens Dietrich[1], Daniel Abou-Ras[2], Thorsten Rissom[2], Thomas Unold[2], Hans-Werner Schock[2], and Christian Boit[1] — [1]Department of Semiconductor Devices, Berlin University of Technology, Einsteinufer 19, 10587 Berlin — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin

Cu(In,Ga)Se_2 absorber layers used in thin-film solar cells exhibit, when grown in a multi-stage process, compositional gradients of gallium and indium, dependent on process parameters such as the Ga content. The high lateral resolution of transmission electron microscopy (TEM) imaging and energy-dispersive X-ray spectroscopy (EDX) allows the determination of lattice defects and the elemental concentrations at identical sample positions. Cross-sectional TEM samples of ZnO/CdS/Cu(In,Ga)Se_2/Mo/glass stacks were prepared with varying [Ga]/([In]+[Ga]) ratio in the absorber. The shape of the Ga distribution was measured by means of EDX and differs for the various [Ga]/([In]+[Ga]) ratios. Linear (dislocations) and planar defects (stacking faults, microtwins) were studied by means of TEM bright field and dark field images along the lengths of the Cu(In,Ga)Se_2 layers. Strong Ga compositional gradients were found even within individual grains. It appears that these Ga gradients correlate with the occurrence of dislocation networks in large grains (diameter $> 1\,\mu$m). We assume that these dislocations compensate for lattice mismatch due to the change in composition in this area of the lattice.

HL 24: Joint Focussed Session: Thin Film Chalcogenide Photovoltaics III

Time: Monday 16:00–17:30 Location: GER 37

HL 24.1 Mon 16:00 GER 37
Time dependent capacitance voltage measurements on Cu(In,Ga)Se_2 Solar Cells — •Tobias Adler[1], Wolfram Witte[2], Dimitrios Hariskos[2], and Andreas Klein[1] — [1]Darmstadt University of Technology, Institute of Materials Science, Petersenstrasse 32, D-64287 Darmstadt, Germany — [2]Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg (ZSW), Industriestrasse 6, D-70565 Stuttgart, Germany

Capacitance Voltage (C-V) measurements are widely used to determine the doping density of semiconductor interfaces in dependence on the width of the space charge layer. In Cu(In,Ga)Se_2 (CIGS) solar cells we observe a time dependent capacitance signal, which can be explained by different models like filling and emptying of electronic (metastable) defect states or by the diffusion of copper ions. The observed capacitance transients are compared to the different models.

HL 24.2 Mon 16:15 GER 37
Charakterisierung der elektrischen Eigenschaften von Korngrenzen an polykristallinen Chalkopyriten — •Sebastian Linke, Thorsten Rissom, Daniel Abou-Ras, Martha Ch. Lux-Steiner und Sascha Sadewasser — Helmholtz-Zentrum für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin

Polykristalline $CuIn_{1-x}Ga_xSe_2$ (CIGSe) Absorberschichten bilden die Grundlage der Dünnschicht-Solarzellen mit dem momentan höchsten Wirkungsgrad. Eine Besonderheit ist, dass polykristalline CIGSe Solarzellen, im Gegensatz zu Dünnschichtzellen auf Siliziumbasis, hö-

here Wirkungsgrade als die monokristallinen Pendants erzielen. Die Gründe dafür sind Gegenstand aktueller Forschung. Der Einfluß der Korngrenzen auf den Ladungstransport, insbesondere in Abhängigkeit vom [Ga]/[Ga+In]-Verhältnis, ist hierbei von großem Interesse. Die Charakterisierung der elektrischen Eigenschaften der Korngrenzen ist Voraussetzung, um ein besseres Verständnis der hohen Wirkungsgrade (> 20%) polykristalliner Absorber zu erhalten. Wir präsentieren Untersuchungen polykristalliner $CuInSe_2$ sowie $CuIn_{0.67}Ga_{0.33}Se_2$ Absorberschichten mittels Rastertunnelspektroskopie (STS) im Ultrahochvakuum bei Raumtemperatur, sowohl im Dunkeln als auch unter Beleuchtung. Bestimmte Korngrenzen zeigen im Vergleich zu ihrer direkten Umgebung eine reduzierte Dichte an Defektzuständen innerhalb der Bandlücke. Dies ist eine mögliche Erklärung für die herausragende Effizienz polykristalliner CIGSe Solarzellen. Unter Beleuchtung nimmt die differentielle Leitfähigkeit ab. Desweiteren wurden Strukturuntersuchungen mittels Elektronenbeugung (EBSD) durchgeführt.

HL 24.3 Mon 16:30 GER 37

Analysis of $Cu_2ZnSn(S/Se)_4$ by Photoluminescence and Raman — •Rabie Djemour, Levent Gütay, and Susanne Siebentritt — Laboratory for Photovoltaics, University of Luxembourg

Kesterites $Cu_2ZnSn(S/Se)_4$ are promising absorber materials for low cost thin film photovoltaic devices, since they are composed of cheap, abundant, and non toxic materials. However, growing single phase $Cu_2ZnSn(S/Se)_4$, turns out to be a difficult task because of the very small existence region, as shown experimentally and theoretically. Thus, for proper optimization of the growth process of kesterites it is essential to detect the occurrence of any secondary phase. Since conventional X-ray diffraction and energy dispersive X-ray analysis are lacking unambiguous phase resolution, we perform photoluminsecence (PL) and Raman measurements, which allow for non-ambiguous identification of the kesterite and co-existing secondary phases. We present a homebuilt system that allows PL and Raman measurements at the same spot with a spatial resolution in the one micron range. We show and discuss characteristic PL spectra for kesterites of different composition and varying crystal quality and demonstrate that even single crystals show compositional and opto-electronic inhomogeneities.

HL 24.4 Mon 16:45 GER 37

Influence of band-gap grading on luminescence properties of Cu(In,Ga)Se_2 — •Jakob Haarstrich[1], Heiner Metzner[1], Carsten Ronning[1], Thorsten Rissom[2], Christian A. Kaufmann[2], Hans-Werner Schock[2], and Andreas Undisz[3] — [1]Institut für Festkörperphysik, Friedrich Schiller Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Solar Energy Research, Institute for Technology, Lise-Meitner-Campus, Hahn-Meitner-Platz 1, 14109 Berlin, Germany — [3]Institute for Material Science and Technology, Metallic Materials, Friedrich-Schiller-University Jena, Loebdergraben 32, 07743 Jena, Germany

Cathodoluminescence (CL) has been measured on Cu(In,Ga)Se_2 with Ga-grading as it is used in high-efficiency thin-film solar cells at 10 K in both cross-section and plain view configuration. In cross-section geometry, we show that the vertical profile of the emission energy represents the Ga-profile in the film and, thus, we are able to measure the band-gap grading present by means of CL methods. At the same time, we observe a strong drift of excited charge carriers towards the minimum of the band-gap which can be explained by the Ga-grading. It is shown by voltage-dependent CL, how these results directly influence the interpretation of luminescence spectra obtained on Ga-graded Cu(In,Ga)Se_2 and, thus, they will have to be considered as a basis for all forthcoming investigations on this topic.

HL 24.5 Mon 17:00 GER 37

Pump-probe investigations on thin film ablation with ultrashort laser pulses — •Matthias Domke, Gerhard Heise, and Heinz Huber — Hochschule München

Laser lift-off processes have been observed during structuring CIGS thin film solar cells. To get a deeper insight in the underlying physical processes a pump-probe setup is used for spatial and temporal investigation of the interaction of ultra-short laser pulses with thin films. The setup consists of a 10 ps-laser pulse at a wavelength of 1064 nm that is split up into a pump and a probe beam. The pump beam is used to ablate thin films with single or multiple pulses. The probe beam illuminates the ablation area after an optically or electronically defined delay. A CCD Camera behind a microscope objective captures an image of the ultra-short exposed region. The probe beam is frequency doubled so that the pump light may be filtered out at the camera. Thus, the development of multiple pulse ablation is investigated in situ by taking pictures after each single pulse. Furthermore, a series of pictures can be taken on a picosecond time-scale by increasing the temporal delay of pump and probe beam. Consequently, the temporal evolution of direct and indirect (lift off) laser ablation of thin films can be studied.

HL 24.6 Mon 17:15 GER 37

Spectroscopic Imaging ellipsometry on arsenic sulphide fibers with a lateral resolution down to one micrometer — •Peter H Thiesen and Christian Röling — Accurion GmbH, Stresemannstr. 30, 37079 Göttingen

The cross section of three different arsenic sulphide fibers with different core diameters and different core/clad ratios were characterized. Ellipsometric contrast micrographs were recorded; wavelength spectra between 360 and 1000 nm at different regions of interest (ROI) and maps with a lateral resolution down to 1 micrometer of Delta and Psi were measured. The optical dispersion of the samples was described by a layer stack including an arsenic sulphide substrate, a roughness layer and air as ambient. The optical dispersion of arsenic sulphide was expressed by a Tauc-Lorentz function and the roughness layer by an effective medium approach. For the transformation of Delta and Psi maps to maps of thickness of roughness layers and maps of refractive index, the Tauc-Lorentz function was substituted by n and k as fitting parameters. Maps of refractive index and of thickness of roughness layer were obtained. Position dependent optical properties of cross sections of arsenic sulphide fibres, with core diameters down to few micrometers, can be characterized by spectroscopic imaging ellipsometry. Refractive index maps were obtained for selected wavelengths with a lateral resolution better than one micrometer.

HL 25: Transport

Time: Monday 15:45–18:15 Location: POT 151

HL 25.1 Mon 15:45 POT 151

Transport properties of BiTe-SbTe superlattices — •Bogdan Yavorsky[1], Nicki Hinsche[1], Peter Zahn[1], Martin Gradhand[2], Michael Czerner[3], and Ingrid Mertig[1,2] — [1]Institut für Physik, Martin-Luther Universität Halle-Wittenberg, D-06120 Halle, Germany — [2]Max-Plank-Institut für Mikrostrukturphysik, D-06099 Halle, Germany — [3]I. Physikalisches Institut, AG Theorie, Justus-Liebig University Giessen, D-35392 Giessen, Germany

During the last decade BiTe-SbTe multilayers attracted much attention due to their enhanced thermoelectric figure of merit compared to the bulk materials. To shed light on the origin of this enhancement, we studied the electronic structure of $(Bi_2Te_3)_x(Sb_2Te_3)_{N-x}$ superlattices with a fully relativistic screened Korringa-Kohn-Rostoker Green's function method. The electrical conductivity was calculated within the relaxation time approximation of the Boltzmann theory. The effect of composition (x) on the transport near the Fermi energy and the consequences for the thermoelectric properties were studied in detail.

HL 25.2 Mon 16:00 POT 151

Thermoelectric properties of strained silicon — •Nicki F. Hinsche[1], Ingrid Mertig[1,2] und Peter Zahn[1] — [1]Martin-Luther-Universität, Institut für Physik, Von-Seckendorff-Platz 1, 06120 Halle/S. — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

Starting from bulk silicon, we study the change in thermoelectric properties due to symmetry breaking in rolled-up and layered Si [1] which might lead to nanostructured thermoelectrics. Valley splitting in strained Si caused by tetragonal distortion was studied recently with respect to the enhancement of electron mobility [2]. Our results show that the tetragonal distortion has a strong influence on the electronic transport properties. The electronic structure is calculated self consistently

within the framework of density functional theory. The transport properties are studied in the diffusive limit applying the Boltzmann theory in relaxation time approximation [3]. In detail, the anisotropy of the electrical conductivity, the thermopower and the resulting powerfactor in the in-plane and off-plane directions are studied in dependence on strain, doping level and temperature [4]. It is shown, that the powerfactor at a given temperature can be enhanced slightly by strain for p-doping, while no enhancement is obtained for n-doping.

[1] F. Cavallo, W. Sigle, and O. Schmidt. *Journal of Appl. Phys.* **103**, 116103 (2008). [2] T. Dziekan, P. Zahn, V. Meded, and S. Mirbt. *Phys. Rev. B* **75**, 195213 (2007). [3] I. Mertig. *Reports on Progress in Physics* **62**, 237 (1999). [4] N.F. Hinsche, I. Mertig and P. Zahn. *submitted*, 2010.

HL 25.3 Mon 16:15 POT 151

Modification of the functional and mechanical properties of Lead Telluride for thermoelectric energy conversion — •Andreas Schmitz, Peter Schorn, and Eckhard Müller — Deutsches Zentrum für Luft- und Raumfahrt e.V., Institut für Werkstoff-Forschung, Linder Höhe, 51147 Köln

Thermoelectric Generators are solid state devices using the Seebeck effect to transform heat differences straight into electricity. Lead telluride is a classical candidate material for thermoelectric conversion in a middle temperature range (250 to 550 °C) and has been used in thermoelectric generator applications for many years. Still the disad*vantageous mechanical properties implicate difficulties for module production and application such as automotive waste heat recovery.

The manufacturing of thermoelectric elements from powders by hot pressing and consecutive pressureless annealing of PbTe leads to a shift of the thermoelectric properties and improved mechanical properties of the material compared to cast PbTe.

Doping is used to optimize the thermoelectric properties of PbTe but may also have an effect on the material*s mechanical properties. Especially doping with acceptor elements has resulted in an increased brittleness of the compound.

In this study the simultaneous effect of doping on the thermoelectric and mechanical properties of sintered PbTe has been studied with a focus on improving mechanical stability and ductility.

HL 25.4 Mon 16:30 POT 151

Tunable transverse rectification in density-modulated 2D-systems — •Andy Quindeau[1], Arkadius Ganczarczyk[1], Martin Geller[1], Axel Lorke[1], Dirk Reuter[2], and Andreas D. Wieck[2] — [1]Experimental Physics and CeNIDE, Universität Duisburg-Essen — [2]Chair of Applied Solid State Physics, Ruhr-Universität Bochum

We investigate tunable transverse rectification in a density-modulated two-dimensinal electron gas (2DEG) at temperatures between 1.8 K and 200 K. The 2DEG is patterned into a Hall bar geometry. Using gate electrodes we induce two stripes of different charge carrier densities running parallel to the channel. The resulting density gradient perpendicular to the channel induces a transverse voltage, which - due to the symmetry of the device - does not change polarity when the current direction is reversed. The experimental results can be reproduced to some extent using a simple ballistic billiard model [1, 2].

To acquire a deeper insight into the physics behind this transverse rectification effect, further experiments and theoretical approaches are presented. For example, we study the voltage probes potentials of an ungated 2DEG-hallbar, where a parabolic source-drain voltage and temperature dependence can be observed. Furthermore, first theoretical results, based on the Boltzmann equation in the relaxation time approximation [3], give further insights into the observed experimental data.

[1] A. Ganczarczyk *et al.*, preprint:arXiv:0804.0689v3 (2009).
[2] A. Ganczarczyk *et al.*, AIP Conf. Proc. 1199, 143 (2009).
[3] S. Rojek, D. Urban, F. Hucht, and J. König, unpublished.

HL 25.5 Mon 16:45 POT 151

Giant negative photoresistance of ZnO single crystals — •Jose Barzola-Quiquia[1], Pablo Esquinazi[1], Silvia Heluani[2], Manuel Villafuerte[3], and Andreas Pöppl[4] — [1]Division of Superconductivity and Magnetism, University of Leipzig, D-04103 Leipzig, Germany — [2]Laboratorio de Física del Sólido, Dpto. de Física, FCEyT, Universidad Nacional de Tucumán, 4000 S. M. de Tucumán, Argentina — [3]Dpto. de Física, Laboratorio de Física del Sólido, FCEyT, Universidad Nacional de Tucumán, Argentina and CONICET, 4000 S. M. de Tucumán, Argentina — [4]Division of Magnetic Resonance of Complex Quantum Solids, University of Leipzig, D-04103 Leipzig, Germany

ZnO is a wide band gap semiconductor exhibiting the largest charge-carrier mobility among oxides. ZnO is a material with potential applications for short-wavelength optoelectronic devices, as a blue light emitting diodes and in spintronics. In this contribution we have measured the temperature dependence (30 K < T < 300 K) of the electrical resistance of ZnO single crystals prepared by hydrothermal method in darkness and under the influence of light in the ultraviolet range. The resistance decreases several orders of magnitude at temperatures T < 200 K after illumination. Electron paramagnetic resonance studies under illumination reveal that the excitation of Li acceptor impurities is the origin for the giant negative photoresistance effect. Permanent photoresistance effect is also observed, which remains many hours after leaving the crystal in darkness.

15 min. break

HL 25.6 Mon 17:15 POT 151

Thermal Probing of Heat Generation in Biased Silicon Nanowires — •Fabian Menges[1,2], Heike Riel[1], Andreas Stemmer[2], and Bernd Gotsmann[1] — [1]IBM Research - Zurich, 8803 Rueschlikon, Switzerland — [2]ETH Zurich, 8092 Zurich, Switzerland

The limited spatial resolution of conventional thermal imaging techniques hinders the local thermophysical characterization of nanoscale electronic devices. In contrast, the demand to study heat conduction and generation in nanosystems is steadily increasing. While novel materials and device geometries tend to impede heat conduction, localized regions of increased heat generation, so-called "hot spots", limit device performance and reliability. New methods are needed to understand the manifold coupling between thermal, electrical and structural device properties. To address this issue, a vacuum-operated scanning thermal microscope was developed to allow for thermal characterization of active nanoscale electronic devices. The key element of the microscope is a microfabricated heatable silicon probe, which allows probing temperature distributions with lateral resolution below 20 nm. Self-heating of a silicon nanowire was studied in-situ as a function of applied voltages. The observed temperature distributions are governed by the ratio of heat conduction along the nanowire and heat dissipation across the nanowire-substrate interface. Furthermore, nanoscopic thermal hot spots were observed at internal junctions of a silicon nanowire diode as a function of current direction. The results are discussed in relation to nanoscale thermal management in electronic devices.

HL 25.7 Mon 17:30 POT 151

Controlling the transport properties of InAs nanowires by Si doping — •Karl Weis[1,3], Stephan Wirths[1,3], Andreas Winden[1,3], Kamil Sladek[1,3], Thomas Weirich[2,3], Thomas Schäpers[1,3], Hilde Hardtdegen[1,3], Hans Lüth[1,3], Nataliya Demarina[1,3], and Detlev Grützmacher[1,3] — [1]Institut für Bio- und Nanosysteme (IBN), Forschungszentrum Jülich, Germany — [2]Gemeinschaftslabor für Elektronenmikroskopie, RWTH Aachen, Germany — [3]JARA, Fundamentals of Future Information Technology

InAs nanowires are attractive building blocks for nanoelectronic devices, e. g. field-effect transistors. For concrete applications, it is important to understand the interplay between their crystal structure and transport properties. By doping, the latter can be tuned.

We fabricated InAs nanowires by selective-area metal-organic vapour phase epitaxy. Using Si_2H_6 as a dopant, samples with five different doping levels, each set comprising 30 to 100 nanowires (typical length and diameter: 3 μm and 100 nm, respectively), were prepared.

From *I-V* measurements and field effect transistor measurements using a SiO_2 back gate, we get a clear positive correlation between doping level and conductivity/carrier concentration/mobility. The conductivity can be tuned between (12.9 ± 0.8) S/cm and (560 ± 120) S/cm. Furthermore, transmission electron micrographs show an influence of doping on the crystal structure of the wires. Magneto-transport measurements are performed to quantify the effect of stacking faults on the conductivity. At low temperatures around 4 K, the *I-V* characteristics show indications of single electron tunneling.

HL 25.8 Mon 17:45 POT 151

Field dependent transport properties and conductance fluctuations of InSb nanowires — •huijun yao[1], h. yusuf günel[1], christian blömers[1], weis karl[1], yennai wang[2], jia grace lu[2], detlev grützmacher[1], and thomas schäpers[1] — [1]Institute of Bio- and Nanosystems (IBN1) and JARA-FIT Jülich-Aachen Research Alliance, Research Center Jülich GmbH, D-52425 Jülich, Germany — [2]Department of Physics & Astronomy, University of Southern Califor-

nia, Los Angeles, California, 9008-0484, USA

Due to the precise structural control, semiconductor nanowires provide a new class of nanoscale building blocks for a broad range of disciplines like quantum optics, electronics, nanosensing, and biotechnology. In this respect, InSb- based nanowires are very promising candidates for applications in spintronics and spin-based quantum information technology, owing to the fact that bulk InSb has a high electron mobility, a strong spin-orbit coupling and a narrow band gap (0.16 eV) at room temperature. The measured InSb nanowires were synthesized by using a physical vapor transport method with gold nanoparticles as a catalyst. The basic transport parameters, e.g., conductivity, electron concentration, and mobility were determined by performing current-voltage and back-gate field-effect measurements in the temperature range from 4.2 to 300 K. Universal conductance fluctuations were studied systematically by performing magnetotransport measurements at temperature down to 0.3 K. From the root-mean square of the fluctuation amplitude and from the correlation field Bc information on the phase-coherence length was obtained.

HL 25.9 Mon 18:00 POT 151

Anomalous galvanomagnetism, cyclotron resonance and microwave spectroscopy of topological insulators — •Ewelina M. Hankiewicz and Grigory Tkachov — Würzburg University

The surface quantum Hall state, magneto-electric phenomena and their connection to axion electrodynamics have been studied intensively for topological insulators. One of the obstacles for observing such effects comes from nonzero conductivity of the bulk. To overcome this obstacle we propose to use an external magnetic field to suppress the conductivity of the bulk carriers. The magnetic field dependence of galvanomagnetic and electromagnetic responses of the whole system shows anomalies due to broken time-reversal symmetry of the surface quantum Hall state, which can be used for its detection. In particular, we find linear bulk dc magnetoresistivity and a quadratic field dependence of the Hall angle, shifted rf cyclotron resonance, nonanalytic microwave transmission coefficient and saturation of the Faraday rotation angle with increasing magnetic field or wave frequency [1].

[1] G. Tkachov and E. M. Hankiewicz, arXiv:1011.2756 (2010).

HL 26: Interfaces and Surfaces

Time: Monday 16:00–17:45 Location: POT 06

HL 26.1 Mon 16:00 POT 06

Focused Ion Beam Structuring of Ag Nanowires with Single Grain Boundaries for Electromigration Experiments — •Simon Sindermann, Christian Witt, Michael Horn-von Hoegen, Guenter Dumpich, and Frank-J. Meyer zu Heringdorf — Address: Faculty of Physics and Center for Nanointegration Duisburg-Essen (CeNIDE) University Duisburg-Essen, D-47057 Duisburg, Germany

Electromigration is decided by the balance of two opposing forces. On one hand the wind force acts via the momentum transfer from the conduction electrons to the atoms, on the other hand the so-called direct force arises from the electric field. Structural features have been shown to change the balance of the forces. Whereas the wind force dominates the electromigration in poly-crystalline Ag and Au nanowires [1], in single-crystalline Ag nanowires, the direct force drives the electromigration opposite to the direction of electron movement [2]. Here we present a new approach to study the electromigration in Ag nanowires with a single grain boundary. Focused ion beam (FIB) is used to structure wires from epitaxially grown Ag islands with two different crystallographic orientations, Ag(001) and Ag(111). While FIB structuring of Ag wires has promising prospects, there are some downsides as well. The issues, e.g. doping of the Si substrate and amorphisation, and possible solutions will be discussed. First electromigration experiments will be presented.

[1] B. Stahlmecke and G. Dumpich, JPCM **19** (2007) 046210
[2] B. Stahlmecke et al. APL **88** (2006) 053122

HL 26.2 Mon 16:15 POT 06

Time Scaling of Silver Nano-Crystal Growth at the Interface of Silver Thick Film Electrodes on n-Type Silicon — •Stefan Kontermann[1,2], Alexander Ruf[1], and Ralf Preu[1] — [1]Fraunhofer Institute for Solar Energy Systems, Heidenhofstr. 2, 79110 Freiburg, Germany — [2]Fraunhofer Heinrich Hertz Institut, Energiecampus, Am Stollen 19, 38640 Goslar, Germany

The interface of silver thick film contacts on n-type silicon features nanoscale silver crystals. They carry the current across such interfaces and hence govern the contact resistance which is a main performance limiting parameter for semiconductor devices. The silver crystals form in pits on the silicon surface at the interface during a high temperature step. In earlier studies we simulated the growth of these pits by considering the probability of removing a silicon surface atom in dependence of its bond energy. In the present work we present a method for introducing a quantitative time scaling for these simulations. This method leads to good quantitative agreement between simulated and experimental data. It enables the prediction of pit formation and hence silver crystal growth for arbitrary process parameters like temperature and duration during silver thick film contact formation on n-type silicon.

HL 26.3 Mon 16:30 POT 06

Nanowire-metal hybrid structures: the influence of the deposition technique on the optical properties — •Apurba Dev, Jan-Peter Richters, and Tobias Voss — Institute of Solid State Physics. University of Bremen. 28359 Bremen

ZnO nanowires (NWs) have drawn widespread attention for their potential use in many optical devices. Recently, surface plasmon resonances of metal nanoparticles (NPs) have been used to increase the quantum efficiency of near-band-edge (NBE) spontaneous emission of these nanowires. However, we observed that the metal NPs deposition process itself significantly influences the optical properties. We investigated the time-integrated and time-resolved photoluminescence (PL) properties of ZnO NWs coated with Au, Ag and Pt NPs which were deposited by DC sputtering in Ar plasma. The influence of the sputtering process was determined by performing the same sputtering treatment while shielding the sample to avoid metal deposition. A strong enhancement of the NBE emission and a quenching of the deep-level emission were observed in all cases. Time-resolved spectroscopy showed a reduction of the radiative lifetime in all samples irrespective of size and kind of metal NPs. PL studies at 4 K revealed a strong hydrogen-donor-bound-exciton line indicating unintentional incorporation of hydrogen. The results can be explained by considering the passivation of deep centers by hydrogen and the introduction of a large amount of hydrogen donors.

HL 26.4 Mon 16:45 POT 06

Lithium Diffusion at Silicon Surfaces — •David Krix, Hatice Karacuban, and Hermann Nienhaus — Faculty of Physics, Center for Nanointegration Duisburg-Essen, University of Duisburg-Essen, 47048 Duisburg, Germany

Lithium-ion batteries are in common use in a large number of modern electrical appliances. In the quest for ever higher storage capacities new electrode materials are needed which will eventually replace the commonly used graphite anodes. Silicon is a promising candidate due to its enormous storage capacity for lithium but suffers from a large density difference between the lithium containing and lithium free phase. Nano-structured materials (particles, wires etc.) promise to remedy this problem. Transport processes at the surface of silicon anode surfaces are therefore of keen interest.

We have studied the diffusion of lithium into silicon under UHV conditions and at low temperatures (150-180 K) using Auger and X-ray photoelectron spectroscopy. Thin layers of lithium were deposited on pristine H-passivated Si(001) and oxygen modified surfaces at a temperature (120 K) that effectively suppresses the diffusion, although a thin layer of silicide forms at the interface right away. At sufficiently high temperatures diffusion of lithium into the bulk sets in, which can be monitored through the attenuation of the silicon signal underneath the metallic lithium film. The formation of surface silicide is a thermally activated process with an activation energy of 0.49 eV.

HL 26.5 Mon 17:00 POT 06

Adsorption of Methanol on Lithium niobate (0001) — •Arthur Riefer, Simone Sanna, and Wolf Gero Schmidt — Theoretische Physik, Universität Paderborn, 33095 Paderborn, Ger-

many

Lithium niobate (LN) is a ferroelectric material with a huge range of applications. While the bulk properties of LN are exploited in optical and acoustic devices, the physics on the different oriented surfaces allows the realization of molecular detectors and other devices at nanoscale level. Temperature programmed desorption measurements of polar molecules, such as Water, Methanol [1], and 2-Propanol [2], on the (0001) LN surfaces show stronger adsorption of these molecules on the positive surface. The mechanisms behind the bonding are still not clear. Recently, structural models for the negative and positive (0001) surface of LN have been proposed on the basis of Density Functional Theory (DFT) calculations. Here, we investigate the behavior of Methanol on the LN surfaces by means of DFT in the Generalized Gradient approximation (GGA). As a first step, we calculate the potential energy surface (PES) for both orientations. We find the preferred position of an adsorption of Methanol near the Oxygen atoms on the positive or near the Lithium atoms on the negative surface, respectively and a bonding-energy difference of about 0.5 eV between the two sites. Also, we investigate the possibility of a dissociation of the molecule on the LN surfaces.

[1] J. Garra *et al.*, Surface Science **603** (2009) 1106 - 1114
[2] Y. Yun *et al.*, J. Phys. Chem. C **111** (2007) 13951-13956

HL 26.6 Mon 17:15 POT 06

Photoemission spectroscopy studies of $SrTiO_3$ and its interface to gold — Susi Wintz[1], Mandy Grobosch[1], •Martin Knupfer[1], Juliane Seibt[2], Florian Hanzig[2], Hartmut Stöcker[2], and Dirk C. Meyer[2] — [1]IFW Dresden, P.O. Box 270116, 01171 Dresden, Germany — [2]Institut für Experimentelle Physik, TU Bergakademie Freiberg, Leipziger Str. 23, 09596 Freiberg, Germany

Motivated by applications of strontium titanate ($SrTiO_3$, STO) in nonvolatile memory devices we studied the surface of STO by means of x-ray and ultra violet photoemission spectroscopy. The focus of the analysis was purity, doping and the annealing time. It could be demonstrated that a surface contamination layer consisting of carbonates and hydroxides exists on surfaces prepared under ambient conditions. In addition, the interface between STO and gold was investigated. We show that there is a weak interaction of these materials, however a Schottky-type $Au/SrTiO_3$ junction is formed. Finally the work function of all STO samples was determined. The work function depends on the modification of the STO surface. This fact should considered for the formation of such a Schottky-type junction.

HL 26.7 Mon 17:30 POT 06

Contributions to the *in situ* RAS signal of MOVPE prepared GaP/Si(100) — •Oliver Supplie, Henning Döscher, Sebastian Brückner, Anja Dobrich, Peter Kleinschmidt, and Thomas Hannappel — Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

High efficient opto-electronic devices based on III-V/Si(100) heterostructures require low defect densities within the active material. Reflection Anisotropy Spectroscopy (RAS) signals from optically isotropic crystals can be related to surfaces, interfaces or defects within the bulk and allow for *in situ* characterization during metal organic vapor phase epitaxy (MOVPE). The (1×2)-like surface reconstruction of P-rich prepared GaP(100) yields a characteristic RA spectrum [1]. Deviations in the RA spectra of thin GaP/Si(100) films of different thicknesses can originate from (1) internal reflections, i.e. interference, (2) the pure surface anisotropy, (3) anti phase disorder induced at the heterointerface, (4) GaP bulk anisotropies, and (5) a possibly anisotropic GaP/Si(100) interface itself. Those contributions can be separated by optical models [2]. The peak intensities of the pure surface signal allow for improved *in situ* quantification of the anti phase domain content at the GaP/Si(100) surface and is in agreement with the GaP(100) surface anisotropy. Neglecting GaP-bulk contributions, an interface anisotropy consistent for different GaP film thicknesses can be extracted.

[1] H. Döscher et al. JAP **107** (2010) 123523. [2] T. Yasuda. TSF **313** (1998) 544, O. Hunderi et al. TSF **472** (2005) 261.

HL 27: Invited Talk: Martin Wagner

Time: Monday 17:00–17:30 Location: POT 51

Invited Talk HL 27.1 Mon 17:00 POT 51

Intraexciton terahertz nonlinear optics in quantum wells — •Martin Wagner[1], Harald Schneider[1], Dominik Stehr[1], Stephan Winnerl[1], Aaron M. Andrews[2], Stephan Schartner[2], Gottfried Strasser[2], and Manfred Helm[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, P.O. 510119, 01314 Dresden — [2]Micro- and Nanostructure Center, Floragasse 7, 1040 Vienna, Austria

Terahertz (THz) light is not only used to probe low-energy material excitations in a spectral region that has become accessible only during the last decades, but at high field strengths it can also induce nonlinear optical effects and enrich our understanding of light-matter interaction. In our contribution we investigate experimentally nonlinear optical effects related to excitonic transitions in undoped GaAs/AlGaAs semiconductor quantum wells. Excitons as bound electron-hole pairs show an energy structure analogous to the hydrogen atom, however, the binding energy is scaled down by a factor of 1000 and lies in the THz spectral range. We make use of the intra-excitonic 1s to 2p transition to explore two basic concepts of nonlinear optics, i.e. the perturbative effect of sideband generation and the non-perturbative Autler-Townes effect. In sideband generation a near-infrared (NIR) laser beam is mixed with the THz beam to generate sidebands at the sum- and difference-frequencies around the NIR frequency. The Autler-Townes or AC Stark effect refers to a splitting of an energy level that is resonantly coupled via intense radiation to an adjacent level. Both effects with their large distinct signatures in the sample's optical response could find applications in future optical modulators.

HL 28: THz Physics

Time: Monday 17:30–18:45 Location: POT 51

HL 28.1 Mon 17:30 POT 51

Density Dependence of the Excitonic 1s-2p Transition Energy in THz Spectroscopy — •Benjamin Breddermann, Mackillo Kira, and Stephan W. Koch — Department of Physics and Material Sciences Center, Philipps-University Marburg, Renthof 5, D-35032 Marburg

Spectroscopy with optical and terahertz (THz) frequencies provides a versatile tool to probe and control semiconductors on a microscopic level. The excitonic resonances depend very strongly on the carrier density n_{eh} excited to the semiconductor yielding several many-body phenomena. In other words, one finds excitation-induced dephasing (EID) that bleaches the excitonic resonances from both optical and THz spectra if n_{eh} is increased enough. All these phenomena are treated fully microscopically with the goal to investigate the influence of these many-body effects in the optical and THz spectra. We report results on the density dependent broadening and red-shift of the 1s-2p transition in the THz spectra and present comparisons with recent experiments.

HL 28.2 Mon 17:45 POT 51

Time-resolved ultrafast photocurrents and terahertz generation in electrically contacted, freely suspended graphene — •Leonhard Prechtel[1], Li Song[2], Nadine Erhard[1], Dieter Schuh[3], Werner Wegscheider[4], and Alex W. Holleitner[1] — [1]Walter Schottky Institut and Physik-Department, TU München — [2]Fakultät für Physik and Center for NanoScience (CeNS), LMU, München — [3]Institut für Experimentelle und Angewandte Physik, Universität Regensburg — [4]Laboratorium für Festkörperphysik, ETH Zürich

We investigate the ultrafast photocurrent dynamics of freely suspended graphene contacted by metal electrodes in the time-domain. At the graphene-metal interface we demonstrate, that built-in electric fields give rise to an ultrafast photocurrent with a FWHM of only a few ps. This suggests the use of graphene for ultrafast photodetectors and photoswitches. We further detect a photo-thermoelectric current with a decay time of about 0.2 ns. We also show that in optically pumped freely suspended graphene plasmon oscillations and terahertz-radiation are efficiently generated.

HL 28.3 Mon 18:00 POT 51

Nanotube Transisors as Quantum Cavity for Terahertz Plasmons — •Diego Kienle — Theoretische Physik I, Universität Bayreuth, 95440 Bayreuth

Since their discovery in 1990, carbon nanotubes (NTs) are believed to be one potential candidate to replace silicon- based electronics due to their exceptional electronic properties. Much effort has been invested in understanding electronic transport at DC, whereas their high-frequency (AC) properties are less explored. In this talk, we employ a newly developed theory for self-consistent AC quantum transport using Non-Equilibrium Green functions and study the AC response of NT transistors in terms of their dynamic conductance with the AC signal applied at the gate terminal. In the ON state, the conductance exhibits pronounced divergent peaks at terahertz frequencies, which are attributed to plasmon excitations. In the OFF-state such collective excitations are suppressed, since the dynamic coherence between the single-particle states is destroyed due to the reflection of electrons at the gate controlled potential barriers. In this case, the AC conductance is oscillatory - a signature of the single-particle excitation spectrum. Importantly, the plasmonic excitations are only captured if the self-consistent charge-potential feedback is an integral part of the AC theory. Higher-order plasmon modes can be excited by varying the length of the NT and thus allows to tune the plasmonic excitation spectrum. [1] D. Kienle and F. Leonard, Phys. Rev. Lett. **103**, 026601 (2009). [2] D. Kienle, M. Vaidyanathan, and F. Leonard, Phys. Rev. B **81** 115455 (2010).

HL 28.4 Mon 18:15 POT 51

Microscopic model of two-dimensional THz spectroscopy: Quantum well intersubband dynamics — •Thi Uyen-Khanh Dang[1], Sebastian Eiser[2], Andreas Knorr[1], Marten Richter[3], Wilhelm Kühn[4], Michael Wörner[4], and Carsten Weber[1] — [1]Institut für Theoretische Physik, Technische Universität Berlin, Germany — [2]European Space Research Institute, Frascati, Italy — [3]Department of Chemistry, University of California Irvine, USA — [4]Max Born Institut, Berlin, Germany

Time resolved two-dimensional spectroscopy combined with field-resolved detection allow important insights into the nonlinear optical response of a sample [1]: A variation of the time delay between the collinear pump and probe pulses enables the simultaneous detection of all orders of n-wave mixing, which can be separated in the frequency domain. Here, a theoretical model is presented to describe the corresponding experimental setup, performed on a GaAs/AlGaAs multiple quantum well sample. Within a density-matrix approach, the equations of motions for the electron density and the intersubband coherence are derived. Focusing on the electron-phonon interaction [2], its influence on the two-dimensional intersubband absorption spectrum is investigated. Experimentally observed signatures are reproduced in the theoretical simulations.

[1] W. Kühn et al., J. Chem. Phys. 130, (2009)
[2] S. Butscher et al., Phys. Rev. B. 72, (2005)

HL 28.5 Mon 18:30 POT 51

Generation of tuneable narrow-band terahertz pulses using large-area photoconductive antennas — Johannes Krause, •Martin Wagner, Manfred Helm, and Dominik Stehr — Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf (HZDR), P.O. Box 510119, 01314 Dresden, Germany

Photoconductive antennas, driven by ultrafast optical pulses, are frequently used as broadband terahertz sources. Due to water vapour absorption in ambient air, these sources are less suitable for free space imaging or addressing small spectral regions. Amongst other techniques, narrow-band THz generation via difference frequency generation in ZnTe crystals [1] and photoconductive antennas [2] were demonstrated, the latter reaching frequencies of only 900 GHz. In this work we generate tuneable narrow-band terahertz pulses from a large-area photoconductive antenna by means of difference frequency generation with two up to 3.3 ps long time-delayed chirped optical pulses. The source is a 250 kHz regenerative Ti:sapphire amplifier. It's output is split into three beams, where one is compressed for field resolved detection. The other two pulses are sent to a Michelson interferometer and get - with an adjustable time delay - recombined and are focussed on the antenna. By using this technique we generated THz pulses tuneable from 0.35 to 2.5 THz with adjustable spectral widths (FWHM) of 200 to 500 GHz.

[1] J.R. Danielson et al., J. Appl. Phys. 104, 033111 (2008).
[2] A.S. Weling and D.H. Auston, J. Opt. Soc. Am. B 13, 2783 (1996).

HL 29: Organic Photovoltaics II: mainly Phtalocyanine

Time: Monday 17:45–18:45 Location: FOE Anorg

HL 29.1 Mon 17:45 FOE Anorg

Band gap states of copper phthalocyanine thin films induced by nitrogen exposure — •Tomoki Sueyoshi[1,2], Haruya Kakuta[1], Masaki Ono[1], Kazuyuki Sakamoto[1], Satoshi Kera[1], and Nobuo Ueno[1] — [1]Graduate School of Advanced Integration Science, Chiba University, Chiba, Japan — [2]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany and JARA-Fundamentals of Future Information Technology

Extensive experimental and theoretical investigations have demonstrated the strong correlation between electronic and structural properties of organic layers. Although understanding of this correlation is very crucial, the question whether the intrinsic or externally induced disorder in the molecular packing structure influences their electronic properties remains obscure.

Here we investigated impact of 1-atm N2 gas exposure on the electronic states of copper phthalocyanine thin films using ultrahigh-sensitivity ultraviolet photoelectron spectroscopy. The highest occupied molecular orbital band of the film showed a drastic reversible change in the bandwidth and band shape as well as in the energy position upon repeated cycles of N2 exposure and subsequent annealing. Furthermore, two types of gap-state densities with Gaussian and exponential distributions appeared after the exposure and disappeared due to the annealing. These changes are ascribed to a weak disorder in the molecular packing structure induced by N2 diffusion into the film.

HL 29.2 Mon 18:00 FOE Anorg

Influence of temperature and illumination on the photovoltage of organic solar cells — •Johannes Widmer, Wolfgang Tress, Karl Leo, and Moritz Riede — Institut für Angewandte Photophysik, TU Dresden, George-Bähr-Straße 1, 01069 Dresden

Temperature plays an essential role in many processes in organic devices, including the current and voltage generation in organic solar cells. In this contribution, we focus on the open-circuit voltage of organic solar cells when varying illumination intensity and temperature in the range of 200K to 400K. Zinc phthalocyanine (ZnPc) and C60 are used as reference system and other materials are investigated in comparison to demonstrate the connection between the effective energy gap and the open-circuit voltage of a photovoltaic device. The use of doped transport layers in a p-i-n diode geometry allows to minimize the energetic losses between the active layers and the contacts and gives access to the quasi Fermi levels in the heterojunction. We can verify the dependence between the effective gap of a heterojunction and the open-circuit voltage. A substantial difference, however, is observed comparing the interplay of temperature and illumination intensity of bulk and flat heterojunction devices. Classic photo-diode like behaviour is observed for the open-circuit voltage of bulk heterojunction devices, as described by generation-recombination dynamics. In the case of a flat heterojunction, however, the influence of temperature and illumination become independent, which is not covered by the established theory. These findings can contribute to the understanding

of the photo-voltage of organic devices.

HL 29.3 Mon 18:15 FOE Anorg

Open circuit voltage as function of mixing ratio in ZnPc:C60 bulk heterojunction organic solar cells — •Steffen Pfuetzner, Wolfgang Tress, Selina Olthof, Max Tietze, Jan Meiss, Karl Leo, and Moritz Riede — Institut für Angewandte Photophysik, Technische Universität Dresden, D-01069 Dresden, Germany

We characterize organic solar cells composed of mixed layers of ZnPc:C_{60} as photoactive layer embedded between a p-doped hole transport (HTL) and an undoped electron transport layer. By varying the mixing ratio of the photoactive bulk heterojunction from 6:1 (ZnPc:C_{60}) to 1:6 by volume, we observe significant changes of V_{OC} from 0.54 to 0.63 V. To exclude that this increase with higher C_{60} content is caused by the increased contact area of C_{60} to the HTL, behaving as an additional exciton separating interface, *J(V)* measurements under spectral narrow red and blue illumination are performed. Independent of where absorption takes place (for red in ZnPc, for blue in C_{60}), V_{OC} is not affected significantly. Hence, we attribute the changes in V_{OC} not to an additional separating interface, but to an intrinsic blend layer effect. Further investigations using ultraviolet photoelectron spectroscopy measurements, absorption measurements, and HTL variations with different highest occupied molecular orbitals indicate as reason HOMO and LUMO shifts of C_{60} and ZnPc as a function of the mixing ratio.

HL 29.4 Mon 18:30 FOE Anorg

In-situ characterization of molecular semiconductor donor-acceptor-blends — Lena Kristin Cornelius, •Max Beu, and Derck Schlettwein — Institute of Applied Physics, Justus-Liebig-University Giessen, Germany. email:schlettwein@uni-giessen.de

Blends of $F_{16}PcCu$ and $PcCu$ were prepared on glass by physical vapour deposition. The acquired thin films had a thickness of around 20nm. The co-evaporation of $PcCu$ and $F_{16}PcCu$ was varied to obtain different molecular mixtures. High admixture of $PcCu$ to $F_{16}PcCu$ as typically used in bulk-hetero-junctions were compared to very low admixtures typical for dopant interactions. The current-voltage characteristics were studied during evaporation (in-situ). High levels of $PcCu$ in $F_{16}PcCu$ (moderate per cent range) disturbed the charge flow in the films. Very little admixture of $PcCu$ in the low per mille range, however, led to an increased conductivity, indicating a successful dopant interaction. Optical transmission spectroscopy consequently showed the disturbance of the $F_{16}PcCu$ solid state structure. The dominant $\beta_{bilayer}$–structure of pure $F_{16}PcCu$ (highly conductive) was partly changed to the herringbone β–structure (less conductive). Consequences for photoconduction in the films will be discussed.

HL 30: Nano Wires: Growth and Characterization

Time: Tuesday 10:15–11:45 Location: FOE Anorg

HL 30.1 Tue 10:15 FOE Anorg

Autocatalytic growth of GaAs nanowires on Si (111) using different SiO_x templates — Daniel Rudolph[1], Simon Hertenberger[1], Xiaodong Wang[1,2], •Watcharapong Paosangthong[1], Max Bichler[1], Gerhard Abstreiter[1], Jonathan J. Finley[1], and Gregor Koblmüller[1] — [1]Walter Schottky Institut, TU München, Garching, Germany — [2]Pohl Institute of Solid State Physics, Tongji Univ., Shanghai, P.R. China

We investigated the autocatalytic growth of GaAs nanowires (NWs) by molecular beam epitaxy on three different kinds of substrate templates: Si (111) coated with (a) an ultrathin layer of amorphous SiO_x, (b) an ultrathin layer of thermal SiO_2, and (c) a layer of thermal SiO_2 with periodic hole patterns defined by electron beam lithography. For the latter, we have investigated the effect of growth temperature and V/III ratio on the vertical NW growth yield and growth selectivity. The grown NWs were characterized using scanning electron microscopy (SEM), high resolution x-ray diffraction (HRXRD), transmission electron microscopy (TEM) and photoluminescence (PL) spectroscopy: SEM images and in-situ reflection high energy electron diffraction studies identified the growth to be mediated by the vapor liquid solid mechanism. A good epitaxial relationship between NWs and the Si substrate is confirmed by HRXRD measurements. TEM analysis revealed the crystal structure to be predominantly zincblende but shows the occurrence of twin boundaries and stacking faults. These results are supported by spatially resolved single NW PL spectroscopy measurements which exhibit the optical signature of zincblende GaAs.

HL 30.2 Tue 10:30 FOE Anorg

MBE growth of axial AlGaAs/GaAs heterostructure nanowires — •Torsten Rieger, Mihail Ion Lepsa, Thomas Schäpers, Hans Lüth, and Detlev Grützmacher — Institute of Bio- and Nanosystems (IBN-1) and JARAFundamentals of Future Information Technology, Forschungszentrum Jülich GmbH, D-52425 Jülich

Nanowire (NW) heterostructures are promising candidates for future (opto-)electronic devices but only little is known about their growth, especially in the case of axial heterostructures containing different group III elements. Here we report about the molecular beam epitaxial (MBE) growth of axial AlGaAs/GaAs heterostructure NWs on GaAs (111)B substrates spin-coated with a thin layer of hydrogen silesquioxan (HSQ). No Au is used to catalyze the growth. We have investigated the influence of Al beam flux, growth time and substrate temperature on the NW growth. It is found that even small amounts of Al reduce the axial growth but strongly promote growth on the amorphous oxide and NW sidewalls leading to unintentionally grown core/shell NWs. Up to an Al amount corresponding to 20%, the axial growth rate is still higher than the layer growth rate. This demonstrates the possibility to grow axial AlGaAs/GaAs heterostructure nanowires using self-catalyzed growth, although the switching back from AlGaAs to GaAs is found to be challenging, mainly due to growth on the amorphous oxide.

HL 30.3 Tue 10:45 FOE Anorg

Doping dependence of the electrochemical properties of GaN:Si nanowires. — •Jens Wallys[1], Florian Furtmayr[1,2], Rudolph Matz[1], Marcus Rohnke[3], and Martin Eickhoff[1] — [1]I. Physikalisches Institut, Justus-Liebig-Universitaet Giessen — [2]Walter Schottky Institut, Technische Universitaet Muenchen — [3]Physikalisch-Chemisches Institut, Justus-Liebig-Universitaet Giessen

Recently, the interest in self assembled nanowires (NW) increased due to their low density of structural defects, the possibility of doping and embedding III-N heterostructures, which allow the realization of novel nanoscale optoelectronic devices, such as light emitters and chemical sensors. For these applications understanding and control of dopant incorporation is an important issue. While investigations based on electron microscopy or optical methods provide valuable information, the determination of the doping concentration in NWs is still problematic since many conventional methods (e.g. Hall measurements) are not applicable.

In this study we investigated various Si-doped GaN NWs grown by plasma assisted molecular beam epitaxy. In order to determine the Si concentration we performed electrical impedance spectroscopy measurements of NW-ensembles. This allows us to extract the surface capacitance and surface resistance via numerical fitting of electrical equivalent circuits to the experimental spectra. The obtained results were compared to time of flight - secondary ion mass spectroscopy measurements as an alternative approach. In addition, the effect of NW-ageing is addressed.

HL 30.4 Tue 11:00 FOE Anorg

Effects of doping profile on the optoelectronic properties of GaN nanowires — •Friederich Limbach[1,2], Tobias Gotschke[1,2], Toma Stoica[1], Carsten Pfüller[2], Oliver Brandt[2], Achim Trampert[2], Sebastian Geburt[3], Carsten Ronning[3], and Raffaella Calarco[1,2] — [1]Institute of Bio- and Nanosystems (IBN-1), Research Centre Jülich GmbH, 52425 Jülich, Germany, and JARA-FIT Fundamentals of Future Information Technology — [2]Paul-Drude-Institute for Solid State Electronics, Hausvogteiplatz 5-7, 10117 Berlin, Germany — [3]University Jena, Inst Solid State Phys, D-07743 Jena, Germany

GaN NWs with two different doping profiles were grown on Si(111) substrates in nitrogen rich conditions without any catalyst using an AlN buffer layer. In one case Si was supplied during the first 2 hours of

the growth followed by 30 min without supply of any doping species, subsequently growth was continuing for an additional 2 hours with supplying Mg (Type-A). In the other case the reverse structure was fabricated, starting with Mg doping and ending with Si doping (Type-B). For all samples of type-B, the DAP signal in PL, μ-PL and CL is less intense than the NBE peak and in some cases almost not detectable. In contrast Type-A samples show a very strong DAP signal. By combining PL, μ-PL and CL results, we concluded that during the first stages of the growth of GaN NWs, the incorporation of Mg is hampered, while in the later phase of the growth, the Mg is more effectively incorporated and acts as an acceptor in the GaN matrix.

HL 30.5 Tue 11:15 FOE Anorg

Kelvin probe force microscopy on doping transitions in single semiconductor nanowires — •Sasa Vinaji[1], Wolfgang Mertin[1], Christoph Gutsche[2], Andrey Lysov[2], Ingo Regolin[2], Werner Prost[2], Franz-Josef Tegude[2], and Gerd Bacher[1] — [1]Werkstoffe der Elektrotechnik & CeNIDE, Universität Duisburg-Essen, Bismarckstr. 81, 47057 Duisburg, Germany — [2]Halbleitertechnologie & CeNIDE, Universität Duisburg-Essen, Lotharstr. 55, 47048 Duisburg, Germany

In order to realize innovative electronic and optoelectronic devices with semiconductor nanowires, controlled doping has to be achieved. Therefore detailed knowledge about the doping level and the local position of the doping transition is essential. This can be accessed by non-contact Kelvin Probe Force Microscopy (KPFM) without damaging the sensitive nanowire [1].

Single GaAs nanowires grown by metal-organic vapour phase epitaxy have been doped with Zn and Sn for p- and n-type doping, respectively, to create a doping transition in axial direction [2]. The nanowires show macroscopic diode-like IV-characteristics. With KPFM single nanowires have been analyzed, and a pn-junction has been localized inside the nanowires with a depletion zone of about 180 nm. Additionally, different biases have been applied and the variation of the depletion width has been investigated.

[1] S. Vinaji, et al., Nanotechnology 20, 385702 (2009), [2] I.Regolin, et al., J. Cryst. Growth (2010), doi:10.1016/j.jcrysgro.2010.08.028

HL 30.6 Tue 11:30 FOE Anorg

Microstructures and electronic properties of one-dimensional ZnO nanostructures — •Peter Hess, Yong Lei, Martin Peterlechner, and Gerhard Wilde — Inst. f. Materialphysik, WWU Münster

One-dimensional (1-D) ZnO nanostructures were systematically investigated concerning their micro-structures and their photoluminescence properties. The main focus of this work is on the assembly of nanowires of different shapes and sizes to investigate their properties. The ZnO 1-D and 2-D structures were prepared using a Chemical Vapour Deposition (CVD) system with ZnO/C mixtures as sources, Au-coated silicon or sapphire as substrates, and an argon and oxygen gas flow as a distributor and oxidation source. Depending on the conditions during the CVD process, different kinds of ZnO nanostructures were obtained. The morphology of the ZnO nanostructures was checked by SEM while the photoluminescence properties were investigated using a spectrometer. Additionally, the crystalline structures, the growth direction, and the lattice spacing of ZnO nanostructures were characterized using TEM. First experiments were also conducted concerning the electrical properties of the Nanowires.

HL 31: III-V-Compounds: Nitrides

Time: Tuesday 10:15–13:30 Location: POT 51

HL 31.1 Tue 10:15 POT 51

Direct measurement of the band gap and Fermi level position at InN(1120) — •Philipp Ebert[1], Sarah Schaafhausen[1], Andrea Lenz[2], Aizhan Sabitova[1], Lena Ivanova[2], Mario Dähne[2], Yu-Liang Hong[3], Shangjr Gwo[3], and Holger Eisele[2] — [1]Institut für Festkörperfoschung, Forschungszentrum Jülich GmbH, 52425 Jülich — [2]Institut für Festkörperphysik, Technische Universität Berlin, 10623 Berlin — [3]Department of Physics, National Tsing-Hua University, Hsinchu 30013, Taiwan

A non-polar stoichiometric InN(1120) surface freshly cleaved inside UHV was investigated by scanning tunneling microscopy and spectroscopy. Due to the absence of intrinsic surface states in the band gap, scanning tunneling spectroscopy yields directly the fundamental bulk band gap EG=0.7 +/- 0.1 eV. The Fermi energy is pinned 0.3 eV below the conduction band minimum due to cleavage induced defect states. Thus, intrinsic electron accumulation can be excluded for this surface. Electron accumulation is rather an extrinsic effect due to surface contamination or material decomposition, but not an intrinsic material property of InN.

HL 31.2 Tue 10:30 POT 51

Growth and characterization of InN by RF MBE — •Andreas Kraus, Ernst Ronald Buss, Heiko Bremers, Uwe Rossow, and Andreas Hangleiter — Technische Universität Braunschweig, Institute of Applied Physics, Mendelssohnstraße 2, 38106 Braunschweig

InN layers were grown on GaN templates by radio frequency molecular beam epitaxy. After a low temperature nucleation layer InN was grown at different substrate temperatures and indium and nitrogen fluxes. With the intention to improve the quality of these thin films the In flux was pulsed by opening and closing the In shutter periodically. A set of samples was grown in this way by varying the In flux, the substrate temperature and the shutter frequency. The growth was monitored in-situ by reflection high energy electron diffraction and by optical reflectometry. The latter shows intensity oscillations following the shutter sequence allowing us to study the growth kinetics of InN on GaN templates.

Comparing both growth methods, the samples grown with a pulsed In flux exhibit improved structural quality in terms of XRD rocking widths and surface roughnesses measured by atomic force microscopy. Furthermore the samples exhibit no significant strain indicating that they are fully relaxed even at thicknesses of approximately 15 nm.

HL 31.3 Tue 10:45 POT 51

Optical gain in GaNAsP heterostructures pseudomorphically grown on silicon — Nektarios Koukourakis[1], Dominic Funke[1], Nils C. Gerhardt[1], Martin R. Hofmann[1], Sven Liebich[2], Christina Bückers[2], Steffen Zinnkann[2], Martin Zimprich[2], Kerstin Volz[2], •Stefan W. Koch[2], Wolfgang Stolz[2], and Bernardette Kunert[3] — [1]Photonics and Terahertztechnology, Ruhr-Universität Bochum, Bochum, Germany — [2]Material Science Center and Faculty of Physics, Philipps-University Marburg, Marburg, Germany — [3]NAsP III/V GmbH, Marburg, Germany

The realization of an electrically pumped semiconductor laser based on silicon remains a huge challenge due to the indirect nature of its band structure. However, a success in this effort would allow for combining the advantage of optical data processing with the well-established silicon processing technology, leading to optoelectronic integrated circuits (OEICs) with drastically improved performance. One promising approach is to grow the novel dilute nitride material Ga(NAsP) lattice matched on silicon. Ga(NAsP) has a direct band gap and has already led to optically and electrically pumped lasers on GaP, that have a lattice constant similar to that of silicon. Here, we analyse the modal gain of the Ga(NAsP) direct band gap material system grown on (001) Si-substrates. We compare the performance of several sample compositions and demonstrate high modal gain values at room temperature, comparable to common high quality laser materials.

HL 31.4 Tue 11:00 POT 51

Surface polarity determination of polar and semi-polar InN — •Daria Skuridina[1], Duc Dinh[1], Michael Kneissl[1], Norbert Esser[1,2], and Patrick Vogt[1] — [1]TU Berlin, Institute of Solid State Physics, Hardenbergstr. 36, 10623 Berlin, Germany. — [2]ISAS Berlin, Albert-Einstein-Str.9, 12489 Berlin, Germany

Over recent years InN has attracted much attention because of its possible applications in electronic devices. However, the growth of high quality InN films still remains a problem. Particularly, the understanding of the structure formation at InN surfaces and the dependency on the InN polarity are still insufficient. In our experiments we have performed X-ray photoelectron spectroscopy (XPS) measurements of the valence band structure of the polar and semi-polar (11-22) InN grown by MOVPE. From the analysis of the peak correlation in the

valence band spectra we could determine the polarity of c-plane InN films with thicknesses even below 100 nm. Our measurements confirm that the polarity of the InN films depends strongly on the nitridation of the sapphire substrate before InN growth. Semi-polar (11-22) InN exhibits columnar surface structure along the c-direction at the angle of 58° with respect to the surface normal. The valence band spectra revealed an In polarity of these surfaces which indicates a [0001] growth direction of the columns on semi-polar InN surface.

HL 31.5 Tue 11:15 POT 51

Time-resolved photoluminescence in GaNAsP heterostructures grown on silicon — •Nektarios Koukourakis[1], Dominic Funke[1], Nils C. Gerhardt[1], Martin R. Hofmann[1], Sven Liebich[2], Steffen Zinnkann[2], Martin Zimprich[2], Kerstin Volz[2], Wolfgang Stolz[2], and Bernardette Kunert[3] — [1]Photonics and Terahertztechnology, Ruhr-Universität Bochum, Bochum, Germany — [2]Material Science Center and Faculty of Physics, Philipps-University Marburg, Marburg, Germany — [3]NAsP III/V GmbH, Marburg, Germany

The new direct band-gap dilute nitride material Ga(NAsP) is a very promising candidate for the realisation of optoelectronic integrated circuits (OEICs) as it can be grown lattice matched on silicon. Electrically pumped lasing of Ga(NAsP) on GaP has already been demonstrated, showing the high quality of the material. Samples grown on silicon have already shown high gain values, comparable to common high-quality laser materials. In this talk we present time-resolved photoluminescence studies of the Ga(NAsP) direct band gap material system grown on (001) Si-substrates. We compare the carrier dynamics of several samples that differ in growth parameters and material compositions to study the radiative and non-radiative recombination mechanisms.

HL 31.6 Tue 11:30 POT 51

Optical properties of quaternary AlInGaN alloys pseudomorphically grown on GaN — •Egidijus Sakalauskas[1], Benjamin Reuters[2], Lars R. Khoshroo[2], Holger Kalisch[2], Michael Heuken[2,3], Rolf H. Jansen[2], Andrei Vescan[2], Gerhard Gobsch[1], and Rüdiger Goldhahn[1,4] — [1]Institut für Physik, TU Ilmenau — [2]Institut für Theoretische Elektrotechnik, RWTH Aachen University — [3]AIXTRON AG — [4]Institut für Experimentelle Physik, OvGU Magdeburg

The optical properties of quaternary $Al_xIn_yGa_{1-x-y}N$ alloy system with $0.28<x<0.74$ and $0.04<y<0.15$ are presented. The (0001)-oriented AlInGaN films are pseudomorphically grown by metal-organic vapour phase epitaxy on thick GaN buffers with sapphire substrates. The ordinary dielectric function of AlInGaN samples was determined in the range 1-10 eV by synchrotron ellipsometry at room temperature (BESSY II). The sharp onset of the imaginary part of the dielectric function defines the direct absorption edge of the alloys. At higher photon energies, the pronounced peaks are observed in the dielectric function, which correspond to high-energy inter-band transitions attributed to the critical points of the band structure (Van Hove singularities), indicating a promising optical quality of the material. An analytical model, which permits to describe accurately the dielectric function (or optical constants) in the range 1-10 eV, is also presented. The band-gap and high-energy inter-band transition values are obtained by fitting the experimental dielectric function with the analytical model. The strain influence on the band gap is evaluated by using k·p formalism.

15 min. break

HL 31.7 Tue 12:00 POT 51

MOVPE von semipolarem AlGaN auf $(10\bar{1}0)$ m-plane Saphir — •Frank Mehnke, Joachim Stellmach, Martin Frentrup, Gunnar Kusch, Tim Wernicke, Markus Pristovsek und Michael Kneissl — Technische Universität Berlin, Institut für Festkörperphysik, Hardenbergstr. 36, 10623 Berlin, Germany

Die Bandlücke von AlGaN variiert von 3,4 eV – 6,2 eV und ermöglicht Leuchtdioden (LEDs) im ultravioletten Spektralbereich. In dieser Arbeit wurden semipolare $(11\bar{2}2)$ AlGaN–Schichten untersucht, die ohne Nukleationschicht direkt auf $(10\bar{1}0)$ m–plane Saphir mittels metallorganischer Gasphasenepitaxie (MOVPE) abgeschieden wurden. Beim Wachstum wurden die TMAl– und TMGa–Partialdrücke bei einer Suszeptortemperatur von 1100 °C unter H_2–Atmosphäre variiert. Die Schichten sind vorzugsweise $(11\bar{2}2)$ orientiert. Die Halbwertsbreite des symmetrischen $(11\bar{2}2)$ Reflexes entlang der $[1\bar{1}00]_{AlGaN}$ Richtung ist mit 2780 arcsec vergleichbar mit der von $(11\bar{2}2)$ GaN Proben auf $(10\bar{1}0)$ Saphir. Die Proben haben eine Oberflächenrauigkeit zwischen 15 nm und 2 nm. Der Al–Gehalt der glattesten Proben liegt bei 60 % und wurde aus Transmissionsuntersuchungen bestimmt. Unterhalb von 60 % Al–Gehalt wird die Morphologie von dreieckigen Strukturen bestimmt, deren Öffnungswinkel sich mit abnehmenden Al–Gehalt erhöht. Oberhalb von 70 % sind zusätzlich inselartige Strukturen zu erkennen. Die Absorbtionskante lag 0,05 eV (bei GaN) bis 0,35 eV (bei AlN) unterhalb der Bandkante von (0001) orientierten AlGaN–Schichten. Weitere Untersuchungen zur Eignung der semipolaren AlGaN–Schichten zur Realisierung von UV–LEDs sind in Vorbereitung.

HL 31.8 Tue 12:15 POT 51

Investigation of the influence from TMIn for the optical properties of MOCVD grown InN — •Stefan Mohn[1], Ronny Kirste[1], Gordon Callsen[1], Öcal Tuna[2], Michael Heuken[2], and Axel Hoffmann[1] — [1]TU Berlin, Institut für Festkörperphysik, Hardenbergstraße 36, 10623 Berlin, Germany — [2]Aixtron AG, Kaiserstr. 98, 52135 Herzogenrath, Germany

Indium Nitride is a member of the III-V semiconductors and has a band gap of approx 0.7 eV. It is a promising candidate for LED, solar cells and other optoelectronic applications. In this talk we report on photoluminescence studies of InN layers grown on sapphire/GaN substrate by metal organic chemical vapor deposition (MOCVD). Commonly used precursors for the growth are of InN Trimethyl Indium (TMIn) and ammonia (NH_3). It is common belief that the ratio between TMIn and NH_3, is the key parameter for the quality of a grown sample. In this contribution we can show that an increase of TMIn flow, while the ammonia flow was constant, leads to to a change of the optical properties. With increasing TMIn content the observed maximas of the photoluminescence measurements shifts to higher energies. At the same time the full width at half maximum (FWHM) is increasing. Therefore we assume a decreasing quality of the grown samples with increasing of the TMIn content. We also observed as decrease in the sample quality, when the TMIn and the ammonia flows are increased while the V/III-ratio remains constant. Theses results are confirmed by a bundle of experimental techniques such as Raman spectroscopy, AFM and XRD.

HL 31.9 Tue 12:30 POT 51

Growth of AlN on c-plane sapphire by pulsed MOVPE — •Hanno Kröncke, Stephan Figge, and Detlef Hommel — Institut für Festkörperphysik, Universität Bremen

Due to it's large bandgap and it's high thermal conductivity Aluminumnitride is of high interest for applications in high power electronics and optoelectronic device emitting in the ultra-violet region. Because Al shows a low surface diffusivity AlN is normally grown at high temperatures up to 1300 °C. An alternative approach is the pulsed or flow modulation MOVPE growth, where an alternating supply of the precursors increases the surface mobility of the atoms.

In this study Al-polar AlN layers with a thickness between 200 nm and 1 μm were directly grown on c-plane sapphire in a closed coupled showerhead MOVPE at temperatures between 1000 and 1250 °C. Beside the variation of the pulse length for precursors, different types of pre-growth treatments have been investigated. The crystal quality, expressed by surface morphology and dislocation density, was mainly characterized by HRXRD, SEM, AFM and also compared to continuously grown samples.

In general the crystal quality is very sensitive to the growth-start and common concepts, known from the growth of GaN, like low temperature nitridation and buffer layers, lead to very rough surface and high mosaicity. With optimized parameter we achieved RMS surface roughness is below 1 nm and dislocation densities, determined by XRD, in the order of $1{\cdot}10^7$ cm^{-2} (screw type) and $3{\cdot}10^{10}$ cm^{-2} (edge type).

HL 31.10 Tue 12:45 POT 51

Carbon doped InAlAs/InGaAs/InAs heterostructures — •Marika Hirmer[1], Dominique Bougeard[1], Dieter Schuh[1], and Werner Wegscheider[2] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, D 93040 Regensburg, Germany — [2]Laboratorium für Festkörperphysik, ETH Zürich, 8093 Zürich, Switzerland

InAlAs/InGaAs heterostructures with a high In content are promising candidates for spintronic applications such as spin-valve mesoscopic devices due to their large Landé g-factor (around 15 in InAs) and the large Rashba effect.

Here, we present results on carbon doped InGaAs/InAlAs heterostructures with embedded InAs channel. We got a two-dimensional hole gas with a hole density of $p = 1.06 * 10^{12}$ cm^{-2} and a hole mobility of $7.26 * 10^3$ cm^2/Vs. Magnetotransport measurements on L-shaped Hall bars along [011], [01-1], [010] and [001] crystal directions exhibit well-developed Shubnikov-de-Haas oscillations and quantum Hall plateaus, indicating the high quality of the material. In the field range from minus 6T to 6T the longitudinal resistance is superimposed with a negative parabolic magnetoresistance background. The minimum of the longitudinal resistance at B = 0T decreases with increasing temperature, and hence, is a sign for weak antilocalization.

HL 31.11 Tue 13:00 POT 51

Point defects in AlN — •Jan E. Stehr[1], Detlev M. Hofmann[1], Bruno K. Meyer[1], and Matthias Bickermann[2] — [1]1st Physics Institute, Justus-Liebig-University Gießen, Heinrich-Buff-Ring 16, 35392 Gießen, Germany — [2]Department of Materials Science 6, University of Erlangen, Martensstraße 7, 91058 Erlangen, Germany

Aluminum nitride (AlN) bulk crystals are due to their high thermal conductivity and the low lattice mismatch a promising substrate material for group III-element-nitrides, e.g. AlGaN. AlN has a band gap of 6.2 eV, but shows a sub-band-absorption, which is a problem for many applications. Therefore it is necessary to understand which defects are responsible for the absorption bands in the crystals. We investigated AlN bulk crystals with UV-VIS spectroscopy and Electron Paramagnetic Resonance spectroscopy (EPR). In the EPR measurements we observe a donor signal with g=1.994 and an acceptor signal with g=2.006. UV-VIS measurements show an optical absorption band at 580 nm. By Photo-EPR we can correlate the absorption band with the EPR signals, which show up after illumination of the sample with light wavelengths shorter than 580 nm. Defect models will be discussed at the conference.

HL 31.12 Tue 13:15 POT 51

Electrical characterization of ion implanted AlN on sapphire — •Niels Henrik Borth, Ulrich Vetter, Tristan Koppe, Marc Brötzmann, Hans-Gregor Gehrke, Kun Zhang, and Hans Hofsäss — II. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

AlN with its large bandgap of 6.2 eV is a promising candidate for application in high power high frequency devices, UV detectors and UV light emitters. Despite the fact that there are a large number of publications concerning the optical activation of dopants in AlN, no attempt was made to achieve electrical activation after ion implantation. In this study we report on the electrical behaviour of ion implanted AlN on sapphire. Silicon, magnesium and fluorine were implanted with several energies forming a boxlike profile. The samples were annealed in a RTP furnace. SIMS measurements were used to investigate the implantation profile before and after the annealing process. Before evaporating contacts the surface was etched by RIE using a Cl_2/BCl_3 plasma. The peak concentrations ranged from 0.05 at% up to 1 at%. Results of the electrical measurements as a function of doping concentration are presented. Additionally sputter and RIE experiments were performed for different fluences and times, respectively. AFM measurements illustrate a smoothening of the surface.

HL 32: Focussed Session: Inorganic/Organic Semiconductor Hybrid Structures I

Time: Tuesday 10:15–13:00 Location: POT 151

Invited Talk HL 32.1 Tue 10:15 POT 151

Self-assembled monolayers on zinc oxide — •Craig L. Perkins — National Renewable Energy Labooratory, Golden, CO USA — Renewable and Sustainable Energy Institute

Two of the most promising schemes for attaching organic molecules to metal oxides are based on the chemistry of the thiol and phosphonic acid moieties. We have made a direct comparison of the efficacy of these two molecular anchors on zinc oxide by comparing the chemical and physical properties of n-hexane derivatives of both. The surface properties of polycrystalline ZnO thin films and ZnO(0001)-O crystals modified with 1-hexanethiol and 1-hexanephosphonic acid were examined with a novel quartz crystal microbalance (QCM)-based flow cell reactor, angle-resolved and temperature-dependent photoelectron spectroscopy, and contact angle measurements. A means of using ammonium chloride as a probe of molecule-ZnO interactions is introduced and used to ascertain the relative quality of self-assembled monolayers (SAMs) based on thiols and phosphonic acids. QCM data shows that a phosphonic acid-anchored alkyl chain only six carbons long can provide significant corrosion protection for ZnO against Brønsted acids, reducing the etch rate relative to the bare ZnO surface by a factor of more than nine. The thermal stability of the two linking groups was also explored and we find that previous claims of highly stable alkanethiolate monolayers on ZnO are suspect. Taken as a whole, our results indicate that the phosphonic acid moiety is preferred over thiols for the attachment of short alkyl groups to ZnO.

Invited Talk HL 32.2 Tue 10:45 POT 151

Inorganic/organic semiconductor heteroepitaxy - towards new hybrid systems for optoelectronics and photonics — •Sylke Blumstengel — Institute of Physics, Humboldt University Berlin, Newtonstr. 15, 12489 Berlin

This talk summarizes our recent efforts to fabricate heterostructures based on ZnO and various conjugated organic materials as well as to tailor their electronic and optical properties. Growth by molecular beam epitaxy of both material components ensures well-defined interfaces and highest structural quality. A unique feature of ZnO and its ternaries ZnCdO and ZnMgO is that films and quantum structures with very good crystalline and optical properties can be epitaxially grown at low temperatures (50°C!) compatible with the stability of organic materials. Thus, not only organic-on-inorganic, but also inorganic-on-organic epitaxy can be performed. Relevant growth mechanisms are discussed. Interfacial energy level alignment including band-offset engineering via the geometric structure of the molecular layer is presented. Direct electronic coupling of the fundamental excitations (Frenkel and Wannier-Mott excitons) across the interface occurs with coupling constants on the meV-energy scale. The superior optoelectronic function of sandwich-type hybrids is demonstrated by the achievement of stimulated emission of the enclosed organic layer at markedly reduced pump thresholds due to efficient energy transfer from ZnO.

15 min. break

Invited Talk HL 32.3 Tue 11:30 POT 151

Electrostatic Field Driven Alignment of Organic Oligomers on ZnO Surfaces — •Fabio Della Sala[1], Sylke Blumstengel[2], and Fritz Henneberger[2] — [1]Nanoscience Institute (CNR), Via per Arnesano, 73100 Lecce — [2]Institut fuer Physik, Humboldt-Universitaet zu Berlin, Newtonstrasse 15, 12489 Berlin, Germany

We present a theoretical study on the physisorption process of organic oligomers on the ZnO($10\bar{1}0$) surface. Using first-principles density-functional theory and non-empirical embedding methods, we find that both in-plane location and orientation of the molecules are completely determined by the coupling of their quadrupole moments to the periodic dipolar electric field present at the semiconductor surface. The adsorption is associated with the formation of a molecular dipole moment perpendicular to the surface, which bears an unexpected linear relation to the molecule-substrate interaction energy. Long oligomers such as sexiphenyl become well-aligned with stabilization energies of several 100 meV along rows of positive electric field, in full agreement with recent experiments. These findings define a new route towards the realization of highly-ordered self-assembled arrays of oligomers/polymers on ZnO($10\bar{1}0$) and similar surfaces.

Invited Talk HL 32.4 Tue 12:00 POT 151

The incorporation of metal nanostructures at organic/inorganic semiconductor interfaces — •Dietrich RT Zahn, Michael Ludemann, Ovidiu Gordan, Philipp Schäfer, and Georgeta Salvan — Semiconductor Physics, Chemnitz University of Technology, 09107 Chemnitz

Raman spectroscopy is applied in situ and online to study the interface formation of organic semiconductors such as perylene derivatives

and phthalocyanines on inorganic semiconductor like gallium arsenide and silicon. Moreover, also the interface formation between metals and organic semiconductors has been extensively investigated. In the latter case the surface enhanced Raman scattering (SERS) effect is observed and it provides useful information regarding e.g. metal reactivity and metal diffusion. More recently well defined metal nanostructures were prepared on oxidised silicon samples using nanosphere lithography. When organic molecules are deposited onto such structured substrates strong enhancement effects are again observed. However, the enhancement effect shows an unusual resonance behaviour at excitation wavelengths well away from the metal cluster plasmon energy. The potential of such structures for application will be illuminated.

HL 32.5 Tue 12:30 POT 151

Fabrication of ZnO/polymer hybride devices using chemical vapor deposition of polymers — •Jan Richters and Tobias Voss — Institut für Festkörperphysik, Universität Bremen, Otto-Hahn-Allee 1, 28359 Bremen

Due to their large surface area and good electrical conductivity, ZnO nanowires are interesting candidates for the fabrication of hybrid inorganic/organic optoelectronic devices. As an example, dye-sensitized solar cells can be prepared using a ZnO nanowire-array as one electrode with a monolayer of dye adsorbed on their surface. An additional hole-conductive material is required to form the connection with the counter electrode, where PEDOT:PSS or similar polymers can be applied. These polymer layers are usually fabricated using liquid-based synthesis-methods such as dip-coating or spin-coating which suffer from a limited penetration depth of the polymer into the pores of the nanowire array.
Here, we present a vapor-transport technique for the fabrication of dye-sensitized solar cells based on ZnO nanowires and the polymers PEDOT and polystyrene. We compare the electrical and optical properties of the devices, describe the microscopic properties of the polymer layers and provide details of the fabrication technique.

HL 32.6 Tue 12:45 POT 151

Electrical investigations of different polymer and substrate materials for dye-sensitized ZnO-NW/polymer hybrid solar cells — •Kay-Michael Günther[1], Julia Waltermann[1], Stefan Kontermann[2], and Wolfgang Schade[1,2] — [1]Clausthal University of Technology, EFZN, EnergieCampus, 38640 Goslar — [2]Fraunhofer Heinrich-Hertz-Institute, EnergieCampus, 38640 Goslar

Dye-sensitized solar cells composed of a n-doped ZnO nanowire (NW) array and a p-doped polymer layer appear to be a promising candidate for low-cost production of environment-friendly solar cells. In this study, we compare the commonly used polymer layers PEDOT:PSS and P3HT. While the former one provides a better conductivity, the latter one shows itself a photoabsorbance below $\lambda = 400$ nm. In addition, we investigate three different TCO substrates (ITO, FTO and ZnO:Al) using Impedance Spectroscopy (IS), current-voltage-measurements (IV), as well as IV-transients. The results show that in our setup an additional polycrystalline ZnO layer beneath the ZnO NWs is needed to prevent short circuits caused by polymer seeping between the NWs towards the counter electrode. Furthermore, the confinement to a simple ZnO layer enables us to optimize the polymer layer independently from the NWs. Hence, we compare devices with and without NWs and with different processing parameters. We achieve the best results with P3HT and FTO substrates. With ZnO:Al, we observe additional RC-combinations which partly result from a Schottky barrier formed at the ZnO:Al interface leading to a significant higher series resistance. An equivalent circuit is derived and discussed.

HL 33: Spin-dependent Transport I

Time: Tuesday 10:15–13:30 Location: POT 251

HL 33.1 Tue 10:15 POT 251

Time-resolved Kerr detection of acoustic spin transport in GaAs (110) quantum wells — •Alberto Hernández-Mínguez, Klaus Biermann, Snežana Lazić, Rudolph Hey, and Paulo V. Santos — Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5-7, D-10117 Berlin, Germany

Surface acoustic waves (SAWs) provide an efficient tool for the transport of spins in semiconductor quantum wells (QWs). The SAW piezoelectric field captures photogenerated electrons and holes in spatially separated locations, thus dramatically increasing the recombination lifetime, and transports them with well-defined velocity. Previous investigations of acoustic spin transport were carried out using spatially resolved photoluminescence, which requires the radiative recombination of the carriers. In this contribution, we demonstrate an alternative spin detection approach based on microscopic Kerr reflectometry in GaAs (110) QWs, where spin dephasing mechanisms associated with spin-orbit interaction result inoperative for electron spins oriented along the growth axis. The spins are generated on the SAW path by a pump laser pulse and are detected by measuring the change δP in polarization of a probe pulse delayed by τ with respect to the pump. Spatial profiles of δP during acoustic transport show a peak at $x = v_{SAW}\tau$, thus revealing the position of the moving spin packet. Measurements under an in-plane applied magnetic field demonstrate the coherent precession of the optically generated electron spins during acoustic transport over several μm, yielding information about the relaxation processes for the acoustically moving spins.

HL 33.2 Tue 10:30 POT 251

InAs spin-filter cascades in perpendicular magnetic fields — •Hauke Lehmann, Till Benter, Jan Jacob, and Ulrich Merkt — Institut für Angewandte Physik und Zentrum für Mikrostrukturforschung, Universität Hamburg, Jungiusstraße 11, 20355 Hamburg

We have experimentally demonstrated the generation and detection of spin-polarized currents by the intrinsic spin Hall effect in two-staged spin-filter cascades fabricated from InAs heterostructures [1]. Applying an external magnetic field perpendicular to the two-dimensional electron system introduces a Lorentz force. This adds to the spin-dependent force of the intrinsic spin Hall effect a spin-independent force dragging the electrons into one of the two outputs of each filter. Thus the magnetic field leads to a change of conductances and spin polarizations in each output. The conductances at the filters' outputs depend on the magnetic field direction and strength. Thus the application of magnetic fields allows inference on the strength of the intrinsic spin Hall effect in low-dimensional semiconductor nanostructures.

[1] J. Jacob, G. Meier, S. Peters, T. Matsuyama, U. Merkt, A. Cummings, R. Akis, and D. Ferry. J. Appl. Phys. **105**, 093714 (2009).

HL 33.3 Tue 10:45 POT 251

Influence of in-plane magnetic fields on the spin-orbit coupling in InAs spin-filter cascades — •Hauke Lehmann, Till Benter, Alexander Buhr, and Jan Jacob — Institut für Angewandte Physik und Zentrum für Mikrostrukturforschung, Universität Hamburg, Jungiusstraße 11, 20355 Hamburg.

In Y-shaped three-terminal junctions of quasi one-dimensional nanowires fabricated from InAs heterostructures an unpolarized current is separated into two oppositely polarized currents by the intrinsic spin Hall effect. The spin polarization can be detected by a second filter stage [1]. Combining the intrinsic spin Hall effect with the spin precession, originating from the spin-orbit interaction, the electrons execute an oscillatory motion - the so-called zitterbewegung. This motion can be tuned by an in-plane magnetic field perpendicular to the electrons' direction of motion, which couples to the effective Rashba field. We present DC biased lock-in transport measurements at millikelvin temperatures on two-staged spin-filter cascades and compare them to simulations [2].

[1] J. Jacob, G. Meier, S. Peters, T. Matsuyama, U. Merkt, A. Cummings, R. Akis, and D. Ferry. J. Appl. Phys. **105**, 093714 (2009).
[2] P. Brusheim and H. Q. Xu, arXiv: 0810.2186v2 (2009).

HL 33.4 Tue 11:00 POT 251

Spin-orbit coupling effects in the quantum oscillatory magnetization of asymmetric InGaAs/InP quantum wells in tilted magnetic fields — •Benedikt Rupprecht[1], Christian Heyn[2], Hilde Hardtdegen[3], Thomas Schäpers[3], Marc A. Wilde[1], and Dirk Grundler[1] — [1]Lehrstuhl für Physik funktionaler Schichtsys-

teme, TU München, James-Franck-Str. 1, D-85747 Garching b. M. — [2]Institute of Applied Physics, Jungiusstr. 11, D-20355 Hamburg — [3]Institute for Bio- and Nanosystems (IBN-1) and JARA Jülich-Aachen Research Alliance, Research Centre Jülich GmbH, D-52425 Jülich

The measurement of the magnetic susceptibility and the de Haas-van Alphen (dHvA) effect was proposed by Bychkov and Rashba in 1984 to study the spin-orbit interaction (SOI) in a structure inversion asymmetric heterostructure and the spin splitting experienced by a two-dimensional electron system (2DES). Micromechanical cantilever magnetometry recently allowed us to measure the magnetization M of asymmetric InGaAs/InP quantum wells. We observe the expected SOI-induced beating patterns in M in both nearly perpendicular and tilted magnetic fields B. Unexpectedly we find phase and frequency anomalies in M vs B which have not been predicted and not been found in magnetotransport experiments. We compare our experimental results with simulations considering SOI, Zeeman splitting and tilted fields. We show that the surprising phase and frequency anomalies go beyond the current theoretical understanding and remain to be clarified. The work is supported via SPP 1285 "Halbleiter-Spintronik" (GR1640/3-2) and the "Nanosystems Initiative Munich" (NIM).

HL 33.5 Tue 11:15 POT 251

Spin polarized photocurrents in InAs:Mn based quantum wells — •P. Olbrich[1], C. Zoth[1], C. Drexler[1], V. Lechner[1], I. Caspers[1], V. Bel'kov[2], S. Weishäupl[1], D. Vogel[1], U. Wurstbauer[3], D. Schuh[1], D. Weiss[1], and S.D. Ganichev[1] — [1]Terahertz Center, Regensburg, Germany — [2]Ioffe Institute, St. Petersburg, Russia — [3]Columbia University, NY, USA

We report on the observation and investigation of terahertz (THz) radiation induced spin polarized currents in manganese doped InAs quantum well structures (QWs). The study is aimed to explore the spin-orbit interaction in this novel material system. The incorporation of Mn into an InAs QW leads to a 2D hole gas with interesting properties as both the g^*-factor and Rashba type of spin-orbit coupling are large. Here, we demonstrate that in Mn-doped InAs QWs the absorption of THz radiation leads to pure spin currents, which we converted into a net electric current by means of an external in-plane magnetic field. Our results, in particular the dependence of the current on the magnetic field strength and temperature, have provided a feedback to the segregation of manganese. We show that as a result of this process only in systems with Mn introduced from the substrate side the spin-dependent scattering and Zeeman effect become enhanced. This result is supported by transport measurements of the longitudinal magnetoresistance. In addition, by applying photogalvanic effects we studied the anisotropy of the band spin splitting and provide the information on the ratio between the Rashba and Dresselhaus terms in InAs:Mn QWs of various designs.

HL 33.6 Tue 11:30 POT 251

Spin polarized electric currents in semiconductor heterostructures induced by microwave radiation — •C. Drexler[1], V.V. Bel'kov[2], B. Ashkinadze[3], P. Olbrich[1], C. Zoth[1], V. Lechner[1], Ya.V. Terent'ev[2], D.R. Yakovlev[2,4], G. Karczewski[5], T. Wojtowicz[5], D. Schuh[1], W. Wegscheider[1], and S.D. Ganichev[1] — [1]THz Center, Regensburg, Germany — [2]Ioffe Institute, St. Petersburg, Russia — [3]Technicon, Haifa, Israel — [4]TU Dortmund, Germany — [5]Polish Academy of Sciences, Warsaw, Poland

We report on microwave (mw) radiation induced electric currents in semi-magnetic CdMnTe and non-magnetic InAs:Si quantum wells subjected to an external in-plane magnetic field. The current generation is attributed to the spin-dependent energy relaxation of electrons heated by mw radiation. The relaxation produces equal and oppositely directed electron flows in the spin-up and spin-down subbands yielding a pure spin current. The Zeeman splitting of the subbands in the external magnetic field leads to the conversion of the spin flow into a spin-polarized electric current, which is proportional to the Zeeman splitting energy in non-magnetic structures. As a result we demonstrate, that the presence of magnetic Mn^{2+} ions yields an additional contribution to the microwave induced current formation which is related to the giant Zeeman spin splitting [1].

[1] C. Drexler *et. al.*, *Appl. Phys. Lett.* **97**, 182197 (2010).

15 min. break

HL 33.7 Tue 12:00 POT 251

Spin and orbital mechanisms of the magneto-gyrotropic photogalvanic effect in GaAs/AlGaAs quantum wells — •V. Lechner[1], L.E. Golub[2], F. Lomakina[1], V.V. Bel'kov[2], P. Olbrich[1], S. Stachel[1], I. Caspers[1], M. Griesbeck[1], M. Kugler[1], M.J. Hirmer[1], T. Korn[1], C. Schüller[1], D. Schuh[1], W. Wegscheider[3], and S.D. Ganichev[1] — [1]University of Regensburg, Germany — [2]Ioffe Institute, St. Petersburg, Russia — [3]ETH Zurich, Switzerland

Here we report on experiments, which allow us to distinguish unambiguously between the spin-dependent [1] and most recently proposed orbital origin [2] of the THz radiation induced magneto-gyrotropic photogalvanic effect (MPGE). To achieve this goal we utilize the qualitative difference in their behavior upon a variation of the g^* factor: In contrast to the orbital effects, the MPGE resulting from the spin-related roots is proportional to the Zeeman spin splitting. To explore this difference, we utilize the fact that in GaAs/AlGaAs QWs the Zeeman splitting changes its sign at a certain QW width. Our experiments show that, for most QW widths, the MPGE is mainly driven by spin-related mechanisms, which results in a photocurrent proportional to the g^* factor [3]. In structures with a vanishingly small g^* factor, however, the MPGE is also detected, proving the existence of orbital mechanisms.

[1] V.V. Bel'kov, S.D. Ganichev, Sem. Sci. Techn. **23**, 114003 (2008),
[2] S.A. Tarasenko, arXiv cond-mat: 1009.0681v1 (2010),
[3] V. Lechner et al., arXiv cond-mat: 1011.4433v1 (2010).

HL 33.8 Tue 12:15 POT 251

Magnetogyrotropic photogalvanic effects in InSb-based quantum wells — •Sebastian Stachel[1], Cynthia Karl[1], Thomas Stangl[1], Peter Olbrich[1], Vasily Bel'kov[2], Steven K. Clowes[3], Tim Ashley[4], and Sergey D. Ganichev[1] — [1]Terahertz Center, University of Regensburg, Regensburg, Germany — [2]Ioffe Institute, St. Petersburg, Russia — [3]Advanced Technology Institute, University of Surrey, UK — [4]QinetiQ, Malvern, UK

We report on the observation of the magnetic-field induced photocurrent in n-doped InSb/InAlSb quantum wells (QWs) excited by terahertz radiation. The photocurrent behavior upon variation of the radiation polarization, magnetic field strength, B, and temperature is studied. While at a moderate magnetic field the photocurrent exhibits a linear field dependence, at high magnetic fields it becomes nonlinear and even changes its sign. The experimental results are analyzed in terms of the magneto-gyrotropic photogalvanic effect (MPGE) based on the asymmetry of optical transitions and/or asymmetric relaxation of carriers in the momentum space [1]. We demonstrate that the sign inversion of the photocurrent is caused by the interplay of two mechanisms: The spin mechanism, which yields a saturation of the current at high magnetic fields due to the large Zeeman splitting in InSb-based QWs, and the orbital mechanism, which depends linearly on B and has an opposite sign. The latter contribution dominates the total current at high magnetic fields.

[1] V.V. Belkov and S.D. Ganichev, Sem. Sci. Tec. **23**, 114003 (2008)

HL 33.9 Tue 12:30 POT 251

Remanent spin injection and spin relaxation in quantum dot light emitting diodes — •Henning Soldat[1], Mingyuan Li[1], Nils C. Gerhardt[1], Arne Ludwig[2], Frank Stromberg[3], Werner Keune[3], Heiko Wende[3], Andreas D. Wieck[2], Dirk Reuter[2], and Martin R. Hofmann[1] — [1]Lehrstuhl für Photonik und Terahertztechnologie, Ruhr-Universität Bochum, D-44780 Bochum — [2]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, D-44780 Bochum — [3]Fakultät für Physik and Center for Nanointegration Duisburg-Essen (CeNIDE), Universität Duisburg-Essen, D-47048 Duisburg

The study of spin-controlled optoelectronic devices has been a field of intensive research over the past few years. We investigate spin injection in remanence into InAs quantum dot (QD) light emitting diodes (LEDs). Our samples are spin LEDs with a Fe/Tb injector with out-of-plane remanent magnetization and a MgO tunnel barrier at the ferromagnetic metal/semiconductor interface to overcome the conductivity mismatch. The active region is an ensemble of InAs QDs. Intrinsic GaAs layers of variable thickness have been implemented between this active region and the spin injector to investigate the influence of transport path length on spin polarization. We have measured the circular polarization of the LED emission in remanence. By investigating the different injection path lengths for the samples we have determined the spin diffusion length in undoped GaAs along with the spin polarization

at the injector interface. Additionally, the spin injection efficiency at the MgO tunnel barrier has been investigated.

HL 33.10 Tue 12:45 POT 251

Perpendicular Spin Injection and Polarization Features in InAs Quantum Dots — •Arne Ludwig[1], Henning Soldat[2], Frank Stromberg[3], Astrid Ebbing[1,4], Anne Warland[3], Mingyuan Li[2], Nils C. Gerhardt[2], Dirk Reuter[1], Oleg Petracic[4], Martin Hofmann[2], Heiko Wende[3], Werner Keune[3], and Andreas D. Wieck[1] — [1]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum — [2]Lehrstuhl für Photonik und Terahertztechnologie, Ruhr-Universität Bochum — [3]Fachbereich Physik and Center for Nanointegration Duisburg-Essen, Universität Duisburg-Essen — [4]Experimentalphysik IV - Festkörperphysik, Ruhr-Universität Bochum

Self assembled InAs quantum dots (QDs) are zero dimensional multilevel systems with long spin relaxation times and thus offer great potential for spin optoelectronic research and applications.

Electrically injected spin polarization is efficiently transferred into circularly polarized photons if the injected spin is oriented perpendicularly to the growth plane. The optical polarization from an ensemble of QDs in a spin-LED is strongly magnetic field dependent due to the orbital character of the transitions of excited carriers. An unambiguous separation of spin injection and Zeeman shift is obtained by investigating the magnetic field dependence of the circular polarisation of the spin-LED emission.

Here we present and analyze perpendicular spin injection from Fe/Tb magnetic injectors at room temperature and in remanence. Polarization features of excited transitions are discussed.

HL 33.11 Tue 13:00 POT 251

Coherent electrical spin-manipulation in strained InGaAs — •Sebastian Kuhlen[1,3], Klaus Schmalbuch[1,3], Markus Hagedorn[1,3], Mihail Lepsa[2,3], Thomas Schäpers[2,3], Gernot Güntherodt[1,3], and Bernd Beschoten[1,3] — [1]II. Physikalisches Institut A, RWTH Aachen University, 52074 Aachen — [2]Institut für Bio- und Nanosysteme IBN-1, Forschungszentrum Jülich, 52425 Jülich — [3]JARA: Fundamentals of Future Information Technology, 52074 Aachen

To realize novel spintronic devices it is important to develop electrical methods both to polarize and to manipulate electron spins.

We have investigated the process of so-called current-induced spin polarization in strained n-InGaAs epilayers, which favorably does not require any ferromagnetic electrodes. An electric field is found to create a Dresselhaus-type internal magnetic field, which is perpendicular and proportional to the E-field ($100\,mT$ per $4 \cdot 10^4\,V/m$). Using electric field pulses, which convert into internal magnetic field pulses, we are able to trigger the phase of the electron spin polarization. The coherence of these spins is probed by spin precession using time-resolved Faraday rotation. Moreover, the internal field pulses can be used to turn on and turn off spin precession of optically pumped coherent spin ensembles in the absence of external magnetic fields. By changing pulse width and amplitude we achieve a full 360° control of the spin direction.

This work has been supported by DFG through FOR912.

HL 33.12 Tue 13:15 POT 251

Separation of Spin and Charge Currents by Photovoltage Measurements in n-InGaAs — •Stefan Göbbels[1,2], Philipp Schäfers[1,2], Klaus Schmalbuch[1,2], Thomas Schäpers[3,2], Mihail Lepsa[3,2], Gernot Güntherodt[1,2], and Bernd Beschoten[1,2] — [1]II. Phys. Institut A, RWTH Aachen University, 52056 Aachen — [2]JARA: Fundamentals of Future Information Technology — [3]Institut für Bio- und Nanosysteme IBN-1, Forschungszentrum Jülich, 52425 Jülich

Spin photocurrents have gained strong attention in the field of spintronics as they convert spin information into electric voltage and spin-polarized currents. Many effects yielding spin-photocurrents have been demonstrated in 2DEGs, e.g. spin-galvanic effect and magneto-gyrotropic photogalvanic effect [1]. However, no direct proof of the spin polarization of these currents has been reported yet.

We present photovoltage measurements on n-InGaAs epilayers combined with Faraday rotation spectroscopy for the detection of the spin polarization. The photovoltage consists of both a light polarization dependent and an independent component which exhibit different energy dependencies. Comparison with the spin sensitive measurements of the Faraday rotation allows us to separate spin from charge voltages.

[1] S. D. Ganichev & W. Prettl, J. Phys. Cond. Mat. 15, R935 (2003)

This work has been supported by DFG through FOR 912.

HL 34: Joint Session: Solid State Photon Sources

Time: Tuesday 10:30–13:00 Location: HSZ 02

HL 34.1 Tue 10:30 HSZ 02

Optical Processes in OLEDs: Molecular Photonics — •Michael Flämmich, Dirk Michaelis, and Norbert Danz — Fraunhofer Institute for Applied Optics and Precision Engineering, 07745 Jena, Germany

Following the OLED display market take-off, huge world wide efforts are spent to develop OLEDs towards competitive sources for general lighting applications. In this context, the light outcoupling problem is well known as the key parameter to improve OLED efficiency in order to tackle existing lighting schemes. From the optical point of view, the device performance is driven (i) by the architecture of the OLEDs layered system and (ii) by the internal features of the emissive material. Studies in recent years have shown that the latter attributes (which are the internal electroluminescence spectrum, the profile of the emission zone, the orientation of the transition dipole moments and the internal luminescence quantum efficiency q) can be determined in situ by measurements of the far-field emission pattern generated by active OLEDs (i.e. in electrical operation) and corresponding optical reverse simulations. Starting from basic considerations of the dipole radiation characteristics, we elaborate specifically how the orientation distribution of the dipole transition moments in the layered system can be analyzed in situ, providing insight into the internal photo-physical processes on the molecular scale of the emitter.

HL 34.2 Tue 11:00 HSZ 02

Single Photon Source with Diamond Nanocrystals on Tapered Optical Fibers — •Almut Tröller[1], Juliane Hermelbracht[1], Markus Weber[1], Wenjamin Rosenfeld[1], Ariane Stiebeiner[3], Arno Rauschenbeutel[3], James Rabeau[4], and Harald Weinfurter[1,2] — [1]Ludwig-Maximilians-Universität, München — [2]Max-Planck-Institut für Quantenoptik, Garching — [3]Johannes-Gutenberg-Universität, Mainz — [4]Macquarie University, Sydney

The development of reliable devices generating single photons is crucial for applications in quantum information as well as for fundamental experiments in quantum optics. Due to its properties the nitrogen-vacancy (NV) color center in diamond is considered a promising candidate for the implementation of such a device. Those properties include an optical transition at 637 nm with a fluorescence lifetime of 11.6 ns, high photostability and the possibility to work at room temperature.

However, the collection efficiency of the fluorescence light in bulk diamond is limited by the high refractive index of diamond. To resolve this issue we use diamond nanocrystals, which – being smaller than the wavelength of the fluorescence light – are not subject to refraction. In order to further enhance the single photon collection efficiency we aim at coupling the emission of a single NV center to the evanescent field of a tapered optical fiber. Here we present data on diamond nanocrystals containing NV centers and the first attempts towards their application to tapered fibers.

HL 34.3 Tue 11:15 HSZ 02

Fiber-integrated diamond-based single photon source — •Tim Schröder, Andreas Wolfgang Schell, Günter Kewes, Thomas Aichele, and Oliver Benson — Nano Optics Group, Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany

The most direct approach to fabricate a reliable single photon source is to mount a single quantum emitter on an optical fibre. It integrates

easily into fibre optic networks for quantum cryptography or quantum metrology applications . For the first time such a fibre-integrated single photon source operating at room temperature is demonstrated. It consists of a single nitrogen vacancy defect centre in a nanodiamond which is directly near-field coupled to the guiding modes of a commercial optical fibre. The coupling is achieved in a bottom-up approach by placing a pre-selected nanodiamond directly on the fibre facet. This configuration is ultra-stable and realignment-free. Its high photon collection efficiency is equivalent to a far-field collection via an objective with a numerical aperture of 0.82. Furthermore, simultaneous excitation of the single defect centre and recollection of its fluorescence light through the fibre is possible introducing a fibre-connected single emitter sensor.

HL 34.4 Tue 11:30 HSZ 02

Near-field infrared spectroscopy of single InAs quantum dots — Rainer Jacob[1], •Stephan Winnerl[1], Harald Schneider[1], Manfred Helm[1], Marc Tobias Wenzel[2], Hans-Georg v. Ribbeck[2], and Lukas M. Eng[2] — [1]Institut für Ionenstrahlphysik und Materialforschung, Helmholtz-Zentrum Dresden-Rossendorf, Postfach 51 01 19, 01314 Dresden, Germany — [2]Institut für Angewandte Photophysik, TU Dresden, George-Bähr-Straße 1, 01069 Dresden, Germany

Scattering-type scanning near-field optical microscopy (s-SNOM) is a versatile technique in optical sciences. It provides optical resolution in the nanometer range, while offering spectroscopic application when combined with a tunable light source. Here, we exploit the combination of a s-SNOM with a widely tunable free-electron laser. With this setup, we were able to perform optical spectroscopy of single InAs quantum dots by means of their near-field signature in the mid infrared. The sample was composed of a single layer of self-assembled InAs quantum dots that were capped by a 70 nm thick GaAs layer. In the s-SNOM-measurements we could obtain a clear near-field contrast between the dots and the surrounding medium at 10.2 um which corresponds to 120 meV. Another clear contrast could be obtained for 85 meV. Both signatures could be attributed to intersublevel transitions in the quantum dot [1]. To our knowledge this is the first time that an optical near-field signature of an intersublevel transition could be demonstrated at a single InAs quantum dot.

[1] P. Boucaud et al., C. R. Physique 9, 840 (2008)

HL 34.5 Tue 11:45 HSZ 02

Quantum-Dot Pyramidal Microcavities as Candidates for Electrically Pumped Efficient Single-Photon Sources — •Daniel Rülke, Christoph Reinheimer, Florian Stockmar, Daniel M. Schaadt, Heinz Kalt, and Michael Hetterich — Institut für Angewandte Physik and DFG Center for Functional Nanostructures, Karlsruhe Institute of Technology (KIT), Wolfgang-Gaede-Straße 1, 76131 Karlsruhe (Germany)

We have investigated InAs-QDs embedded in reversed pyramidal GaAs microcavities in order to fabricate optically and electrically pumped single-photon sources. As a great advantage of the pyramidal shape the total number of QDs inside the cavity can be controlled by the position of the QD layer during molecular-beam epitaxial growth. Thus, by placing the QD layer close to the tip of the reversed pyramid, a very low number of QDs in the cavity can be achieved, while the facets act as a retroreflector for the emitted light. The pyramidal cavities were fabricated by a a combination of e-beam lithography and a selective wet-chemical etching process. In order to pump QDs electrically they have been embedded in the intrinsic layer of a pin-junction and individual cavities have been connected via bridges to a larger contact pad. To this end, a second non-critical e-beam alignment step had to be added after the wet-chemical etching process before metalisation and a subsequent lift-off process.

HL 34.6 Tue 12:00 HSZ 02

Realisation of a robust and compact fibre-coupled diamond based single photon source implemented with gradient-index lenses — •Philip Engel, Tim Schröder, and Oliver Benson — Nano Optics Group, Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin

Single photons play an important role for many quantum information technologies. Quantum cryptography schemes and other experiments with single photons have already been implemented in rather large laboratory setups. To reduce the size and cost and increase the scalability of such experiments we designed a diamond based single photon source which uses gradient-index (GRIN) lenses with integrated thin film filters to collect and couple single photons into a single-mode fibre. GRIN lenses can be fabricated in such a way that a collimated incoming beam has its focal plane overlaying with the surface of the lens where nanodiamonds containing single defect centres can be deposited via spin-coating. In this manner the GRIN lens serves as holder for single photon emitters as well as light collection objective. Furthermore a solid immersion lens like behaviour increases the emission of a dipole into the direction of the GRIN lens. Depending on the defect centre type we expect more than 100 kcts/s of fibre coupled single photons. This high count rate combined with its easy experimental realisation, moderate cost for components and its small dimensions of about 3 mm by 3 mm by 30 mm makes this device interesting for robust and low cost single photon implementations.

HL 34.7 Tue 12:15 HSZ 02

A spintronic circularly-polarized single-photon source — •Andreas Merz, Pablo Asshoff, Robin Schwerdt, Heinz Kalt, and Michael Hetterich — Karlsruhe Institute of Technology (KIT)

Diluted magnetic semiconductors (DMS) are among the most promising materials for efficient spin-injection into semiconductors. They are thus ideal materials for designing a spin-polarized single photon source pumped by an electrical current. As a model system we investigate a spin light-emitting diode with the DMS ZnMnSe and an InGaAs quantum dot as single photon source. With an applied magnetic field of 2 T, a pronounced spin-polarization of $\sim 65\,\%$ is achieved, while at B = 6 T it even approaches 95 %. Autocorrelation measurements in pulsed operation mode prove the light emitted being non-classical.

HL 34.8 Tue 12:30 HSZ 02

On-demand single photon source in (311)A GaAs quantum dots — •Snežana Lazić, Rudolf Hey, and Paulo Santos — Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5–7, 10117 Berlin, Germany

We demonstrate the generation of single photons on demand using an acousto-electric effect in GaAs/AlGaAs quantum well (QW) grown by molecular beam epitaxy on pre-patterned (311)A GaAs substrates. In this process, a surface acoustic wave (SAW) is employed to control the transfer of carriers, photogenerated in the QW, to an array of quantum dots (QDs) embedded at well-defined positions within the high-mobility QW transport channel. The embedded QD arrays form during the growth at the edges of etched triangular trenches due to monolayer fluctuations of the QW thickness. The photoluminescence from these acoustically-pumped arrays of QDs consists of a series of sharp lines which are attributed to the recombination of carriers in discrete quantum states. Time-resolved studies show that the population of the emitting states within the array, as well as the subsequent emission of single photons is governed by the SAW. The photons are emitted when the electrons captured within the array recombine with holes brought in a subsequent SAW cycle. The mechanism for the emission of non-classical light from QD arrays was investigated by analyzing the statistics of the emitted photons using the Hanbury Brown and Twiss approach.

HL 34.9 Tue 12:45 HSZ 02

Tunnel Injection in Electrically Pumped Single Photon Emitters — •Alexander Dreismann[1], Murat Öztürk[1], Ole Hitzemann[1], Erik Stock[1], Waldemar Unrau[1], Askhat K. Bakarov[2], Aleksandr I. Toropov[2], Ilia A. Derebezov[2], Vladimir Haisler[2], and Dieter Bimberg[1] — [1]Institut für Festkörperphysik, TU-Berlin, 10623 Berlin, Germany — [2]Institute of Semiconductor Physics, 630090 Novosibirsk, Russia

Electrically pumped InGaAs/GaAs quantum dot (QD) based Resonant-Cavity LEDs (RC-LEDs) represent powerful semiconductor based single photon and potential entangled photon emitters with high out-coupling efficiencies as required for quantum key distribution [1]. To achieve high photon emission rates the exciton luminescence intensity should be as high as possible; in the case of entangled photon sources exciton and biexciton luminescence intensities should be comparable.

To optimize the operation of our RC-LED in this regard we investigate the dependence of the luminescence intensity on the applied bias as well as on the temperature. We observe resonant tunneling injection of charge carriers into the QDs before the flat band condition of the diode structure is reached [2]. The influence of the dark state of the exciton on the luminescence is studied by comparing experimental data with a rate equation model. This work was partly funded by the SFB 787.

[1] D. Bimberg et. al., IEEE Photonics Journal, 1, 58 (2009)

[2] A. Baumgartner et. al., Phys. Rev. Lett. accepted (2010)

HL 35: Joint Session: Organic Semiconductors II: Solar Cells B

Time: Tuesday 10:30–13:00 Location: ZEU 222

Topical Talk HL 35.1 Tue 10:30 ZEU 222

Modelling charge transport in organic semiconductors — •Denis Andrienko — MPI for Polymer Research, Mainz, Germany

The role of material morphology on charge carrier mobility in partially disordered organic semiconductors is discussed for several classes of materials: derivatives of hexabenzocoronenes,[1] perylenediimides,[2] triangularly shaped polyaromatic hydrocarbons,[3] Alq3,[4] polypyrrole and a variety of organic crystals. Simulations are performed using a package developed by Imperial College, London and MPI for Polymer Research, Mainz (www.votca.org[5]). This package combines: quantum chemical methods for the calculation of molecular electronic structures and reorganization energies; molecular dynamics and systematic coarse-graining approaches for simulation of self-assembly and relative positions and orientations of molecules on large scales; kinetic Monte Carlo and master equation for studies of charge transport.

[1]. J. Kirkpatrick, V. Marcon, J. Nelson, K. Kremer, D. Andrienko, *Phys. Rev. Lett.*, 98, 227402, 2007

[2]. V. Marcon, W. Pisula, J. Dahl, D. W. Breiby, J. Kirkpatrick, S. Patwardhan, F. Grozema, D. Andrienko, *J. Am. Chem. Soc.*, 131, 11426, 2009

[3]. X. Feng, V. Marcon, W. Pisula, M. R. Hansen, J. Kirkpatrick, F. Grozema, D. Andrienko, K. Kremer, and K. Müllen, *Nature Materials* 8, 421, 2009

[4]. A. Lukyanov, D. Andrienko, *Phys. Rev. B*, 82, 193202, 2010

[5]. V. Rühle, C. Junghans, A. Lukyanov, K. Kremer, D. Andrienko, *J. Chem. Theor. Comp.* 5, 3211, 2009

HL 35.2 Tue 11:00 ZEU 222

Performance of density functional theory for donor-acceptor systems: a case study for TTF and TCNQ molecules — •Viktor Atalla[1], Mina Yoon[1,2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany — [2]Oak Ridge National Laboratory, USA

Organic materials are promising candidates for a next generation of electronic devices, since they offer a variety of new intriguing properties. However, from a theoretical point of view these materials are challenging because they are often composed of donor-acceptor systems, for which density-functional theory (DFT) with state-of-the-art exchange-correlation (XC) functionals is often suspected to fail. Here we study the performance of DFT in describing electron affinities, ionization potentials, and charge transfer for clusters of the prototypical electron donor molecule TTF and acceptor molecule TCNQ.

For the indivdual molecules we calculate the dependence of the HOMO and LUMO levels on the fraction of exact exchange and the screening length [1]. We find that conventional semilocal and hybrid XC functionals severely underestimate HOMO-LUMO gaps. For weakly bound TTF-TCNQ dimers all investigated XC functionals consistently give charge transfer from the donor to the acceptor, however the amount of transfered charge is strongly functional dependent - in particular all semilocal functionals have significant aritificial charge transfer in the asymptotic limit.

[1] A. Krukau *et al.*, J. Chem. Phys. **125**, 2006

HL 35.3 Tue 11:15 ZEU 222

Sub-Bandgap Absorption in Polymer-Fullerene Solar Cells — •Martin Presselt[1], Felix Herrmann[1], Marco Seeland[1], Maik Bärenklau[1], Roland Rösch[1], Wichard J. D. Beenken[2], Erich Runge[2], Sviatoslav Shokhovets[1], Harald Hopp[1], and Gerhard Gobsch[1] — [1]Experimental Physics I, Institute of Physics & Institute of Micro- und Nanotechnologies, Ilmenau University of Technology, Weimarer Str. 32, 98693 Ilmenau, Germany — [2]Theoretical Physics I, Institute of Physics, Ilmenau University of Technology, Weimarer Str. 25, 98693 Ilmenau, Germany

We present external quantum efficiency (EQE) studies of P3HT:PCBM based bulk heterojunction polymer solar cells with improved intensity resolution in the sub-bandgap (SBG) region, i.e. the energy range below the optical bandgaps of the pristine materials. Varying the P3HT:PCBM blending ratio, we find that in addition to a Gaussian profile an exponential tail is needed for a quantitative description of the SBG EQE spectra. To gain insights into the origin of the single contributions, absorption and emission spectra covering several decades of intensity and SBG EQE signals are discussed in detail.

HL 35.4 Tue 11:30 ZEU 222

Quantitative analysis of optical spectra and solar cell performance of P3HT:PCBM blends — •Sarah T. Turner, Patrick Pingel, Robert Steyrleuthner, and Dieter Neher — Institute of Physics and Astronomy, University of Potsdam, Germany

The properties of solar cells made from a blend of regioregular poly(3-hexylthiophene) (P3HT) with [6,6]-phenyl-C_{61}-butyric acid methyl ester (PCBM) are known to depend largely on the layer morphology. Here, we present the results of optical studies on P3HT:PCBM blends coated from chloroform and dichlorobenzene with subsequent thermal annealing. A recently established analytical model developed by Spano for the absorption of weakly interacting H-aggregates was used to obtain information about the fraction of crystallized chains, the width of the aggregates, and the energetic disorder in the P3HT phase [1]. In terms of an increased aggregate width and a decreased energetic disorder in the P3HT phase, thermal annealing was found to have little effect on the films prepared from dichlorobenzene and an appreciable effect on the films prepared from chloroform. The results from the model were compared with the performance of solar cell devices and single-carrier devices with the same active layer. Most importantly, the initial increase in P3HT aggregate size upon thermal annealing showed a good correlation with an increase in hole mobility. Further increases in solar cell device performance at higher annealing temperatures were correlated with a decrease in P3HT energetic disorder and an increase in PCBM aggregation.

[1] F.C. Spano, J. Chem. Phys. 2005, 122, 234701.

HL 35.5 Tue 11:45 ZEU 222

Influence of Phase Segregation on the Dynamics of Charge Carriers in Organic Solar Cells — •Andreas Baumann[1], Tom J. Savenije[3], Dharmapura H. K. Murthy[3], Martin J. Heeney[4], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Physical Institute, Julius-Maximilians-University of Würzburg, Am Hubland, D-97074 Würzburg — [2]Bavarian Center for Applied Energy Research (ZAE Bayern), Am Hubland, D-97074 Würzburg — [3]Optoelectronic Materials Section, Department of Chemical Engineering, Delft University of Technology, 2628 BL Delft, The Netherlands — [4]Department of Chemistry, Imperial College London, London, SW7 2AZ, United Kingdom

The morphology of a bulk heterojunction solar cell plays an important role in the dynamics of charge carriers, whereas the donor–acceptor ratio have a great impact on the extent of phase segregation. A fine phase intermixing is believed to be beneficial for an efficient photogeneration. However, the charge transport is strongly related to percolated pathways to the electrodes. We studied the influence of phase segregation on the dynamics in the blend system poly(2,5-bis(3-dodecyl thiophen-2-yl) thieno[2,3-b]thiophene) (pBTCT) mixed with [6,6]-phenyl-C61-butyric acid methyl ester. We used the technique of charge extraction by linearly increasing voltage and transient microwave conductivity to study the macroscopic and microscopic transport properties, respectively. We found an enhanced geminate recombination in the 1:1 ratio blends due to fine phase intermixing, whereas extensive phase segregation in the 1:4 ratio led to an efficient polaron pair dissociation.

HL 35.6 Tue 12:00 ZEU 222

Charge separation at molecular donor-acceptor interfaces: correlation between interface morphology and solar cell performance — •Andreas Opitz, Julia Wagner, Mark Gruber, Ulrich Hörmann, and Wolfgang Brütting — Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

Combinations of organic electron and hole conductive materials are widely used for ambipolar charge carrier transport and donor/acceptor photovoltaic cells. Thereby the efficiency of these excitonic solar cells is correlated to the morphology of the interface between the donor and

the acceptor materials.

In this contribution we show the effect of crystallization behaviour on molecular bulk and planar heterojunction solar cells [1]. Different donor (copper phthalocyanine – CuPc, diindenoperylene – DIP) and acceptor (Fullerene – C_{60}, per-fluorinated copper phthalocyanine – F_{16}CuPc) materials are analysed for their growth morphology in planar and mixed films as well as for their performance in photovoltaic cells. The morphology of the blended layer ranges from molecularly mixed films in the case of the two phthalocyanines to phase-separated films when mixing CuPc or DIP with C_{60}. A corrugated interface is found for bilayered structure of DIP/C_{60} [2]. Additionally a good crystallization behaviour of DIP improves the solar cell performance even for its lower absorption in comparison to CuPc.

[1] A. Opitz et al., IEEE J. Sel. Top. Quant. (2010), early view.

[2] J. Wagner et al. Adv. Func. Mater. (2010), early view.

HL 35.7 Tue 12:15 ZEU 222

Towards Ideal Morphology of Polymer Bulk Heterojunction Solar Cells — •Chetan Raj Singh[1], Michael Sommer[2,3], Marcel Himmerlich[1], André Wicklein[3], Stefan Krischok[1], Mukundan Thelakkat[3], and Harald Hoppe[1] — [1]Institute of Physics, Ilmenau University of Technology, Germany — [2]Department of Chemistry, University of Cambridge, United Kingdom — [3]Applied Functional Polymers, University of Bayreuth, Germany

We present the thorough optimization of block copolymer (BCP) based polymer solar cells utilizing a blend of a self-assembling P3HT-b-PPerAcr BCP and an PPerAcr acceptor homopolymer. As an effect of increasing acceptor content in the block copolymer/homopolymer blend, we observe a continuous rise in the open circuit voltage (Voc) and the short circuit current (Isc) leading to an overall improved photovoltaic performance. The improved performance with increasing acceptor content is attributed to (a) an increase of the acceptor domain size leading to improved charge transport and to (b) a reduced recombination of charge carriers at the cathode interface due to the surface segregation of the acceptor. The surface segregation of the acceptor is identified by atomic force microscopy and X-ray photoelectron spectroscopy. Furthermore we show that by deliberately introducing an acceptor buffer layer at the cathode interface, we are able to control Voc at relatively high values (˜ 640 mV), independently of the bulk heterojunction morphology underneath.

HL 35.8 Tue 12:30 ZEU 222

Triplet Excitons and Cations in dicyanovinyl end-capped quaterthiophenes with varying side chain length — •Christian Koerner[1], Hannah Ziehlke[1], Roland Fitzner[2], Egon Reinold[2], Peter Bäuerle[2], Karl Leo[1], and Moritz Riede[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden — [2]Institut für Organische Chemie II und Neue Materialien, Universität Ulm

Dicyanovinyl end-capped oligothiophenes (DCV-nT) are highly suitable for systematical investigations of energy and charge transfer processes in donor-acceptor blends because of the tunability of electronic and morphological properties by varying e.g. length of backbone or side chains. Moreover, it has been shown to work well as absorber in small molecule organic solar cells (OSC) achieving up to 5.2% power conversion efficiency (PCE) for DCV-5T in a bulk heterojunction (BHJ) device[1].

We use photoinduced absorption spectroscopy (PIA) to probe the long-living (μs-ms) excited states (triplet excitons, cations) after photoexcitation of DCV-nT:C_{60} blends. With PIA, their generation and recombination behaviour can be investigated. Here, we report our results obtained on a series of DCV-4Ts with varying side chains from none to methyl side chains which supposedly mainly influences the morphology of the thin film. We complement our studies by exploring the potential of these materials as absorber layer in planar and BHJ solar cells. For example, DCV-4T without side chains gives an open circuit voltage of 1V and PCEs of 1.9% in a BHJ solar cell with C_{60}.

[1] Fitzner et al., Adv. Func. Mat., accepted

HL 35.9 Tue 12:45 ZEU 222

Surface structure of organic heterojunction solar cells — •M. Zerson[1], E.-C. Spitzner[1], C. Riesch[1], A. Sperlich[2], H. Kraus[2], A. Förtig[2], C. Deibel[2], V. Dyakonov[2], R. Lohwasser[3], M. Thelakkat[3], and R. Magerle[1] — [1]Chemische Physik, TU Chemnitz — [2]Experimental Physics VI, Julius-Maximilians-University of Würzburg — [3]Makromolekulare Chemie I, Univ. Bayreuth

In organic heterojunction solar cells based on P3HT and PCBM, the charge transfer within the active layer as well as the charge transport towards the electrodes are determined by the electronic properties of the interfaces and their microstructure. The surface of semicrystalline polypropylene has been shown to be covered by a thin layer of amorphous material. We aim at investigating potential similarities between organic semiconductors for photovoltaics. We report on 3D depth profiling of the surface structure of different types of P3HT and blends of P3HT with PCBM using amplitude modulation atomic force microscopy. From a map of amplitude-phase-distance curves, the tip indentation into the soft (compliant) amorphous surface layer is measured. This spatial information serves as depth coordinate for reconstructing high resolution cross sections and 3D depth profiles of the top 10 nm of the specimen. Furthermore, the shape of the unperturbed (true) surface and the thickness of the amorphous top layer are determined. The latter is found to be between 4 and 10 nm thick, depending on the type of material and the sample preparation conditions (thermal and solvent annealing). We discuss the impact of the thickness of the amorphous top layer on the efficiency of organic solar cells.

HL 36: Joint Focussed Session: Transparent Conductive Oxides II

Time: Tuesday 11:15–13:15 Location: WIL B122

Topical Talk HL 36.1 Tue 11:15 WIL B122

Experimental Electronic Structure of In_2O_3 and Ga_2O_3 — •Christoph Janowitz — Brandenburgische Technische Universität Cottbus — Humboldt Universität zu Berlin, Institut für Physik

Transparent conducting oxides (TCO's) pose a number of serious challenges. Besides the strive for high quality single crystals and thin films their application has to be preceded by a thorough understanding of their peculiar electronic structure. It is of fundamental interest to understand why materials transparent up to the UV spectral regime behave also as conductors. In this talk two binary oxides -In_2O_3 and Ga_2O_3 from the group of TCO's showing the smallest respectively largest optical gap- will be explored experimentally. The investigations on the electronic structure were performed on high quality n-type single crystals showing carrier densities of 10^{19} cm^{-3} (In_2O_3) and 10^{17} cm^{-3} (Ga_2O_3). Subjects addressed are the determination of the band structure along the high symmetry directions, effective masses and fundamental gap by angular resolved photoemission (ARPES). Also by resonant ARPES and a combination of X-ray photoemission and X-ray absorption complementary information on the orbital character of the valence- and conduction band regime and on the band gap are obtained. The observations are discussed by reference to calculations of the electronic structure and models for the conductivity mechanism.

Topical Talk HL 36.2 Tue 11:45 WIL B122

Transparent Electronics Using Oxide Materials — •Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II

We discuss all-oxide transparent electronic devices, such as diodes, photodiodes, transistors and inverters, based on rectifying, transparent Schottky contacts from metal oxides, transparent semiconducting oxides and transparent substrates. In particular, MESFET devices are presented with crystalline and amorphous oxides as channel, exhibiting low operation voltage and voltage swing. Inverters built from such transistors exhibit high gain (>200). Directions of further research will be discussed.

Topical Talk HL 36.3 Tue 12:15 WIL B122

Optical properties of undoped and doped ZnO — •Axel Hoffmann and Markus R. Wagner — Institut für Festkörperphysik, TU Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

A spectroscopic study of optical transitions and lattice dynamics of ZnO under the influence of external fields is reviewed. A comparative study of different ZnO single crystals and doped and undoped ZnO films reveals pronounced differences in the free and bound exci-

ton luminescence which can be related to different impurity centers and strain levels. A correlation between the localization energies of excitons bound to the same chemical element in the neutral and ionized charge state is reported. The properties of the shallow impurity bound excitons are compared to defect related deeply bound excitons. The lattice dynamics of ZnO crystals are studied by Raman spectroscopy under the influence of external pressure. A variety of important material parameters is derived including high precision values of the hydrostatic pressure coefficients and Grüneisen parameters of all Raman active modes. For the Born transverse effective charge, an incorrect pressure dependence in the literature is discovered and revised. Raman measurements of ZnO single crystals under uniaxial pressure are reported. In combination with the hydrostatic pressure measurements on the same samples, the first experimental determination of the phonon deformation potentials of all Raman active modes in ZnO is achieved.

HL 36.4 Tue 12:45 WIL B122

Thermodynamic stability, stoichiometry and electronic structure of bcc-In_2O_3 surfaces — •Peter Agoston and Karsten Albe — TU Darmstadt, Petersenstr. 32, 64287 Darmstadt

The thermodynamic stability of all experimentally observed low index surfaces of bcc-indium oxide (In_2O_3) have been investigated by means of density functional theory calculations. The effect of a changing environment has been studies as well as the influence of hydrogen and water. It is found that the (001) surfaces have the most complex behavior. For this surface additionally the effects due to dopants (Sn) as well as the in-plane lattice strain has been studied. Finally, scanning tunneling microscopy images are presented and discussed in the light of previous experiments.

HL 36.5 Tue 13:00 WIL B122

Growth and characterization of In_2O_3 single crystals — •Valentina Scherer, Peter Hlawenka, Christoph Janowitz, Alica Krapf, Helmut Dwelk, and Recardo Manzke — Institut für Physik, Humboldt-Universität zu Berlin

The scientific interest in transparent conducting oxides (TCOs) such as ZnO, Ga_2O_3, In_2O_3 and SnO_2 increases significantly. However, information on the electronic structure and the doping behaviour is very scarce. This is in part due to the challenging problem of growing high purity single crystals and substrates for homoepitaxy, which also limits the attainable progress in device production. High quality In_2O_3 single crystals were grown using the chemical vapor transport method (CVT). The crystals were of body centered cubic bixbyite-type structure with a lattice parameter $a = 10.12$. The temperature-dependent resistivity, Hall-constant, and mobility were measured and an electron density in the range of $\sim 10^{19} cm^{-3}$ was determined. The crystals were then investigated using high resolution photoemission and transport measurements. Emission from the valence band and the partially filled conduction band at the Γ-point yielded a direct band gap of ~ 3 eV. The weak conduction band emission near the Fermi edge enabled a Fermi-map and the determination of the Fermi surface. The obtained results are in good agreement with theoretical band structure calculations and with the previously experimental results of the thin films.

HL 37: Joint Focussed Session: Theory and Computation of Electronic Structure: New Frontiers II

Time: Tuesday 11:15–13:00 Location: TRE Phy

Topical Talk HL 37.1 Tue 11:15 TRE Phy

Electronic and Optical Excitations in Magnetic Insulators — •Claudia Rödl, Frank Fuchs, and Friedhelm Bechstedt — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

With the advent of electronic devices exploiting also the spin degree of freedom, magnetic materials attract more and more interest due to potential technological applications. However, describing the excitation properties of insulators with strongly localized and partially occupied d states by means of *ab-initio* methods remains a considerable challenge. Here, we focus on the antiferromagnetic transition-metal oxides (TMO) MnO, FeO, CoO, and NiO and ferromagnetic $CrBr_3$ as prototypical representatives for the class of magnetic insulators.

A perturbative treatment of Hedin's *GW* approximation based on (semi)local approaches to exchange and correlation in the subjacent density-functional calculation fails to reproduce the experimental photoemission spectra. Instead, we use the non-local HSE03 exchange-correlation functional to obtain a reasonable starting point for the *GW* calculation. The spin-polarized extension of the Bethe-Salpeter equation (BSE) is solved to calculate optical absorption spectra including excitonic and local-field effects. The spectra are analyzed in terms of dipole-allowed and dipole-forbidden transitions. For instance, it turns out that the main absorption peaks in the TMOs are due to d-d excitations which are dipole-forbidden at the Γ point. Further, the occurrence of spin-allowed and spin-forbidden Frenkel-like bound excitonic states within the fundamental band gap is investigated.

HL 37.2 Tue 11:45 TRE Phy

LSDA+DMFT calculations of FeNi disordered alloys and Fe/Au(001) thin films — •Jan Minar, Jurgen Braun, Ara Cho, and Hubert Ebert — Dep. Chemie und Biochemie, LMU University of Munich, Germany

The combination of the local spin density approximation (LSDA) and the dynamical mean field theory (DMFT) provide a powerful tool to treat correlations beyond plain LSDA. The KKR or multiple scattering approach implemented on this basis allows among others to deal with alloy and surface systems as well as to study spectroscopic properties on equal footing [1].

Here, we present a LSDA+DMFT study of FeNi disordered alloys using the coherent potential approximation (CPA). In particular the influence of correlation effects on magnetic properties will be discussed. Special emphasis will be put on the additional information supplied by the spin-polarised relativistic mode allowing to deal with the spin-orbit coupling induced properties like orbital magnetic moments and dichroism. A detailed comparison to recent angle resolved photoemission with high resolution [3] allows for a discussion on the influence of correlations with the increasing Ni concentration. In the second part the results of fully self-consistent LSDA+DMFT calculations for the Fe/Au(001) system are presented. In particular the creation of quantum well states has been followed by angular resolved photoemission.

1. J. Minar et al., prb 72, 0415125 (2005), J. Sanchez-Barriga et al., prl 103, 267203 (2009) and Phys. Rev. B 82, 104414 (2010)

HL 37.3 Tue 12:00 TRE Phy

Effective on-site Coulomb interaction in transition metals from constrained RPA — •Ersoy Sasioglu, Christoph Friedrich, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Effective on-site Coulomb interaction (Hubbard U) between localized d electrons in $3d$, $4d$, and $5d$ transition metals are calculated employing the recently developed constrained random-phase approximation (cRPA) within the full-potential linearized augmented plane-wave (FLAPW) method [1] using Wannier functions [2]. The obtained Hubbard U parameters lie between 1 and 5 eV and show a non-monotonic behavior across the transition-metal series. We find that the U depends on the crystal structure, spin polarization, d-electron number and filling of the d orbitals rather than d-character of the elements. For most of the isovalent transition metals, U assumes similar values. The obtained U parameters for the $3d$ series are in good agreement with previous studies as well as available experimental data. Using calculated U parameters we discuss the strength of the electronic correlations and instability of the paramagnetic state towards the ferromagnetic one for $3d$ transition metals. This work has been supported in part by DFG-FOR-1346.

[1] www.flapw.de
[2] F. Freimuth, Y. Mokrousov, D. Wortmann, S. Heinze, and S. Blügel, Phys. Rev. B. **78**, 035120 (2008).

HL 37.4 Tue 12:15 TRE Phy

Ab-initio description of spin-dependent transport in disordered alloys — •Diemo Ködderitzsch, Stephan Lowitzer, and Hubert Ebert — Ludwig-Maximilians-Universität München, Department Chemie und Biochemie, Physikalische Chemie, Butenandtstraße 11, D-81377 München, Germany

Spin-orbit induced couplings are the source of many interesting physical phenomena like the anomalous- and spin-Hall-effects (AHE, SHE), which recently received a lot of attention due to their potential application in the field of spintronics. During the last years several theoretical works have dealt with the intrinsic AHE and SHE, based on the band structure of pure materials and only few of them use a parameter free *ab initio* approach.

We present a coherent *ab initio* description of both, the AHE and SHE, that is applicable to pure **and** disordered alloys by treating all sources, i.e. intrinsic as well as extrinisic contributions, on equal footing. We use an implementation of the Kubo-Středa equation employing the fully relativistic Korringa-Kohn-Rostoker (KKR) Green's function method in conjunction with the Coherent Potential Approximation (CPA) alloy theory. For discussing spin currents we employ our recently devised relativistic spin projection scheme [1] and a corresponding generalization of the Kubo-Středa equation. We illustrate the power and versatility of the approach by giving several examples.

[1] S. Lowitzer, D. Ködderitzsch and H. Ebert, Phys. Rev. B 82, 140402(R) (2010).

HL 37.5 Tue 12:30 TRE Phy

Applying hybrid-functional and many-body methods to rare earths: a study of Cerium — •Marco Casadei[1], Xinguo Ren[1], Joachim Paier[2], Patrick Rinke[1], Angel Rubio[1,3], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der MPG (TH), Berlin, Germany — [2]Humboldt Universitaet (Institut fuer Chemie), Berlin, Germany — [3]UPV/EHV, San Sebastian (Fisica Materiales), Spain

The presence of localized, partially occupied f-electron states dictates many of the peculiar physical properties of rare-earth materials. In particular, the description of the iso-structural α-γ phase transition in Ce metal poses great challenges to density-functional theory (DFT) based approaches since local/semilocal (LDA/GGA) functionals completely fail to produce the phase transition. Here we address this problem by investigating bulk-like Ce clusters of increasing size using hybrid functionals, that incorporate a portion of exact-exchange, and full exact-exchange plus correlation at the level of the random phase approximation (EX+cRPA). In all clusters we find two stable configurations with different lattice constants and distinct electronic and magnetic properties, resembling the bulk situation. However, all hybrid functionals predict that the high volume phase (linked to the γ-Ce phase) is lower in energy at zero temperature, in contrast to experiment. Decreasing the amount of exact-exchange in the hybrid functional eventually restores the correct phase ordering, at the expense of introducing an adjustable parameter. We show that EX+cRPA – a physically meaningful screening of exact-exchange – achieves the same effect from first principles.

HL 37.6 Tue 12:45 TRE Phy

Issues with J-dependence in the LSDA+U method for non-collinear magnets — •Eric Bousquet[1,2] and Nicola Spaldin[1] — [1]Department of Materials, ETH Zurich, Switzerland — [2]Physique Théorique des Matériaux, Université de Liège, B-4000 Sart Tilman, Belgium

We re-examine the commonly used density functional theory plus Hubbard U DFT+U method for the case of non-collinear magnets. While many studies neglect to explicitly include the exchange correction parameter J, or consider its exact value to be unimportant, here we show that in the case of non-collinear magnetism calculations the J parameter can strongly affect the magnetic ground state. We illustrate the drastic J-dependence of magnetic canting, magnetoelectric response and magnetocrystalline anisotropy by calculating trends in the magnetic lithium orthophosphate family $LiMPO_4$ (M = Fe and Ni) and difluorite family MF_2 (M = Mn, Fe, Co and Ni). These results can be readily understood by expanding the usual DFT+U equations within the spinor scheme. On the flip side, it is clear that non-collinear magnetic systems provide a challenging case for testing the correctness of new exchange correlation functionals within the density functional formalism.

HL 38: Polaritons and Polariton Lasing

Time: Tuesday 12:00–13:15 Location: FOE Anorg

HL 38.1 Tue 12:00 FOE Anorg

Non-polar III-nitride microcavities for polariton lasing — •Georg Rossbach[1], Jacques Levrat[1], Amélie Dussaigne[1], Henryk Teisseyre[2], Gatien Cosendey[1], Marlene Glauser[1], Munise Cobet[1], Izabella Grzegory[2], Raphaël Butté[1], Tadeusz Suski[2], and Nicolas Grandjean[1] — [1]ICMP, Ecole Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland — [2]Institute of High Pressure Physics, Polish Academy of Sciences, 01-142 Warsaw, Poland

Owing to their ultra-low effective mass and bosonic character, exciton-polaritons are promising candidates for a significant reduction of the threshold of electrically driven semiconductor coherent light emitters. In this context polariton lasing at room temperature has been demonstrated recently in III-nitride (MCs) under optical pumping. However, due to the hexagonal symmetry of III-nitrides, heterostructures grown along polar orientation suffer from the presence of the quantum-confined Stark-effect. The latter reduces the oscillator strength and the exciton binding energy in wide quantum wells, which can potentially prevent the formation of polaritons. In order to circumvent these effects the growth of non-polar orientations looks well suited even though the achievement of high crystal quality is challenging.

Here, we present first results obtained on a non-polar III-nitride MC grown by molecular beam epitaxy on m-plane bulk GaN. Photoluminescence and reflectivity studies were carried out (in the temperature range 4 - 300 K) showing linear and non-linear effects in the strong light-matter coupling regime combined with a pronounced optical anisotropy as expected from selection rules.

HL 38.2 Tue 12:15 FOE Anorg

From polariton condensates to highly photonic quantum degenerate states of bosonic matter — •Franziska Veit[1], Marc Assmann[1], Jean-Sebastian Tempel[1], Manfred Bayer[1], Arash Rahimi-Iman[2], Andreas Löffler[2], Sven Höfling[2], Stephan Reitzenstein[2], Lukas Worschech[2], and Alfred Forchel[2] — [1]Experimentelle Physik 2, Technische Universität Dortmund,44221 Dortmund — [2]Technische Physik, Physikalische Institut und Wilhelm Conrad Röntgen Research Center for Complex Material Systems, Universität Würzburg, 97074 Würzburg

Bose-Einstein condensation (BEC) of exciton-polaritons in microcavities is considered to be a non-equilibrium process of a degenerate polariton gas in self-equilibrium. We are able to show several key signatures of Bose Einstein condensation BEC without fulfilling the self-equilibrium condition in a highly photonic quantum degenerate non-equilibrium system. Using a planar GaAs/GaAlAs microcavity we observe a buildup of a macroscopic ground state occupation, supressed quantum fluctuations and a linearization of the excitation spectrum.

HL 38.3 Tue 12:30 FOE Anorg

Distinguishing photon and polariton lasing from GaAs microcavities by spectral and temporal analysis of the two-threshold behavior — •Lars Erik Kreilkamp[1], Jean-Sebastian Tempel[1], Franziska Veit[1], Marc Assmann[1], Arash Rahimi-Iman[2], Andreas Löffler[2], Sven Höfling[2], Stephan Reitzenstein[2], Lukas Worschech[2], Alfred Forchel[2], and Manfred Bayer[1] — [1]Experimentelle Physik 2, Technische Universität Dortmund, D-44221 Dortmund, Germany — [2]Technische Physik, Physikalisches Institut, Wilhelm Conrad Röntgen Research Center for Complex Material Systems, Universität Würzburg, D-97074 Würzburg, Germany

We present the excitation-power dependent evolution of the emission of a planar GaAs/GaAlAs microcavity from thermal polariton photoluminescence to polariton lasing and to photon lasing. For the emission from the lower energy-momentum dispersion branch we find a two-threshold behavior of the ground state in the input-output curve where each transition is accompanied by characteristic changes of the in-plane mode dispersion. By studying the second-order correlation

function $g^{(2)}(\tau)$ of the emission, using a streak camera set-up with appropriate time resolution, we show in particular, that the thresholds are unambiguously reflected in the photon statistics. Moreover, the evolution of the emission pulse duration confirms the occurence of two distinct transitions.

HL 38.4 Tue 12:45 FOE Anorg

Magnetic Field Interaction of Exciton-Polaritons in GaInAs Quantum Well-Microcavities — •Arash Rahimi-Iman, Christian Schneider, Julian Fischer, Matthias Amthor, Sven Hoefling, Stephan Reitzenstein, Martin Kamp, and Alfred Forchel — Technische Physik, Universität Würzburg, D-97074 Wuerzburg, Germany

Polaritons formed by excitons and photons in strongly coupled quantum well (QW) semiconductor microcavities have initiated intensive studies of multiple particle physics in solids during the last decade. Bose-Einstein condensation of these quasi particles and the so-called polariton-lasing represent very interesting physical phenomena investigated in different material systems (Deng et al. 2002, Kasprzak et al. 2006). Since condensation is not feasible in ideal 2D systems, it only occurs in planar cavities if natural or artificial traps are provided.

We have studied polariton emission from artificial traps in planar cavities in the presence of external magnetic fields up to 5 T, The work focuses on the interaction of the spin-resolved excitonic component of trapped polaritons due to the Zeeman effect. We report on trap-size dependent Zeeman splittings up to 100 μeV and diamagnetic coefficients up to 0.025 meV/T^2 of exciton-polaritons spatially confined by photonic quantum boxes in a planar single GaInAs QW-microcavity at 5 T. Providing a size variation of the traps ranging from 0.5 to 10 μm on a wide detuning range, quantized polariton modes were observed under non-resonant optical pumping.

HL 38.5 Tue 13:00 FOE Anorg

Balistic exciton polariton propagation in CdZnTe crystals — •Tillmann Godde[1], Ilya Akimov[1], Dimitri Yakovlev[1], Henri Mariette[2], and Manfred Bayer[1] — [1]Experimentelle Physik 2a, Technische Universität Dortmund, 44227 Dortmund, Germany — [2]CEA-CNRS group Nanophysique et Semiconductors, Institute Néel, CNRS and Université Joseph Fourier, 25 Avenue des Martyrs, 38042 Grenoble, France

We study the propagation of lower branch exciton polaritons in 200 μm - 800μm thick $Cd_{0.88}Zn_{0.12}Te$ samples using time resolved photoluminescence (PL) and time of flight techniques. The PL spectrum comprises of two peaks consistent with emission from upper and lower polariton branches with a resonance frequency of $\hbar\omega_0 = 1.664$ eV. The lifetimes of the exciton polaritons in the upper and lower branches are 1.5 ns and 3 ns, respectivly.

In time of flight measurements we observe significant delay of 1 ps optical pulses, which increases to 350 ps at $\hbar\omega = 1.661$ eV in a 745 μm thick sample. Femtosecond-pulses get stretched and allow to obtain the dispersion in a single streak camera measurement. We reproduce the measured delays using a single oscillator model for the lower polariton branch dispersion.

The propagation is ballistic, which follows from the observation of reflected replica pulses. Assuming that the exciton polariton scattering on optical and acoustical phonons is mainly inelastic, we conclude that the propagation is coherent. We estimate the coherence time to be about 300 ps.

HL 39: Photovoltaics: Chalcopyrites I

Time: Tuesday 13:30–15:15 Location: FOE Anorg

HL 39.1 Tue 13:30 FOE Anorg

Excess carrier depths profiles in Cu(In,Ga)(S,Se)$_2$ absorbers from spectral photoluminescence — •Nils Könne[1], Sebastian Knabe[1], Wolfram Witte[2], Dimitrios Hariskos[2], Alexander Meeder[3], and Gottfried H. Bauer[1] — [1]Institute of Physics, CvO University Oldenburg, Germany — [2]Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg (ZSW), Stuttgart, Germany — [3]SULFURCELL Solartechnik GmbH, Berlin, Germany

The polycrystalline structure of chalcopyrite absorbers, such as Cu(In,Ga)(S,Se)$_2$ and their complex metallurgical composition results in lateral and depth dependent inhomogeneities. The spectral photoluminescence (PL) recorded from front and rear side of these chalcopyrite thin-film systems shows a distinct different behavior in particular of the high energy PL-wing which is strongly governed by absorption/emission approaching unity, as well as by re-absorption of emitted PL-photons and their depth dependent origin, say excess carrier depth profile. We define a contrast parameter for the high energy PL-yield of the fluxes recorded from front side and rear side and we proof the origin of the experimental contrast with numerical simulations of spectral PL-yields via Planck's generalized law for different depth profiles of excess carriers and band gap/absorption coefficients. By comparison of experimental contrast parameters with results from numerical simulations we conclude a set of regimes of realistic combinations of depth profiles for excess carriers and band gaps.

HL 39.2 Tue 13:45 FOE Anorg

Investigation of recombinatoric loss mechanisms in Cu(In,Ga)Se$_2$ Thin Film Solar Cells — •Robin Knecht[1], Torben Klinkert[1], Jürgen Parisi[1], Ingo Riedel[1], Raymund Schäffler[2], and Bernhard Dimmler[2] — [1]Thin Film Photovoltaics, Energy- and Semiconductor Research Laboratory, University of Oldenburg, D-26111 Oldenburg — [2]Würth Solar GmbH & Co. KG, Alfred-Leikam-Straße 25, D-74523 Schwäbisch-Hall

Today solar cells based on the compound semiconductor Cu(In,Ga)Se$_2$ (CIGSe) present the highest lab scale efficiency among all thin-film technologies. The performance of elementary cells in photovoltaic modules might however be different due to thicker conductive ZnO:Al window layers, missing anti-reflection coating and occasionally less defined absorber formation on large scales. One approach to improve the elementary cell efficiency is to fine-tune the absorber composition and the in-depth band gap grading. In this work we investigated CIGSe samples with varied absorber composition in order to quantify the minority carrier collection efficiency (CE). CE is directly related to the electron diffusion length $L_{D,n}$ and the characteristics of the space charge region (SCR). $L_{D,n}$ was deduced by relating the inverse internal quantum efficiency to the penetration depth of incident photons and the SCR characteristics were obtained from capacitance-profiling of the samples. Based on these results we discuss the different photovoltaic performance observed for samples with varied CIGSe absorber composition.

HL 39.3 Tue 14:00 FOE Anorg

Dynamics of light-induced changes in CIGSe2 solar cells with electroplated absorber — •Anton Werth[1], Janet Neerken[1], Jörg Ohland[1], Jürgen Parisi[1], Ingo Riedel[1], and Juan Rechid[2] — [1]Carl-von-Ossietzky Universität Oldenburg, Carl-von-Ossietzky-Straße 9-11, D-26129 Oldenburg — [2]CIS Solartechnik GmbH & Co. KG, c/o Aurubis AG, Hovestr. 50, D-20539 Hamburg

In this work we studied the transient evolution of the J-V-characteristics of CIGSe2 solar cells during light soaking (LS). The failure of the dark-light superposition (cross over - CO) evolves already within seconds whereas the positive effect of the LS procedure shows up on large time scales (several hours up to days). We focus on the evolution and relaxation dynamics of these mechanisms in CIGSe2-solar cells with CdS and an alternative buffer layer. The investigations include IV-analysis and space charge profiling on different time scales (miliseconds up to several hours). The influence of the spectral composition of the irradiation used for LS was also considered. We discuss our results in terms of photoinduced changes of the conduction band offset and the metastable interface characteristics of the buffer-absorber interface.

HL 39.4 Tue 14:15 FOE Anorg

Impact of thickness reduction of the ZnO:Al window layer on opto-electronical properties of CIGSSe solar cells — •Jan Keller[1], M. Knipper[1], J. Parisi[1], I. Riedel[1], T. Dalibor[2], and A. Avellan[2] — [1]Thin Film Photovoltaics, University of Oldenburg, D-26111 Oldenburg — [2]AVANCIS GmbH & Co. KG, D-81739 Munich

The application of highly doped transparent conducting oxides in chalcopyrite solar cells requires an optimized trade-off between optical transmission and sheet-conductivity. In this respect we stud-

ied the thickness variation of ZnO:Al films used as window layer in Cu(In,Ga)(Se,S)$_2$ (CIGSSe) thin film solar cells. Thin ZnO:Al layers (200nm) on glass exhibit significantly enhanced transmission at wavelengths λ<400nm while a considerable sub-bandgap absorption at λ>800nm appears in thicker films which is attributed to free charge carrier absorption. The IV-characteristics of CIGSSe solar cells with $d_{ZnO:Al}$=200nm exhibit a strong enhancement of the short-circuit current density J_{SC} (ΔJ_{SC}=3mA) as compared to samples with conventional ZnO:Al-film thickness. However, the reduced parallel (R_p) and increased series (R_s) resistance of samples with thin ZnO:Al-layer cause reduction of the fill factor, which has direct consequences for the series connection of cells in a CIGSSe-module. XRD-diffractograms suggest that the high R_s in thin ZnO:Al is not only related to the thickness but also due to reduced (002)-texture that appears to be beneficial for lateral conductivity. By thermographic investigations we are able to directly locate the cell-regimes responsible for the decreased R_p.

HL 39.5 Tue 14:30 FOE Anorg

Investigation of the initial interface formation between CuInSe2 (112) and ZnO grown by ALD — •Eike Janocha and Christian Pettenkofer — Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Deutschland

The interface between a solar cell absorber and its transparent conductive oxide (TCO) defines the electrical properties and thus the efficiency of chalcopyrite solar cells. Since large conduction band offsets lower the solar cell photocurrent usually a CdS buffer layer is deposited by chemical bath deposition (CBD) between chalcopyrite absorber and TCO. Due to its toxicity and the interruption of the in-line production process by CBD an alternative buffer layer material would be advantageous.

To improve the efficiencies of chalcopyrite solar cells a detailed understanding of the electronic band structure between absorber and TCO is necessary. Therefore, we investigated a model system of a single crystalline CuInSe2 absorber material grown in the technological important (112) orientation by molecular beam epitaxy and an epitaxial ZnO TCO grown layer-by-layer via atomic layer deposition (ALD). ALD is known for being a deposition technique allowing the growth of a single monolayer due to its self-limiting growth characteristics.

In situ characterization of the initial growth has been performed after each ZnO deposition step by photoelectron spectroscopies (XPS/UPS/SR-PES) in an UHV growth and analysis system resulting in a detailed view of the interface formation and binding characteristics of the involved elements.

HL 39.6 Tue 14:45 FOE Anorg

Spatially and time resolved cathodoluminescence spectroscopy of CuGaSe$_2$ — •Torsten Schwarz[1], Mathias Müller[1], Frank Bertram[1], Jürgen Christen[1], Daniel Abou-Ras[2], Thorsten Rissom[2], Thomas Unold[2], and Hans-Werner Schock[2] — [1]Otto-von-Guericke-University Magdeburg, Germany — [2]Helmholtz Zentrum Berlin for Materials and Energy, Germany

The luminescence properties of polycristalline CuGaSe$_2$ as an efficient absorber material for thin film solar cells has been studied comprehensively using spatially and time resolved cathodoluminescence (CL) spectroscopy. The Mo/glass substrate of a complete solar cell grown by a three-stage process was lifted off to investigate the back side of the absorber layer. CL spectra recorded at 6 K, exhibit a strong, dominating emission at 1.64 eV. In addition, an emission peak around 1.57 eV as well as a peak around 1.45 eV is found in several microscopic regions. In excitation density dependent CL measurements a blueshift of 6.4 meV/decade and 4.3 meV/decade for the peaks at 1.64 eV and 1.57 eV is observed as well as a sublinear increase of the peak intensities with slopes of 0.66 and 0.77. ps-time resolved CL was performed using a long rectangular shaped electron excitation pulse of 710 ns width to ensure reaching steady state and a low repetition rate (200 kHz) to reach the thermal equilibrium between the pulses. A redshift in onset (6 meV) and decay (36 meV) is found. Furthermore, monochromatic transients show an increase of the initial lifetime of carrier recombination processes from 10 ns at 1.67 eV up to 150 ns at 1.55 eV. Both are characteristic fingerprints for strong relaxation processes.

HL 39.7 Tue 15:00 FOE Anorg

Luminescence investigation of Cu(In,Ga)Se$_2$solar cells with different Ga-contents grown in a three-stage-process on glass substrate — •Kristin Wendt[1], Mathias Müller[1], Thomas Hempel[1], Frank Bertram[1], Jürgen Christen[1], Daniel Abou-Ras[2], Thorsten Rissom[2], Thomas Unold[2], and Hans-Werner Schock[2] — [1]Institute of Experimental Physics, Otto-von-Guericke-University Magdeburg, Germany — [2]Helmholtz-Zentrum Berlin for Materials and Energy, Germany

A fundamental advantage of Cu(In,Ga)Se$_2$ (CIGS) alloys as absorber materials in thin-film solar cells is their direct band gap energies which can be varied between 1.04 eV (CuInSe$_2$) and 1.68 eV (CuGaSe$_2$). Photoluminescence (PL) spectra of complete CIGS solar cells with a systematic variation of the Ga-content in the absorber layer will be presented. The CIGS cells investigated were grown on a Mo back contact sputtered on soda lime glass and have a Ga-concentration ranging over the entire range from CuInSe$_2$ to CuGaSe$_2$. Samples with Ga-contents between 100 % and 33 % show two broad luminescence bands. In contrast, CuInSe$_2$ exhibits only one broad luminescence band. Each band is composed of two or three different transitions. Varying excitation density over four orders of magnitude results for samples with Ga-content of 0 % and 33 % in a blueshift of the main peak with increasing excitation density. For higher Ga-concentrations, first a blue- and then a redshift of the dominating peak with increasing excitation density is visible. The temperature dependence of the PL spectra is investigated going from 4 K to 300 K.

HL 40: Joint Session: Organic Semiconductors III: Aggregation and Nanostructures

Time: Tuesday 14:00–15:15 Location: ZEU 222

HL 40.1 Tue 14:00 ZEU 222

Substituted Perylene Diimides as Electron Acceptors in Organic Solar Cells: Suppressing Aggregate Formation to Increase Device Efficiency — •Valentin Kamm, Glauco Battagliarin, Ian A. Howard, Michael Hansen, Hans W. Spiess, Alexey Mavrinskiy, Wojciech Pisula, Chen Li, Klaus Müllen, and Frédéric Laquai — Max-Planck-Institut für Polymerforschung, Mainz, Deutschland

Perylene diimide (PDI) is a promising electron acceptor material for high open circuit voltage bulk heterojunction organic solar cells. However, many PDI molecules have the drawback of strong aggregation leading to intermolecular excited state formation that results in exciton trapping. These traps can effectively limit the diffusion of excitons to the interface where charge separation occurs and thus strongly reduce the charge generation efficiency. In this contribution we study the influence of substitution of PDI molecules with side groups attached to the terminal and to the perylene core positions on the formation of aggregates. In particular transient photoluminescence and absorption spectroscopy are used to probe the impact of aggregation on the dynamics of charge generation and recombination in bulk heterojunction solar cells. Besides, AFM, x-ray and solid state NMR techniques are used to get further insight into the solid state morphology of polymer:PDI blends on different length scales. Finally, we correlate the photophysical properties of the PDI derivatives with the efficiency of bulk heterojunction organic solar cells and present unprecedented efficiencies from polymer:PDI solar cells.

HL 40.2 Tue 14:15 ZEU 222

Near-field spectroscopic mapping of the nanoscale phase separation of low band-gap polymer:fullerene blend film — •xiao wang[1], hamed azimi[2], hans-georg mack[1], mauro morana[2], hans-joachim egelhaaf[3], alfred j. meixner[1], and dai zhang[1] — [1]Institute of Physical and Theoretical Chemistry, Auf der Morgenstelle 18, University of Tübingen, Germany — [2]Konarka Austria F&E GmbH, Linz, Austria — [3]Konarka Technologies GmbH, Nürnberg, Germany

We present the study of the influences of the additive 1,8-octanedithiol (ODT) on the nanometer scale morphology and local photophysics properties of low band-gap polymer blends, PCPDTBT and PCBM. Near-Field spectroscopic mapping provides the possibility to obtain si-

multaneously morphology and spectroscopic (photoluminescence and Raman) information correlated with high spatial resolution.[1] We observe the phase separations of the PCPDTBT:PCBM blend film induced by ODT by the dramatically increased PL emission from PCPDTBT that was originally largely quenched, by the fluctuations of spectral features at different locations of the sample surface, by the fibril-shaped topographic features evolve to spherical bumps. The correlations between the local photo physics properties and the morphology of the blend film with/without ODT at both the micrometer and nanometer scales were revealed by the confocal and high-resolution near-field spectroscopic mapping technique. 1.Wang, X.; Zhang, D.; Braun, K.; Egelhaaf, H. J.; Brabec, C. J.; Meixner, A. J. Adv. Funct. Mater. 2010, 20, (3), 492-499.

HL 40.3 Tue 14:30 ZEU 222

High Crystallinity and Nature of Crystal–Crystal Phase Transformations in Regioregular Poly(3-hexylthiophene) — •Ovidiu F. Pascui[1,3], Ruth Lohwassser[2], Michael Sommer[2], Mukundan Thelakkat[2], Thomas Thurn-Albrecht[1], and Kay Saalwächter[1] — [1]Institut für Physik, Martin-Luther-Univ. Halle-Wittenberg, Halle, Germany — [2]Makromolekulare Chemie I, Universität Bayreuth, Germany — [3]Experimentelle Physik III, TU Dortmund, Germany

Molecular weight and stereoregularity affect the morphology and the crystallinity of conjugated polymers and are thus of pivotal relevance for the mobility of charge carriers in electro-optical device applications. We use ^{13}C solid-state NMR to determine the crystallinity and details on crystal–crystal phase transformations in regioregular head-to-tail poly(3-hexylthiophene) of well-defined molecular weight and demonstrate that the crystallinity was previously severely underestimated. Typical crystallinities are at least around 37% for the lowest molecular weights and as high as about 64% upon increasing MW, corresponding to a corrected maximum value for the reference melting enthalpy of $\Delta H_\mathrm{m} \approx 37$ J/g for use in DSC experiments. Using one- and two-dimensional NMR, we observe that the crystal-crystal phase transition between a 3D- and a 2D-ordered crystalline phase at around 60°C entails a structural disordering process of the alkyl side chains, while not affecting the backbones. The formation of the 3D-ordered phase is kinetically suppressed at higher molecular weights.

see: O. F. Pascui et al., *Macromolecules* **43**, 9401 (2010).

HL 40.4 Tue 14:45 ZEU 222

Self-Assembled Ultralong Organic Semiconducting Nano/Microwires — Julia Lambrecht, •Tobat P. I. Saragi, and Josef Salbeck — Macromolecular Chemistry and Molecular Materials (mmCmm), Department of Mathematics and Science and Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, Heinrich-Plett-Strasse 40, D 34132 Kassel, Germany

We report on the simple process in fabrication of spiro-substituted perylene diimide nano/microwires (NMWs) by using self-assembly approach, namely drying under solvent atmosphere. This method results in a controllable number of NMWs on the substrate, which enables us to fabricate single NMW electronic device. Furthermore, we are able to control the growth direction of NMWs by using a structured substrate. An aspect ratio as high as ~9200 can be obtained in our experiment and the longest wire is determined to be 5.5 mm. The resistivity of the single NMW is characterized and the value is in the range of 100 Ohm m and 10000 ohm m.

HL 40.5 Tue 15:00 ZEU 222

Plasmonic enhancement of light absorption in organic semiconductors using silver nanowire arrays — •Matthias Handloser[1], Ricky Dunbar[2], Philipp Altpeter[2], Lukas Schmidt-Mende[2], and Achim Hartschuh[1] — [1]Department Chemie and CeNS, Ludwig-Maximilians-Universität, München, Germany — [2]Department Physik and CeNS, Ludwig-Maximilians-Universität, München, Germany

Plasmonics can be used to improve light absorption in photovoltaic devices, permitting a considerable reduction in the physical thickness of absorber layers, and yielding new options for solar-cell design [1]. We investigated arrays of aligned silver nanowires embedded in different organic polymers via confocal microscopy in combination with Time Correlated Single Photon Counting (TCSPC) and Pump-Probe techniques. The wires had a length of 10 um, a height of 20 nm, and variable widths and spacings. Thin films of different organic semiconductors were then deposited onto these arrays. Plasmon modes were excited through one and two photon absorption between 500 to 900 nm and photoluminescence maps and transients of the arrays were recorded. We observed a clear correlation between photoluminescence intensity, lifetime and nanowire spacing. We analyzed our data to distinguish between absorption and radiative rate enhancement and energy transfer to the metal followed by quenching. [1] H.A.Atwater, A.Polman, Nature Materials 9, 205 (2010)

HL 41: Nitrides: InGaN

Time: Tuesday 14:15–15:15 Location: POT 51

HL 41.1 Tue 14:15 POT 51

Systematics of nonradiative recombination in blue and green emitting GaInN/GaN quantum wells — •Torsten Langer, Andreas Kruse, Markus Göthlich, Holger Jönen, Heiko Bremers, Uwe Rossow, and Andreas Hangleiter — Institut für Angewandte Physik, Technische Universität Braunschweig

Light emitters based on GaInN/GaN quantum wells (QW) exhibit a strong drop of efficiency for increasing peak emission wavelengths known as "green gap". In this contribution, we analyze its origin by temperature dependent time-resolved photoluminescence spectroscopy, separating non-radiative and radiative contributions to the carrier recombination processes. We control the peak emission wavelength by varying the indium mole fraction x_In between 18% and 38%. The QW thickness is kept below 2 nm to reduce both the risk of lattice relaxation and the diminishing influence of piezoelectric fields on the oscillator strength (especially for c-plane QWs). While the influence of piezoelectric fields is experimentally observed by an increase of radiative lifetimes towards higher x_In and thicker QWs, a strong reduction of nonradiative lifetimes τ_nr occurs for high x_In ($> 25\%$). As the experiments were performed in the low carrier density regime, the nonradiative recombination rate $R_\mathrm{nr} \propto 1/\tau_\mathrm{nr}$ is of defect-related nature following an exponential temperature dependence $R_\mathrm{nr} \propto \exp(-E/(kT))$ with an activation energy E. We compare the lifetimes of uncapped multi quantum well (MQW) structures with efficiency optimized structures as well as samples grown on different substrates: sapphire and HVPE-grown pseudo-bulk GaN.

HL 41.2 Tue 14:30 POT 51

Preparation of reconstructed $\mathbf{In_xGa_{1-x}N(0001)}$ surfaces — •C. Friedrich[1], A. Biermann[1], V. Hoffmann[2], N. Esser[1,3], M. Kneissl[1], and P. Vogt[1] — [1]TU Berlin, Inst. f. Festkoerperphysik EW6-1, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Ferdinand-Braun-Institut, Leibniz-Institut, Gustav-Kirchhoff-Str. 4, 12489 Berlin, Germany — [3]Leibniz-Inst. fuer Analytische Wissenschaften - ISAS e.V., Albert-Einstein Str. 9, 12489 Berlin, Germany

The $In_xGa_{1-x}N(0001)$ is a promising alloy system to investigate the principal mechanisms for the formation of group-III-nitride surface reconstructions, such as metal adlayer formation on reconstructed GaN(0001) or intrinsic surface electron accumulation on InN(0001). However, there is still not much known about the atomic structure of $In_xGa_{1-x}N(0001)$ grown by metal organic vapour phase epitaxy (MOVPE) mainly because the preparation of such surfaces is crucial for measurements in ultra high vacuum (UHV). Here were present results on $In_{0.15}Ga_{0.85}N(0001)$ surfaces after annealing under UHV conditions and alternatively in nitrogen plasma at temperatures between 500 °C and 800 °C. Auger electron spectroscopy, low energy electron diffraction and atomic force microscopy measurements were performed to elucidate the chemical composition, symmetry and morphology. On clean surfaces we obtained a (1+1/6) symmetry similar to the pseudo-(1×1) surface as reported for GaN(0001). By changing the preparation conditions a (2×2) and $(\sqrt{3}\times\sqrt{3})$R30° symmetry is formed. All surfaces exhibit different group-III to group-V ratios and differ significantly in morphology and roughness.

HL 41.3 Tue 14:45 POT 51

InGaN quantum wells in quaternary AlInGaN barriers — •Julian Mack, Clemens Wächter, Alexander Meyer, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen and Research Center SCoPE, University of Stuttgart, Pfaffenwaldring 57, D-70569 Stuttgart, Germany

The luminescence efficiency of green emitting InGaN quantum wells grown in between c-plane GaN barriers suffers from strong electrical fields. To overcome this problem we have grown InGaN quantum wells embedded in quaternary AlInGaN barriers by metal-organic vapor phase epitaxy. By using a growth sequence for the barriers with pulsed metal-organic supply we enhanced the photoluminescence efficiencies of these structures. The amount of material was varied, resulting in AlInGaN barriers with constant thickness and indium contents between 1% and 20%. We have analyzed the material properties by x-ray diffraction (XRD) and ensemble photoluminescence (PL) measurements. The observed XRD-spectra and the PL-intensity show the high quality of the deposited material. The Pl spectra of the InGaN quantum wells shift from 2.60 eV to 2.75 eV with decreasing indium content of the barrier. This shift can be attributed to a reduction of the internal electric fields at the heterointerface between InGaN and AlInGaN and the associated quantum confined stark effect (QCSE).

HL 41.4 Tue 15:00 POT 51

effect of mocvd growth parameters on high In content InGaN layers — •öcal tuna[1], hannes behmenburg[1,2], christoph giesen[1], egidijus sakalauskas[3], rüdiger goldhahn[3], holger kalisch[2], rolf h. jansen[2], and michael heuken[1,2] — [1]AIXTRON AG, Kaiserstr. 98, 52134 Herzogenrath, Germany — [2]Chair of Electromagnetic Theory, RWTH Aachen University, Kackertstr. 15-17, 52072 Aachen, Germany — [3]Institut für Micro- und Nanotechnologien, Technische Universität Ilmenau, PF 100565, 98684 Ilmenau, Germany

In this study, several growth parameters have been varied to investigate MOCVD of high-quality InGaN bulk layers using AIXTRON reactors. TMIn, TMGa and NH3 have been used as precursors, N2 as carrier gas and GaN layers as templates. Structural and optical properties have been studied by X-ray diffraction, atomic force microscopy and spectroscopic ellipsometry, respectively. The growth temperature increment from 705 to 755oC results in higher crystal quality but reduced In incorporation due to the low InN dissociation temperature. Also the effect of TMIn and TMGa flows on InGaN growth was investigated. With increasing TMIn flow from 2.5 to 4.4 *mol/min, In incorporation increased from 11.5% to 16.3% without diminishing quality (clear layer fringes observed in ω-2θ X-ray scans). Increasing TMGa flow causes a growth rate enhancement from 22 nm/hr to 37 nm/hr and a simultaneous increment of In content from 16.8% to 17.4% which were calculated by fitting ω-2θ X-ray scans. Even at that high In content, we still have fully strained InGaN layers with observable layer fringes and low RMS roughness around 1.1 nm.

HL 42: Focussed Session: Inorganic/Organic Semiconductor Hybrid Structures II

Time: Tuesday 14:15–15:15 Location: POT 151

Invited Talk HL 42.1 Tue 14:15 POT 151

Interfacial charge-carrier energetics probed by electromodulated absorption spectroscopy: implication for organic-inorganic hybrid photovoltaic devices — •Peter Ho — Dept of Physics, National University of Singapore

The transition from vacuum-level alignment to Fermi-level pinning of the organic semiconductor contact as the work function of the "metallic" electrode crosses a certain threshold value has been well-established by numerous careful ultraviolet photoemission spectroscopy stuides. In this talk, I will discuss the use of electromodulated absorption spectroscopy to probe this transition within the devices directly through the built-in potential measured at the Stark feature, and also the interface polaron density measured in the subgap. Therefore the results are particularly relevant to the operation of light-emitting diodes and photovoltaic cells. We found that the pinning crossover occurs surprisingly at different work-function threshold values. The implications of this result for energy-level alignment and contact optimisation in light-emitting diodes and photovoltaic devices, and in hybrid inorganic-organic semiconductor photovoltaic devices, will also be discussed.

Invited Talk HL 42.2 Tue 14:45 POT 151

Organic layers on Si, SiC, and diamond substrates: structural and electronic properties — •Martin Stutzmann, Ian D. Sharp, Jose Antonio Garrido, and Martin S. Brandt — Walter Schottky Institut, Technische Universität München, Am Coulombwall 4, 85748 Garching, Germany

In this contribution, we address the structural and electronic properties of hybrid heterostructures of organic functional layers on silicon, silicon carbide, and diamond substrates. For the covalent grafting of alkenes or phenyls on H- or OH-terminated surfaces, distinct differences in the reactivity of the different substrates and the quality of the resulting self-assembled monolayers are observed. These surfaces can be further functionalized with proteins such as enzymes or photosystems to investigate charge transfer processes between the solid substrate and the bioorganic layer. In addition, we have investigated the electronic properties of thin films of P3HT or pentacene deposited on Si, SiC, and diamond by spin coating or organic MBE. Based on current-voltage characteristics of such heterojunctions in the dark and under illumination we discuss basic questions of band alignment and charge transfer at the different heterointerfaces.

HL 43: Spin-dependent Transport II

Time: Tuesday 14:30–15:15 Location: POT 251

HL 43.1 Tue 14:30 POT 251

Electrical Spin injection into Zinc Oxide — •Christoph Schwark[1,3], Christian Weyer[1,3], Gernot Güntherodt[1,3], Matthias Althammer[2], Sebastian T.B. Goennenwein[2], Matthias Opel[2], Rudolf Gross[2], and Bernd Beschoten[1,3] — [1]II. Physikalisches Institut A, RWTH Aachen University, Aachen, Germany — [2]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [3]JARA - Fundamentals of Future Information Technology, Aachen, Germany

We have investigated the feasibility of electrically injecting spin-polarized carriers into ZnO. For this purpose we have used Co/n-ZnO heterostructures deposited on sapphire substrates by pulsed laser deposition. Electrical spin injection was demonstrated at 10 K by optical means using Kerr rotation measurements in Hanlé geometry. Spin injection can be observed up to a temperature of 35 K with a temperature independent spin dephasing time of 1 ns, which has been determined from the width of the Hanlé curves.

Financial support by DFG through SPP 1285 is gratefully acknowledged.

HL 43.2 Tue 14:45 POT 251

Doping density dependence of electron spin relaxation in bulk wurtzite GaN — •Jan Heye Buss, Jörg Rudolph, Sebastian Starosielec, and Daniel Hägele — AG Spektroskopie der kondensierten Materie, Ruhr-Universität Bochum, Bochum, Germany

GaN is a prototypical wide-gap semiconductor with wurtzite structure. Nevertheless, the spin relaxation for moderate to very high doping densities has not been investigated so far. We measure the doping density dependence of electron spin relaxation in 11 different n-type bulk wurtzite GaN samples by time-resolved Kerr-rotation measurements up to a density of 1.5×10^{19} cm^{-3}. The spin relaxation time shows a non-monotonic dependence on doping density, with a decrease of the spin lifetime for increasing doping density in the highly degenerate regime. The decrease in spin lifetimes is much less dramatic

than the decrease known from zincblende semiconductors. We present an analytical expression for the density-dependent spin relaxation tensor in wurtzite semiconductors based on Dyakonov-Perel theory in the degenerate regime that shows good agreement with the experiment.

HL 43.3 Tue 15:00 POT 251

Long room-temperature electron spin lifetimes in highly doped cubic GaN — •Jörg Rudolph[1], Jan Heye Buss[1], Thorsten Schupp[2], Donat As[2], Klaus Lischka[2], and Daniel Hägele[1] — [1]AG Spektroskopie der kondensierten Materie, Ruhr-Universität Bochum, Germany — [2]Universität Paderborn, Department Physik, Warburger Str. 100, 33095 Paderborn, Germany

The wide-gap semiconductor GaN is a promising material for spin-optoelectronic applications in the blue spectral region. The metastable cubic phase of GaN is especially interesting due to its higher symmetry and therefore weaker spin-orbit coupling as compared to the wurtzite phase. We demonstrate very long electron spin relaxation times in highly n-doped cubic GaN ($n_D = 1 \times 10^{19}$ cm^{-3}) exceeding 500 ps up to room-temperature. Time-resolved Kerr-rotation measurements show an almost temperature independent spin relaxation time between 80 and 295 K [1], confirming an early prediction of Dyakonov and Perel for a degenerate electron gas.

[1] J. H. Buß et al., Appl. Phys. Lett. **97**, 062101 (2010)

HL 44: Poster Session I

Time: Tuesday 18:00–21:00 Location: P3

HL 44.1 Tue 18:00 P3

Antiferromagnetic semiconductor LiMnAs — Vit Novak[1], Tomas Jungwirth[1], Miroslav Cukr[1], •Stepan Svoboda[1,2], Zbynek Soban[1,3], Xavier Marti[2], Vaclav Holy[2], Petra Horodyska[2], and Petr Nemec[2] — [1]Institute of Physics AS CR, Cukrovarnicka 10, Praha, Czech Republic — [2]Charles University, Ke Karlovu 5, Praha, Czech Republic — [3]Czech Technical University, Technicka 2, Praha, Czech Republic

LiMnAs belongs to the theoretically predicted class of I-Mn-V semiconductors with the antiferromagnetic ordering of Mn atoms. We report its first successful preparation in form of a thin film by molecular beam epitaxy. Structural properties of the material were examined in-situ by RHEED, and ex-situ by XPS and XRD, confirming the tetragonal crystal structure with its [100] direction oriented along the [110] direction of the InAs substrate. Transparency of LiMnAs in the spectral range of 870 to 1400 nm confirms the existence of an optical gap and indicates the band-gap energy above 1.4 eV. Magnetic properties measured by SQUID magnetometry show nearly compensated net magnetic moment in temperatures up to 400 K and magnetic fields up to 7 T, in a clear contrast to the ferromagnetic character of MnAs or to the paramagnetic behavior of the same amount of uncoupled Mn atoms.

HL 44.2 Tue 18:00 P3

Electric field induced transition phenomena in phase change materials — •Martin Wimmer, Gunnar Bruns, Philipp Merkelbach, Carl Schlockermann, Martin Salinga, and Matthias Wuttig — I. Physikalisches Institut (IA), RWTH Aachen University

Phase change materials have already been successfully applied in rewriteable optical media like DVD-RW and Blu-ray RW. Prototypes of electrical storage devices based on phase change memories provide key features like non-volatility and ultrafast read and write speeds. The information is stored by the distinct difference of optical or electrical properties between the amorphous and crystalline structure.

The electrical switching behaviour of GeSbTe-based phase change memory devices needs to be investigated. The phenomenon of threshold-switching, a sudden drop in resistivity in the picosecond timescale at high electric fields, is important for applications, in particular if high data transfer rates are required. To investigate very fast switching events, a high frequency optimised setup for electrical testing has been established. Time resolved measurements on the picosecond timescale during the switching process are performed, which provide detailed knowledge of the electronic switching mechanism.

HL 44.3 Tue 18:00 P3

Drift in amorphous phase change materials — •Rüdiger M. Schmidt, Gunnar Bruns, Jennifer Luckas, Carl Schlockermann, Martin Salinga, and Matthias Wuttig — I. Physikalisches Institut (IA), RWTH Aachen University

While phase change materials have been successfully applied in rewriteable data storage, they are also used for novel non-volatile electronic data storage devices. The material has the ability to be switched within nanoseconds between the two phases, which show a large optical and electrical contrast. The low resistive crystalline phase is associated with a logic zero state and the high resistive amorphous phase with a logic one state.

While the resistance of the crystalline phase does not change over time, the amorphous phase shows a resistance drift with time and temperature. This drift needs to be understood, especially in order to increase the storage density by employing multi level storage. To gain a deeper insight into the temperature and time dependant drift phenomena, a custom made setup was designed. The setup can perform measurements of sheet resistances up to 100 GΩ in a temperature range from 300 K to 625 K and has a temperature stability of 0.01 K. Our results show that drift is correlated to the activation energy and the number of bond-bending and bond-stretching constraints.

HL 44.4 Tue 18:00 P3

Black silicon with femtosecond double laser pulses — •Anna Lena Baumann[1], Thomas Gimpel[2], Kay-Michael Günther[2], Christian Lehmann[3], Augustinas Ruibys[1], Stefan Kontermann[1], and Wolfgang Schade[1,2] — [1]Fraunhofer Heinrich-Hertz-Institute, Am Stollen 19, 38640 Goslar — [2]Clausthal University of Technology, EFZN, EnergieCampus, Am Stollen 19, 38640 Goslar — [3]FU Berlin, Fachbereich für Physik, Arnimallee 14, 14195 Berlin

We investigate the influence of double femtosecond laser pulses on topology, absorption, series and shunt resistance of p-doped silicon in 500 Torr SF_6. A Michelson interferometer splits the laser pulses into pairs. The topology of p-doped silicon processed with laser pulse pairs at delay times from $\Delta t = 16$ fs to 30000 fs is different from single pulse black silicon, but similar for all delay times greater $\Delta t = 0$ fs. We process samples with 5 and 500 laser pulses per spot at delay times $\Delta t = 50$ fs and $\Delta t = 100$ fs. Optical characterization reveals the absorption characteristics in the visible and near-infrared range. We metalize the samples with an indium front and an aluminum back contact and measure series and shunt resistance. Overall absorption is greater for 500 pulse samples. In the visible range 5 pulse samples at $\Delta t = 50$ fs have slightly higher absorption. In the near-infrared both 5 and 500 pulse samples at $\Delta t = 100$ fs exhibit higher absorption values, with a difference greater 10% for the 5 pulse samples. All samples feature similar series and shunt resistance for the two delay times, while all 5 pulse samples display increased shunt resistance values.

HL 44.5 Tue 18:00 P3

Visibility of graphene on gadolinium and dysprosium oxide thin films — •I. Petrov[1], T. Toader[1], C. Bock[1], U. Kunze[1], A. Milanov[2], A. Devi[2], R. A. Fischer[2], L. Thekkekara[3], D. A. Schmidt[3], and M. Havenith[3] — [1]Werkstoffe und Nanoelektronik, Ruhr-Universität Bochum — [2]Anorganische Chemie II, Ruhr-Universität Bochum — [3]Physikalische Chemie II, Ruhr-Universität Bochum

In this work we study the visibility of monolayer graphene exfoliated on gadolinium (Gd_2O_3) and dysprosium oxide (Dy_2O_3), respectively. The rare earth oxides are deposited by thermal chemical vapour deposition on top of a highly n-doped silicon substrate. Due to the higher dielectric constant of the rare earth oxides ($\epsilon_r \approx 8-9$) compared to SiO_2 ($\epsilon_r = 3.9$), we expect an improved screening of charged impurities [1] for graphene-based devices and therefore an enhanced charge carrier mobility. In order to identify the monolayer graphene on the rare earth oxides we calculated the contrast as a function of the wavelength for different oxide thicknesses using a Fresnel-law-based model [2]. The thickness of the flakes is measured by atomic force microscopy while the contrast of the flakes for several wavelengths is determined by optical microscopy. Finally, Raman spectroscopy was performed to verify the exact thickness of the graphene flake. The calculated contrast val-

ues are in good agreement with the experimental data, proving optical microscopy is reliable identification tool for monolayer graphene.

[1] S. V. Morozov, *et al.*, Phys. Rev. Lett. **100**, 016602 (2008).
[2] P. Blake, *et al.*, Appl. Phys. Lett. **91**, 063124 (2007).

HL 44.6 Tue 18:00 P3

Ab initio study of the phase-change magnetic material — Yan Li and •Riccardo Mazzarello — RWTH Aachen, Aachen, Germany

Phase-change materials based on chalcogenide alloys are of great technological importance due to their ability to undergo reversible and fast transitions between the amorphous and crystalline phases upon heating. This property, together with the strong optical and electronic contrast between the two phases, is exploited in rewritable optical discs (CDs, DVDs, Blu-Rays discs) and prototype non-volatile memories. Up to now, very few works have addressed the properties of chalcogenide phase change materials doped with magnetic impurities. In [1] it was shown that Ge_2Sb_2Te_5 doped with Fe exhibits phase-change behavior for not too large concentrations of Fe and that both the amorphous and the crystalline phases are ferromagnetic at low enough temperatures. Moreover, the two phases were found to have different ferromagnetic properties. However, very little is known about how magnetic impurities affect the atomic-scale mechanisms of the phase transition in these systems and also about the relationship between magnetism and structural properties. To shed light on these issues, we have investigated the structural, electronic and magnetic properties of amorphous and crystalline Ge_2Sb_2Te_5 doped with magnetic impurities from first principles. Models of the amorphous phases were generated by quenching from the melt by means of ab-initio molecular dynamics simulations. [1] W. Song, L. Shi, X. Miao and C. Chong, Adv. Mater. 20, 2394 (2008)

HL 44.7 Tue 18:00 P3

Optical Transitions in the Charged NV^--Center in Diamond — •Florian Hilser and Guido Burkard — University of Konstanz

The electronic configuration of the NV^--center in diamond is well known from spectroscopic data and the electronic states are established theoretically by linear combination of sp^3-hybridized dangling bonds forming p-like orbitals [1]. Spin-orbit interaction and strain lead to orbital symmetry-breaking and the degeneracy of the electronic states is lifted. The ordering of energy levels is determined using group theoretical considerations [2]. Furthermore the energies of the degenerate spin-triplet-states can be split by applying a magnetic field. We determine the electric dipole matrix elements for optical excitation and derive an effective Hamiltonian for optically induced spin-flip transitions.

[1] A. Lenef, S. Rand, Phys. Rev. B **53**, 13441 (1996).
[2] J. R. Maze, A. Gali, arXiv 1010.1338v1.

HL 44.8 Tue 18:00 P3

Dynamische Separation von Kohlenstoffnanoröhren — •Frieder Ostermaier, Juliane Posseckardt und Michael Mertig — TU Dresden, Professur für Physikalische Chemie, Mess- und Sensortechnik, 01062 Dresden, Germany

Einwandige Kohlenstoffnanoröhren (SWCNT) haben aufgrund ihrer besonderen elektronischen Eigenschaften großes Potenzial als Bausteine einer zukünftigen nanoskaligen Elektronik. Metallische mSWCNT sind dabei als Leiterbahnen geeignet und halbleitende scSWCNT können zur Herstellung von Feldeffekttransistoren verwendet werden. Für diese Anwendungen ist es erforderlich, SWCNT mit definierten elektronischen Eigenschaften zur Verfügung zu stellen. Bisher gibt es allerdings noch kein Herstellungsverfahren, das nur mSWCNT oder nur scSWCNT produziert. Deshalb ist eine Sortierung der SWCNT für technische Anwendungen unbedingt erforderlich. Mit bekannten Batch-Verfahren, wie der Dichtegradienten-Ultrazentrifugation, können nur geringe Mengen sortierter SWCNT hergestellt werden.

Wir haben deshalb die kontinuierliche Sortierung von SWCNT durch Dielektrophorese (DEP) in einem mikrofluidischen Kanal untersucht. Dabei wird eine quer zur Strömung gerichtete DEP-Kraft genutzt, die oberhalb einer Grenzfrequenz für mSWCNT und scSWCNT ein unterschiedliches Vorzeichen besitzt.

Zur Dispergierung der SWCNT wurde Sodiumcholat und das organische Lösungsmittel N-Methyl-2-pyrrolidon verwendet. Letzteres ermöglicht die Sortierung bei sehr viel kleineren Frequenzen. Zur Analyse der sortierten Dispersionen wurde UV/VIS-Spektroskopie verwendet.

HL 44.9 Tue 18:00 P3

Phonon dynamics in graphite observed with time-resolved terahertz spectroscopy — •Martin Scheuch[1,2], Konrad von Volkmann[1,3], Luca Perfetti[4], Tobias Kampfrath[2], Christian Frischkorn[1,2], and Martin Wolf[2] — [1]Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin — [2]Fritz-Haber-Institut der MPG, Faradayweg 4-6, 14195 Berlin — [3]APE GmbH Plauener Str. 163-165 Haus N, 13053 Berlin — [4]Laboratoire des Solides Irradiés, Ecole polytechnique, 91128 Palaiseau cedex, France

Time-resolved terahertz spectroscopy in the range from 10 to 30 THz is used to monitor the relaxation of highly oriented pyrolytic graphite (HOPG) that has been excited by a laser pulse (wavelength 790 nm, duration 10 fs). The measured pump-induced changes in the complex dielectric function $\Delta\varepsilon(\omega)$ show that most of the electron excess energy is transferred to few strongly coupled optical phonon modes (SCOPs) on a sub-picosecond timescale. Cooling of the hot SCOPs occurs on a picosecond time scale [1]. Temperature-dependent measurements of the SCOP lifetimes in the range from 10 to 300 K were performed to identify the decay into A_1' and E_{2g} phonons. The results are in agreement with theoretical predictions [2] and show that the A_1' mode at the K point provides the dominant relaxation channel. Additional measurements on naturally grown graphite show no differences to HOPG.

[1] T. Kampfrath *et al.*, Phys. Rev. Lett. **95**, 187403 (2005); [2] N. Bonini *et al.*, Phys. Rev. Lett. **99**, 176802 (2007)

HL 44.10 Tue 18:00 P3

Controlling exciton decay in semiconducting carbon nanotubes by surface acoustic waves — Markus Regler[1,2], Hubert J. Krenner[2], Alexander A. Green[3], Mark C. Hersam[3], Achim Wixforth[2], and •Achim Hartschuh[1] — [1]Department Chemie & CeNS, Ludwig Maximilians Universität München, Germay — [2]Department Physik, Universität Augsburg, Germany — [3]Department of Materials Science and Engineering, Northwestern University, Evanston, Illinois, USA

Single-walled carbon nanotubes (SWNTs) are quasi-1 dimensional direct-bandgap materials with unique properties making them promising candidates for a variety of technological applications including photonics, optoelectronics and sensing. The excited states of semiconducting SWNTs are formed by strongly bound luminescent excitons that can be populated either by light absorption or electrically [1]

We show that the decay dynamics of excitons in SWNTs can be controlled by surface acoustic waves (SAWs) launched in piezoelectric substrates. The photoluminescence (PL) intensity of nanotube films deposited on LiNbO3 was found to be reduced by up to 40% depending on the SAW amplitude. Time-resolved PL measurements reveal that the intensity reduction is caused by a SAW-induced decrease of the radiative exciton recombination rate that results from the electric fields associated with the SAW.

[1] P. Avouris, M. Freitag, V. Perebeinos, Nature Photon. 2, 341 (2008)

HL 44.11 Tue 18:00 P3

Magnetotransport Studies of Graphene on GaAs — •Nils Gayer, Karen Peters, Alina Tittel, Andreas Graf, Vera Paulava, Ursula Wurstbauer, and Wolfgang Hansen — Institut für Angewandte Physik und Zentrum für Mikrostrukturforschung, Universität Hamburg, Germany

We study graphene on GaAs substrates, the preferred material for ultrafast and optical device applications. With temperature dependent magnetotransport measurements the influence of the GaAs substrates on the properties of graphene is investigated. Our substrates contain a Si-doped GaAs backgate grown by means of molecular beam epitaxy. The investigated graphene flakes were prepared by mechanical cleavage of natural graphite. Due to the very low contrast of graphene on GaAs, we established a method to enhance the visibility of graphene that facilitates the detection of graphene on this substrate using optical microscopy. For this purpose, the prepared graphene samples are spin-coated with PMMA e-beam resists of optimized layer thickness. We demonstrate that it is possible to determine the number of layers of graphene on GaAs even through the PMMA resist layer using Raman spectroscopy. We discuss our findings as well as according calculations of the contrast of graphene on GaAs as a function of the wavelength of the incident light and the PMMA layer thickness.

HL 44.12 Tue 18:00 P3

Micromechanical sensor for magnetization studies on few layer graphene — •Amadeus K. Mlynarski[1], Paul Berberich[1], Matthias Brasse[1], Karthik Sridhara[1], Benedikt Rupprecht[1],

Stefanie Heydrich[2], Marc A. Wilde[1], and Dirk Grundler[1] — [1]Lehrstuhl für Physik funktionaler Schichtsysteme, Technische Universität München, Physik Department, James-Franck-Str. 1, D-85747 Garching b. München, Germany — [2]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, D-93040 Regensburg

Graphene is a strictly two-dimensional material exhibiting novel electronic properties due to its peculiar band structure. For graphene, magnetic edge states, a diverging magnetic susceptibility around the charge neutrality point and an unconventional de Haas - van Alphen effect have been predicted. Measuring the magnetization $M = -\partial U/\partial B$ for a temperature T→0 yields direct access to the ground state energy U of the charge carriers in graphene. Thermodynamic energy gaps in the density of states between neighboring Landau levels can be measured directly.

We intend to measure M of chemical-vapor-deposited few layer graphene (FLG) down to 300 mK and high magnetic fields up to 16 T. The FLG is characterized using magnetotransport measurements prior to the magnetization experiments. A specially designed micromechanical sensor is fabricated to allow for high sensitive magnetization measurements.

We thank the DFG for financial support in the SPP1459 grant no. WI3320/1-1.

HL 44.13 Tue 18:00 P3

Spin orbit mediated entanglement in graphene — •Alexander Lopez[1,2] and John Schliemann[1] — [1]Institute for Theoretical Physics, University of Regensburg, D-93040 Regensburg, Germany — [2]Centro de Fisica, Instituto Venezolano de Investigaciones Cientificas, Apartado 21874, Caracas 1020-A, Venezuela

We analyze the Spin-Orbit mediated two and three qubit entanglement production in single layer graphene. We found the striking result that, within experimentally feasible parameter values, it is possible to thermally increase the two qubit quantum concurrence, even near room temperature. We also find a cooperative effect resulting from the interplay of scattering and SO coupling. The experimental and technologically relevant implementations are further discussed.

HL 44.14 Tue 18:00 P3

Crystallographically Anisotropic Etching of Graphene — •Florian Oberhuber, Dieter Weiss, and Jonathan Eroms — Institute for Experimental and Applied Physics, University of Regensburg

We report crystallographically anisotropic carbothermal etching of graphene on SiO_2 substrates in an argon gas flow at atmospheric pressure. The samples were prepatterned with antidot lattices by electron beam lithography and reactive ion etching. The hexagonal form of the antidots obtained by the carbothermal reaction suggests the absence of armchair edges [1]. We studied the dependence of the etching rate on the number of graphene layers.

Furthermore we conducted electron transport measurements on a set of single- and bilayer samples patterned by lattices of hexagonal antidots. From temperature dependent investigation of the clearly resolved weak localization peak we deduce the phase coherence length as well as lengths for inter- and intravalley scattering.

[1] P. Nemes-Incze et al., Nano Res. **3**, 110 (2010)

HL 44.15 Tue 18:00 P3

Fabrication of top gates with ALD deposited Al_2O_3 on graphene structures — •Franz-Xaver Schrettenbrunner, Dieter Weiss, and Jonathan Eroms — Institut für Experimentelle und Angewandte Physik, Universtität Regensburg, 93040 Regensburg

We report the fabrication and transport measurements of top gated graphene devices. The insulating Al_2O_3 top gate was realized using atomic layer deposition. Usually, a seed layer (e.g. oxidized aluminum, NO_2/TMA process, etc.) has to be grown in order to achieve uniform oxide layers with low impurities. Previously, we have shown that a 100°C TMA/H_2O-process with low purge times of five seconds creates a stable top gate dielectric on graphene resulting in strong n-doping of the sample (impurity carrier density: $n_{\mathrm{ind}} = 5.2 \cdot 10^{12}\mathrm{cm}^{-2}$). Now this process was improved by growing 10nm Al_2O_3 at 100°C as a seed layer on which further material was deposited while heating the ALD reaction chamber up to 225°C. This "in-situ" annealing step forms a stable gate dielectric on our graphene structures with impurity carrier density $n_{\mathrm{ind}} = 3.6 \cdot 10^{11}\mathrm{cm}^{-2}$.

HL 44.16 Tue 18:00 P3

Paramagnetic surface-states in μc-3C-SiC as efficient acceptor in solar cells — •Andre Konopka, Siegmund Greulich-Weber, Uwe Gerstmann, Eva Rauls, and Wolf Gero Schmidt — Physics, University of Paderborn, Paderborn, Germany

Microcrystalline silicon carbide (μc-SiC) have become an attractive new class of advanced microstructured materials for heterojunction photovoltaic (PV) devices due to their wide band gap and lower absorption in the visible region while retaining their higher conductivity. We use a sol-gel process for growing μc-SiC with sizes up to several 100 μm allowing arbitrary doping. The initial material is insulating, indicating that the resulting sol-gel SiC is almost free from usually unavoidable nitrogen donors. As an analytic tool for the control of doping success we used electron paramagnetic resonance (EPR). The spectra obtained are clearly different from those known for usual shallow donors and acceptors in bulk SiC. Obviously, in microcrystals at least some of the defects seen by EPR are no longer bulk-like, but are surface-related. PV measurements support our finding that the required acceptor behavior of μc-SiC is caused by surface-related defects in combination with an appropriate position of the fermi level, which is determined by donor or acceptor doping. Based on this knowledge, the microscopic structure of the responsible defect structure at the clean surface of the microcrystallites is discussed with the help of total energy calculations in the framework of density functional theory. For possible dangling-bond related structures the elements of the electronic g-tensor are calculated and compared with the experimental values.

HL 44.17 Tue 18:00 P3

Stoichiometric defects in silicon carbide — •Guido Roma[1], Ting Liao[2], and Olga Natalia Bedoya-Martínez[1] — [1]CEA-Service de Recherches de Métallurgie Physique, Saclay, France — [2]Institute of Metal Research, Shenyang, China

Defect structures showing odd-membered rings are known features of several tetrahedral semiconductors as well as carbon nanostructures; examples of them are bond defects in crystalline and amorphous silicon, Stone-Wales defects in fullerenes and carbon nanotubes, and the core structure of partial dislocations in some tetrahedral semiconductors. We investigate, using Density Functional Theory, two types of stoichiometry-conserving defects, which we call SCD and antiSCD and which are metastable structures presenting five- and seven-membered rings, both in the cubic and in the hexagonal 4H-SiC polytypes. We also investigate the annealing properties of the two mentioned variants and find that one of them (SCD) easily disappears, turning back to a normal site, while the other (antiSCD) transforms to an antisite pair, overcoming a barrier of 0.21 eV. The very short lifetimes at ambient conditions explain why those defects have not been observed up to now, but they suggest they should be observable at very low temperature and we provide local vibrational modes to facilitate their identification.

HL 44.18 Tue 18:00 P3

Spin Noise Spectroscopy and Selection Rules in Highly Purified ^{28}Silicon — •Nils Scharnhorst[1], Georg Müller[1], Helge Riemann[2], Jens Hübner[1], and Michael Oestreich[1] — [1]Institute for Solid State Physics, Leibniz Universität Hannover, Appelstr. 2, D-30167 Hannover, Germany — [2]Institut für Kristallzüchtung, Max-Born-Str. 2, D-12489 Berlin, Germany

We present our most recent experimental setup and results in qualifying the spin-lifetime and spin-selection rules of donor-bound and free electrons in highly purified ^{28}Silicon and natural silicon. Isotopically pure ^{28}Silicon is promising very long spin-coherence times due the missing inhomogeneous spin decoherence via nuclear hyperfine-interaction. The fragile measurements on localized spins in ^{28}Silicon will be realized by spin-noise spectroscopy based upon weakly interaction off-resonant Faraday-rotation [1] while spin selective pump-probe measurements yield the spin selection rules at the Δ-band minimum in natural, slightly n-doped silicon.

[1] G. M. Müller, M. Oestreich, M. Römer, and J. Hübner, Semiconductor spin noise spectroscopy: Fundamentals, accomplishments, and challenges, Physica E **43**, 569 (2010).

HL 44.19 Tue 18:00 P3

Structural and electronic properties of silicon polymorphs — •Tobias Sander, Claudia Rödl, Kaori Seino, and Friedhelm Bechstedt — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

Currently, silicon has been assigned to 12 different high pressure phases from which two are still undetermined in their atomic geometries. Due

to the occurrence of complex structures and metastable phases, a complete investigation of structural or even electronic properties has not been completed yet. The possible chance to find crystalline Si structures that may be applicable in photovoltaic devices has enforced the interest in a detailed investigation. Since it is little known about the atomic distributions, we performed ground-state calculations for three distinct exchange and correlation functionals (LDA, PBE, AM05) to obtain parameters like lattice constants, bulk moduli, or cohesive energies. Reflecting structural properties for semiconducting structures best, the AM05 functional has been used to investigate electronic properties such as band gaps, band offsets, and density of states (DOS). From that we classify four polymorphs to be semiconducting, including Si-XIII which has not been observed experimentally yet. We also investigated quasiparticle band structures within the *GW* method and compare band gap results from AM05+*GW* and HSE03+*GW* calculations. Finally, the results are completed by optical absorption spectra.

HL 44.20 Tue 18:00 P3

Investigation of the direct bandgap-emission of highly doped strained germanium layers — •Michael J. Drexler[1], Niko S. Köster[1], Kolja Kolata[1], Giovanni Isella[2], Daniel Chrastina[2], Hans von Känel[2], Hans Sigg[3], and Sangam Chatterjee[1] — [1]Faculty of Physics and Material Sciences Center, Philipps-Universität Marburg, Renthof 5, D-35032 Marburg, Germany — [2]Dipartimento di Fisica del Politecnico di Milano, Polo di Como, via Anzani 42, I-22100 Como, Italy — [3]Labor für Micro- und Nanotechnologie, Paul Scherrer Institut, Schweiz

One of the key components of Si photonics is an all integrated laser light source emitting in the C-band at 1550 nm. A promising approach is using highly doped tensile strained germanium. Optical gain in this material system has been shown [1]. We processed structures with several cavity lengths to investigate the edge- emitted light from the direct band-gap transitions. The system is pumped with a Q-switched laser at 1054nm with 70 ns pulses and the emitted light is spectrally resolved with a double monochromator and detected with a liquid nitrogen cooled Ge-detector.

[1] J. Liu et al, Opt. Lett. 34 (11), p. 1738-40, 2009

HL 44.21 Tue 18:00 P3

Giant dynamical Stark shift in germanium quantum wells — •Ronja Woscholski[1], Niko Steffen Köster[1], Kolja Kolata[1], Christoph Lange[1,3], Giovanni Isella[2], Daniel Chrastina[2], Hans von Känel[2], and Sangam Chatterjee[1] — [1]Faculty of Physics and Material Sciences Center, Philipps-Universität Marburg, Renthof 5, D-35032 Marburg, Germany — [2]Dipartimento di Fisica del Politecnico di Milano, Polo di Como, via Anzani 42, I-22100 Como, Italy — [3]present address: University of Toronto, Department of Physics, 60 St. George St., Toronto ON, M5S 1A7, Canada

One of the goals in semiconductor research is to realize the necessary components for silicon photonics, like detectors, emitters, and modulators. Here, we show the potential of Ge/SiGe quantum well structures to work as optical modulators. We investigate the dynamical Stark effect by using polarization-resolved ultrafast pump and white-light probe spectroscopy. This method offers insight on both the modulation bandwidth and the switching speeds achievable in this material system. A strong blue shift of more than 150meV is found for a sample temperature of 10K, which exceeds the values typically for III-V materials. The experimental results are in good agreement with the dressed exciton model. We conclude that the ultrafast coherent dynamics are mainly governed by the direct transition; the indirect minima play only a minor role.

HL 44.22 Tue 18:00 P3

Structural modification of SHI irradiated amorphous Ge layers — •Tobias Steinbach[1], Claudia S. Schnohr[1], Leandro L. Araujo[2], Raquel Giulian[2], David J. Sprouster[2], Mark C. Ridgway[2], Daniel Severin[3], Markus Bender[3], Christina Trautmann[3], and Werner Wesch[1] — [1]Institute of Solid State Physics, Friedrich Schiller University Jena — [2]Department of Electronic Materials Engineering, Australian National University, Canberra — [3]GSI Helmholtz Centre for Heavy Ion Research GmbH

During SHI irradiation of amorphous Ge a strong volume expansion of the amorphous layer accompanied by an enhanced plastic flow process was observed. To study the effect of high electronic energy deposition ϵ_e on a-Ge layers in more detail samples were irradiated at RT and LT with Au-ions having high energies in the range of several hundred MeV. In order to quantify the swelling of the sample one half was masked to distinguish the irradiated from the unirradiated reference. We demonstrate for all used irradiation conditions that a strong swelling of the irradiated areas can be observed, which depends linearly on the ion fluence as well as on ϵ_e. XSEM revealed the transformation of the a-Ge layer into a porous structure with irregularly shaped voids thus establishing that swelling was a consequence of void formation. Moreover, an electronic energy deposition threshold has been estimated, at which the swelling, i.e. the formation of voids, begins. Furthermore, we report on the early stages of void formation in a-Ge by means of SAXS and TEM investigations, which demonstrates that voids are formed due to the imperfect resolidification of molten ion tracks.

HL 44.23 Tue 18:00 P3

Electronic structure of III-V hexagonal polytypes — •Christian Panse and Friedhelm Bechstedt — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Germany

Semiconducting nanowires (NW) are of great interest due to their potential in electronic and optoelectronic applications. With increasing success on the control over the crystal structure in the last years it became possible to grow pure layers of zinc blende (ZB/3C), wurtzite (WZ/2H) and also small segments of the hexagonal 4H polytype. As this offers a new degree of freedom for NW device design, investigations of the electronic properties of different hexagonal polytypes are needed for the design of polytypic superlattice nanowire devices.

We perform *ab-initio* calculations within the density functional theory (DFT) and discuss the results on the electronic and optical properties of III-V compounds (GaAs, InAs, InP, InSb) with respect to the different WZ/ZB stacking sequences. The bulk phases of different polytype structures (3C, 2H, 4H, 6H) are especially studied. The electronic properties are calculated versus the hexagonality of the polytypes using the LDA-1/2 method, even including spin-orbit coupling, which leads to quasiparticle band structures but with the effort of conventional DFT. We present results on effective masses, fundamental gaps, spin-orbit and crystal-field splittings and band discontinuities and how these band parameters are modified by the polytypism. Special attention is given to the impact of the cell internal structure.

HL 44.24 Tue 18:00 P3

Electronic and Optical Properties of Group-III Nitride Alloys from ab-initio Methods — •Luiz Cláudio de Carvalho, André Schleife, Abderrezak Belabbes, Cláudia Rödl, and Friedhelm Bechstedt — Institut für Festköpertheorie und -optik, Friedrich-Schiller-Universität, Max-Wien-Platz 1, 07743 Jena, Germany

Group-III mononitrides and their alloys are subject of intense investigations due their interesting electronic and optical properties. First-principles calculations based on the density functional theory, hybrid functionals, and an iterative solution of the quasiparticle equation with the exchange-correlation self-energy in GW approximation have demonstrated to give electronic structures in good agreement with spectroscopic data. Recently, a new approach called LDA-1/2, was proposed based on the concept of half occupation. Applied to excitation energies in solids one overcomes the band-gap problem and obtains reliable electronic properties with less computer-time demands. In the present work, electronic and optical properties of wurtzite group-III nitrides alloys are studied within the cluster expansion approximation. Three different cluster statistics, GQCA, SRS and MDM, are applied in order to illustrate different preparation techniques. The calculations are performed using implement atoms in the VASP code. Based on the LDA-1/2 method electronic structures, are derived optical absorption spectra including electron-hole interaction and local-field effects are computed as a function of composition by solving the Bethe-Salpeter equation. The computed spectra are analyzed and compared to available experimental data.

HL 44.25 Tue 18:00 P3

Band Parameters of (Al, Ga, In)N Polytypes from Different XC Functionals — •Luiz Cláudio de Carvalho, André Schleife, Frank Fuchs, and Friedhelm Bechstedt — Institut für Festköpertheorie und -optik, Friedrich-Schiller-Universität, Max-Wien-Platz 1, 07743 Jena, Germany

Actually a detailed knowledge of the band parameters of the group-III nitrides is necessary to interpret experimental data and understand theoretical results. The most successful theoretical approach is the Density Functional Theory (DFT), but its accuracy depends on the exchange-correlation (XC) functional. Different XC functionals yield slightly varying results for the structural and electronic properties.

However, this effect is less important in comparison to the drastic changes of the electronic band structures by solving the quasiparticle (QP) equation. In this work we present and discuss the qualitative and quantitative influence of the XC functionals LDA, GGA, and AM05 induced by structural changes on the band parameters of the AlN, GaN and InN mononitrides. DFT as implemented in VASP code is used to calculate the structural and elastic properties of zinc-blende and wurtzite polytypes. The QP band structures including the XC self-energy within Hedin's GW approximation are obtained taking almost self-consistency into account using HSE03 hybrid XC functional as a starting point. The gap energies, crystal-fields splittings, momentum matrix elements, effective masses and spin-orbit coupling are computed from the QP band structures. We compare our results with experimental values reported in the literature.

HL 44.26 Tue 18:00 P3

Determination of the valence band offset at selected oxide/InN interfaces — Georg Eichapfel[1], •Marcel Himmerlich[1], Anja Eisenhardt[1], Stefan Krischok[1], Andreas Knübel[2], Thorsten Passow[2], Chunyu Wang[2], Fouad Benkhelifa[2], and Rolf Aidam[2] — [1]Institut für Physik and Institut für Mikro- und Nanotechnologien, TU Ilmenau, PF 100565, 98684 Ilmenau, Germany — [2]Fraunhofer-Institut für Angewandte Festkörperphysik, Tullastraße 72, 79108 Freiburg, Germany

The valence band offsets (VBO) at different oxide/InN(0001) interfaces are investigated for TiO_2, HfO_2, Al_2O_3 and In_2O_3 using X-ray photoelectron spectroscopy. These oxide materials might be potential candidates for the use as barrier material in InN based transistors. The precise knowledge of the band alignment at the oxide/InN interface is relevant to understand the carrier transport characteristics in electronic devices. InN films with a thickness of 1 μm were grown by PAMBE on GaN(0001)/Al_2O_3 templates. Thin oxide films were grown on top of these InN layers, within a series of varying thickness (1-5 nm). TiO_2 and HfO_2 were deposited by plasma-assisted e-beam evaporation, while for Al_2O_3 a remote plasma ALD process was used and In_2O_3 was grown by MOCVD. Thickness dependent changes of the barrier could only be found for TiO_2 which exhibited the strongest degree of process-induced InN interface oxidation. The VBO values, which were determined by linear extrapolation of the thickness dependence, are 1.8 eV, 1.2 eV, 2.65 eV and 1.5 eV for the TiO_2/InN, HfO_2/InN, Al_2O_3/InN and In_2O_3/InN heterointerface, respectively.

HL 44.27 Tue 18:00 P3

Epitaxial growth and characterization of InN and GaN on C-face SiC($\bar{1}\bar{1}\bar{1}$)/Si(111) — •Anja Eisenhardt, Marcel Himmerlich, Pierre Lorenz, Katja Tonisch, Jörg Pezoldt, and Stefan Krischok — Institut für Mikro- und Nanotechnologien, TU Ilmenau, PF 100565, 98684 Ilmenau, Germany

We studied the epitaxial growth and characterized the surface properties of thin GaN and InN films grown by plasma-assisted molecular beam epitaxy on Si(111) substrates carbonized via rapid thermal processing (RTP). This RTP process results in a 2-3 nm thick 3C-SiC($\bar{1}\bar{1}\bar{1}$) film with C-polarity. As characterization methods for the InN and GaN layers in-situ reflection high energy electron diffraction (RHEED), photoelectron spectroscopy (UPS, XPS) and atomic force microscopy (AFM) were used. Furthermore structural properties were ex-situ determined using X-ray diffraction (XRD) measurements. The results are compared to InN(0001) and GaN(0001) grown on sapphire and SiC(0001) substrates, respectively, as well as InN(000$\bar{1}$) and GaN(000$\bar{1}$) grown on 6H-SiC(000$\bar{1}$). The electronic properties of the GaN and InN films grown on carbonized C-face SiC($\bar{1}\bar{1}\bar{1}$)/Si(111) are comparable to metal-face GaN and InN and therefore indicate metal-polarity and not the expected N-polarity. InN on C-face SiC($\bar{1}\bar{1}\bar{1}$)/Si(111) exhibits occupation of the conduction band due to the detected electron emission up to the Fermi level. The InN work function of about 4.0 eV is significantly lower compared to InN(0001)/sapphire ($\sim$ 4.6 eV) and InN(000$\bar{1}$)/6H-SiC ($\sim$ 4.8 eV) samples. All InN and GaN epitaxial films were tensily strained.

HL 44.28 Tue 18:00 P3

Ex-situ activation of magnesium acceptors in InGaN/LED-structures — •Gunnar Kusch, Martin Frentrup, Joachim Stellmach, Tim Kolbe, Tim Wernicke, Markus Pristovsek, and Michael Kneissl — Technische Universität Berlin, Institut für Festkörperphysik, Hardenbergstr. 36, 10623 Berlin, Germany

One of the main problems limiting the output power of group-III-nitride compound light emitting diodes (LEDs) and laser diodes (LD) is the p-doping of nitrides with magnesium (Mg). During metal-organic vapor phase epitaxy (MOVPE) growth of (Al)GaN:Mg magnesium acceptors are passivated by hydrogen (H). By thermal annealing under nitrogen atmosphere the Mg-H bond can be cracked, thus activating the Mg acceptor.
We have investigated ex-situ Mg-activation of the p-GaN layer and p-AlGaN electron blocking layer (EBL) in LEDs grown by MOVPE. Especially the activation of the AlGaN EBL is crucial. Simulations show, that a high doping level is required for effective electron blocking and a high injection efficency. Additionally the acceptor activation energy is expected to increase with increasing Al-content, reducing the free hole concentration in the EBL. Electroluminescence spectroscopy (EL) was performed to determine the influence of the activation on the external quantum efficiency of the LED structure. Furthermore we used CV measurements to determine the Mg-acceptor concentration.

HL 44.29 Tue 18:00 P3

Temperaturabhängigkeit des elektrischen Feldgradienten in $Al_xGa_{1-x}N$ — •Ronnie Simon[1], Sahar Hamidi[1], Patrick Kessler[1], Sérgio Miranda[2], Katharina Lorenz[2], Reiner Vianden[1] und ISOLDE Collaboration[3] — [1]Helmholtz Institut für Strahlen- und Kernphysik, Universität Bonn — [2]Instituto Tecnológico e Nuclear, 2686-953 Sacavém, Portugal — [3]CERN, Genf, Schweiz

Ternäre Verbindungen von Gruppe III-Nitriden, unter anderem das hier untersuchte $Al_xGa_{1-x}N$, finden zahlreiche Anwendungen in optoelektronischen Bauteilen wie LEDs.

In Abhängigkeit vom Al-Anteil x wurden Messungen mit der gestörten γ-γ-Winkelkorrelation (PAC) durchgeführt. Dazu wurden ^{111m}Cd(^{111}Cd), ^{117}Cd(^{117}In) und ^{111}In(^{111}Cd) als Sonden verwendet. Die bei der Implantation der Sonden entstehenden Gitterschäden wurden bei 1200K ausgeheilt. Die Auswirkungen des Al-Anteils in $Al_xGa_{1-x}N$ auf den elektrischen Feldgradienten des Gitters wurden untersucht. Dabei wurden Messungen bei Temperaturen zwischen 300K und 1000K durchgeführt.

PAC Messungen mit ^{111}In in GaN haben gezeigt, dass es zur Bildung eines Defektkomplexes aus einem substitutionellen Indiumatom und einer Stickstoffleerstelle kommt (In-V_N). In-V_N weist ein reversibles Temperaturverhalten auf und ist bis zu hohen Temperaturen stabil. Dieser Komplex ist auch in $Al_xGa_{1-x}N$ beobachtbar und zeigt eine hohe Abhängigkeit vom Al-Anteil x.

HL 44.30 Tue 18:00 P3

$In_xGa_{1-x}N$ films for use in photo-electrochemical cells — •Y.H. Wu[1,2], Philipp R. Ganz[1,2], D.Z. Hu[1,2], and Daniel M. Schaadt[1,2] — [1]Institut für Angewandte Physik, Karlsruher Institute of Technology, 76131 Karlsruhe, Germany — [2]DFG-Center for Functional Nanostructures, Karlsruher Institute of Technology, 76131 Karlsruhe, Germany

Development of renewable and clean energy is becoming interesting. Photo-electrochemical cells (PECs) are a new and promising possibility of generating hydrogen by splitting water. A PEC consists of a semiconductor electrode and a metal counter electrode and is embedded in an electrolyte or water. A possible material for the semiconductor electrode is $In_xGa_{1-x}N$, because it has an appropriate band-edge potentials, which straddles the redox potentials of water. We have characterized $In_xGa_{1-x}N$ films for use in PECs. The carrier concentrations were investigated by Hall measurement and the surface morphology by atomic force microscopy. The films were exposed to various electrolytes with different PH levels and their potential for hydrogen generation was explored.

HL 44.31 Tue 18:00 P3

Effect of nitridation on the MOVPE growth of InN on *c*-, *r*- and *a*-plane sapphire — •Sergej Solopow, Duc Dinh, Markus Pristovsek, and Michael Kneissl — TU Berlin, Institute of Solid State Physics, Hardenbergstr. 36, 10623 Berlin, Germany.

Growth of high quality InN is still challenging because of a narrow growth window and lack of suitable substrates. We report on the growth of InN on different oriented sapphire substrates, i.e. a-plane ($11\bar{2}0$), c-plane (0001), m-plane ($10\bar{1}0$) and r-plane ($10\bar{1}2$) using metalorganic vapor phase epitaxy (MOVPE).

To grow InN directly on the sapphire substrate, a nitridation process is used to improve crystallinity and optical properties. We have grown InN layers after nitridation for 2min at different temperatures from 500 °C to 1050 °C. We found that the nitridation temperature strongly affects the morphology as well as the orientation of InN layers. Atomic

force microscopic (AFM) measurements on the grown samples showed smoother surfaces at higher nitridation temperatures. *c*-oriented InN was grown on *c*-plane sapphire with in-plane relationship of $[10\bar{1}0]$ || $[11\bar{2}0]_{Sapphire}$. On the *a*-plane sapphire we obtained *c*-oriented InN with in-plane relationship of $[1\bar{1}00]_{InN}$ || $[0001]_{Sapphire}$ and $[11\bar{2}0]_{InN}$ || $[1\bar{1}00]_{Sapphire}$ at nitridation temperature higher than 900 °C and additional in-plane relationship by temperatures below 900 °C. We have grown also *a*-oriended InN on *r*-plane sapphire at nitridation temperature higher than 800 °C. At nitridation temperatures below 800 °C this orientation disappears.

HL 44.32 Tue 18:00 P3

Spin Noise Spectroscopy — •Fabian Berski[1], Jens Hübner[1], Fanny Greullet[2], Georgy Astakhov[2], and Michael Oestreich[1] — [1]Institute for Solid State Physics, Leibniz Universität Hannover, Appelstr. 2, D-30167 Hannover, Germany — [2]Faculty of Physics and Astronomy, Julius-Maximilians-Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

We study the intrinsic magnetization fluctuations of the magnetic semiconductor GaMnAs at its phase transition by spin noise spectroscopy [1]. Spin noise spectroscopy avoids generating additive holes and is therefore a promising tool to unreveal unperturbed spin dynamics and has been widely applied to study spin-dynamics of non magnetic semiconductors by investigating the stochastic deviation from vanishing spin polarization at thermal equilibrium. In this contribution we explore the advancement of spin noise spectroscopy to diluted magnetic semiconductors with the aim to observe the transition from random spin fluctuations to the rise of a collective order. We examine a thin GaMnAs film deposited on a sapphire substrate. GaMnAs can easily be integrated in existing GaAs growth procedures and is consequently an attractive candidate to engineer spintronic devices and serves as an ideal model system to study the effects of combining semiconducting and ferromagnetic properties.

[1] G. M. Müller, M. Oestreich, M. Römer, and J. Hübner, Semiconductor spin noise spectroscopy: Fundamentals, accomplishments, and challenges, Physica E 43, 569 (2010).

HL 44.33 Tue 18:00 P3

Experimental realisation of ultrafast spin noise spectroscopy — •Jan Gerrit Lonnemann, Georg Müller, Jens Hübner, and Michael Oestreich — Institute for Solid State Physics, Leibniz Universität Hannover, Appelstr. 2, D-30167 Hannover, Germany

Semiconductor spin noise spectroscopy has evolved as a powerful experimental technique to explore spin dynamics in close vicinity to thermal equilibrium [1], however, the application of a continuous wave laser limits the detectable spin frequencies to the bandwidth of the photoreceivers. Sampling the spin fluctuations with pulsed laser light allows detection of spin noise at GHz frequencies that are only limited by the inverse pulse width [2]. However this implementation is in general restricted to spin dephasing rates that are smaller than the laser repetition rate. We present the experimental relalization of a complementary technique [3] that is exclusively sensitive to spin dephasing rates that exceed the repetition rate of the laser system. This experiment will pave the way towards application of spin noise spectroscopy even at room temperature.

[1] Georg M. Müller, Michael Oestreich, Michael Römer, and Jens Hübner; Semiconductor spin noise spectroscopy: Fundamentals, accomplishments, and challenges; *Physica E*, 43(2):569 - 587, 2010.

[2] Georg M. Müller, Michael Römer, Jens Hübner, and Michael Oestreich; Gigahertz spin noise spectroscopy in n -doped bulk GaAs; *Phys. Rev. B*, 81(12):121202, Mar 2010.

[3] Sebastian Starosielec and Daniel Hägele; Ultrafast spin noise spectroscopy; *Applied Physics Letters*, 93(5):051116, 2008.

HL 44.34 Tue 18:00 P3

Photoluminescence spectra of weakly n-doped GaAs in view of spin noise spectroscopy — •Carsten Schulte[1], Jens Hübner[1], Dirk Reuter[2], Andreas Wieck[2], and Michael Oestreich[1] — [1]Institute for Solid State Physics, Leibniz Universität Hannover, Appelstr. 2, D-30167 Hannover, Germany — [2]Chair for Applied Solid State Physics, Ruhr-Universität Bochum, D-44780 Bochum, Germany

We measure the photoluminescence signal of a weakly n-doped GaAs sample ($n_D \leq 10^{14}\,\mathrm{cm}^{-3}$) in preparation of prospective spin noise spectroscopy (SNS) on non-interacting donor spins. Spin noise spectroscopy [1] is a powerful tool in semiconductor quantum optics and is capable of delivering important information on the dynamics of non-interacting spins with the long-term goal of entangled electron spin ensembles in semiconductors. The spin noise spectra provide valuable information on the dominant limitation of the spin relaxation time due to hyperfine interaction with nuclear spins. The photoluminescence and transmission spectra are used to select the sample and determining its suitability for the entanglement of spin ensembles.

[1] G. M. Müller, M. Oestreich, M. Römer, and J. Hübner, Semiconductor spin noise spectroscopy: Fundamentals, accomplishments, and challenges, Physica E 43, 569 (2010).

HL 44.35 Tue 18:00 P3

Semiconductor spin noise spectroscopy in oblique magnetic fields — •Georg Müller, Fabian Berski, Jens Hübner, and Michael Oestreich — Abteilung Nanostrukturen, Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstraße 2, D-30167 Hannover

Spin noise spectroscopy (SNS) is a powerful experimental technique to resolve equilibrium electron spin fluctuations in semiconductor systems [1]. Here, we present spin noise measurements in bulk GaAs with an arbitrary angle between magnetic field and the direction of light propagation. Usually, a magnetic field is applied in SNS in Voigt geometry, i.e., transverse to the direction of probe light propagation, to modulate the detected spin fluctuations with the Larmor frequency. This traditional experimental scheme is applied for measurements of the transverse spin dephasing time $T_2^{(*)}$. A magnetic field along the light wave vector, i.e., in Faraday geometry, introduces a splitting of the probed spin states. Correspondingly, energy relaxation accompanies the spin fluctuations and SNS with a longitudinal magnetic field is sensitive to the spin relaxation time T_1. The new experimental geometry presented in this contribution allows simultaneous detection of spin dephasing and relaxation in a single measurement. The strength of SNS in this particular experiment lies in the fact that spin dephasing and relaxation are separated in the spin noise spectrum by the Larmor frequency while these different dynamics would overlap in the time domain in corresponding measurements via pump-probe techniques.

[1] G. M. Müller *et al.*, Physica E **43**, 569 (2010).

HL 44.36 Tue 18:00 P3

Fabrication of a μ-Schottky diode using molecular beam epitaxy and ion beam lithography — •Ashish K. Rai[1], P. Szary[2], O. Petracic[2], H. Zabel[2], H.-W. Becker[3], A. Ludwig[1], D. Mantei[4], S. Gordon[4], A. Zrenner[4], D. Reuter[1], and A. D. Wieck[1] — [1]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, D-44780 Bochum, Germany — [2]Experimentalphysik IV, Ruhr-Universität Bochum, D-44780 Bochum, Germany — [3]Fakultät für Physik und Astronomie, Ruhr-Universität Bochum, 44780 Bochum, Germany — [4]Center for Optoelectronics and Photonics Paderborn,Uni. Paderborn, 100 33098 Paderborn, Germany

Schottky junctions of the metal-intrinsic-n-doped type are widely used to control the charge in quantum dots (QDs) underneath them by an electrical field.It is significant technological challenge to apply this concept to single QDs and requires μ-Schottky diodes with an active area of approximately 1μm x μm.In this contribution,we present a novel approach to create such μ-diodes:After growing the basic layer sequence by molecular beam epitaxy,we define a buried stripe in the n-layer by optical lithography and subsequent O ion implantation in opened stripe-like resist window.After that,a metal line oriented perpendicular to the buried stripe is defined on the surface by electron beam lithography,so that the active area of the junction is only the over-lap region of both stripes.The diode characteristic was confirmed by I-V measurements at room temperature as well as at low temperature (4.2K).It is intended to perform PLV (voltage dependent Photoluminescence of single QDs)or Electroluminescence on these structures.

HL 44.37 Tue 18:00 P3

Diffusionslängen in GaAs — •Sergej Markman, Markus K. Greff und Andreas D. Wieck — Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum

Eine mögliche Charakterisierung und Optimierung der elektrischen Güte von III-V-Solarzellen für die Photovoltaik ist die Diffusionslänge der Minoritätsladungsträgern, die sowohl die Ladungsträgerbeweglichkeit als auch die Lebensdauer beinhaltet. Durch fokussierte Ionenstrahlen (FIB) können elegant laterale pn-Übergänge geschrieben werden, die oberflächennah sind. Da dann vom eingestrahlten Licht keine hoch dotierten Schichten durchquert werden müssen und so eine potenzielle Absorption entfällt, kann die Effizienz der Ladungsträgergeneration in

den verarmten Bereichen zwischen p- und n-Gebiet erhöht werden.

Es sollen dann die Diffusionslängen von Elektronen bzw. Löchern in GaAs in Abhängigkeit der Dotierstoffkonzentration untersucht werden. Dazu soll, mittels eines fokussierten Ionenstrahls, Kohlenstoff in ein n-HEMT implantiert und so p-überkompensiert werden, da Kohlenstoff in GaAs einer der flachsten Akzeptoren darstellt. Komplementär dazu soll ebenfalls ein p-HEMT lokal n-dotiert werden. Die Diffusionslängen werden anschließend mittels eines OBIC-Aufbaus (eng. Optical beam induced current) gemessen. Über eine optische Abbildung der im LED-Betrieb erzeugten Infrarotstrahlung durch eine CCD-Kamera soll ebenfalls ermöglicht werden, die Diffusionslängen direkt zu beobachten.

HL 44.38 Tue 18:00 P3

Hole spin dynamics in 2D hole systems in [113]-grown GaAs/AlGaAs quantum wells at low temperatures — •Stephan Furthmeier[1], Michael Kugler[1], Tobias Korn[1], Michael Griesbeck[1], Marika Hirmer[1], Dieter Schuh[1], Werner Wegscheider[2], and Christian Schüller[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Germany — [2]Solid State Physics Laboratory, ETH Zurich, Switzerland

For the realization of scalable solid-state quantum-bit systems, spins in semiconductor quantum dots are promising candidates. This has led to studies of low-temperature hole spin dynamics in two-dimensional hole systems (2DHS) in GaAs/AlGaAs quantum wells (QW) grown in the crystallographic direction [001]. Recently, calculations and experiments have shown that the effective hole g-factor g* can have different values for a magnetic field B applied in the direction normal to the plane of the 2DHS compared to in-plane. For directions other than the high-symmetry directions [001] and [111], it is theoretically predicted that, even for a purely in-plane B, g* can depend strongly on the orientation of B with respect to the crystal axes [1].

Here, we report on our experimental findings of hole spin dynamics in [113]-grown GaAs/AlGaAs QWs at low temperatures after optical excitation. Using the all-optical time-resolved Faraday rotation technique, we observe long-lived hole spin dephasing times in our sample at a temperature of 1.2 K. A complete angle-dependent series on the direction of the in-plane B with respect to the crystal axes is planned.

[1] R. Winkler et al., Phys. Rev. Lett. 85, 4574-4577 (2000).

HL 44.39 Tue 18:00 P3

Carbon implantation in GaAs by focused ion beam and electrical activation by rapid thermal annealing — •Markus K. Greff, Arne Ludwig, Dirk Reuter, and Andreas D. Wieck — Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum

Since its development at the end of the 70s, focused ion beam implantation has become a powerful tool for maskless, local implantation or sputtering with a lateral resolution about 10 nm. Because carbon is one of the shallowest acceptors in GaAs, it is desirable to create a focused carbon beam employing a suitable liquid metal ion source[1]. Also one could think about possible applications such as implantation of carbon in diamond or organic materials as well as working with carbon nanotubes or graphene.
In this contribution we would like to present first results for carbon implantation in GaAs by focused ion beam and subsequent electrical activation of implanted carbon by rapid thermal annealing.

[1] P. Mazarov, A.D. Wieck, L. Bischoff, and W. Pilz, Journal of Vacuum Science and Technology B **27**, L47 - L49 (2009).

HL 44.40 Tue 18:00 P3

Exciton-mediated lattice distortions in InAs/GaAs quantum dots — •Sebastian Tiemeyer[1], Michael Bombeck[2], Michael Paulus[1], Christian Sternemann[1], D. C. Florian Wieland[1], Oliver H. Seeck[3], Manfred Bayer[2], and Metin Tolan[1] — [1]Fakultät Physik / DELTA, TU Dortmund, D-44221 Dortmund, Germany — [2]Experimentelle Physik II, TU Dortmund, D-44221 Dortmund, Germany — [3]HASYLAB, DESY, D-22607 Hamburg, Germany

The confinement of charge carriers to length scales comparable to the de Broglie wavelength in semiconductor heterostructures such as quantum wells and quantum dots leads to a considerable modification of the density of states (DOS). In particular quantum dots represent zero-dimensional structures possessing a DOS similar to that of atoms.

Indium Arsenide (InAs) and Gallium Arsenide (GaAs) exhibit a lattice mismatch of 7% giving rise to strain fields in quantum dot heterostructures. The strain affects significantly the electronic properties of quantum dots e.g. the band structure and band gap. Previous x-ray studies have determined the strain distribution in non-excited quantum dots and the surrounding crystalline structure. The lattice distortion by optically excited carriers has been monitored up to now only indirectly by high resolution continuous wave or non-linear time-resolved optical spectroscopy. In this study we have investigated the laser-induced strain in InAs quantum dots grown on and capped with GaAs by means of anomalous x-ray diffraction at the beamlines BL9 (DELTA, TU Dortmund) and P08 (HASYLAB, DESY Hamburg).

HL 44.41 Tue 18:00 P3

MOVPE grown InAs quantum dots: Towards long wavelength emission — •Matthias Paul, Daniel Richter, Elisabeth Koroknay, Wolfgang-Michael Schulz, Marcus Eichfelder, Robert Rossbach, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen, University Stuttgart, Allmandring 3, 70569 Stuttgart, Germany

In recent years, investigations on semiconductor quantum dots (QDs) have been motivated by their potential application in the field of quantum information processing. Therefore, optically or electrically addressable single quantum dots are needed on a mass production scale using metal-organic vapor-phase epitaxy (MOVPE). QD emission in the telecom wavelength bands around 1.3 μm and 1.55μm reduces optical losses in fibers to a minimum. Furthermore, low densities of QDs will allow for single-photon sources, one key device in quantum information networks. Two approaches are pursued to reach emission wavelengths of 1.3μm and 1.55μm, respectively. First, embedding InAs QDs in an InGaAs well grown on GaAs substrates the InAs QD emission is shifted to long wavelengths. Second, even longer wavelengths can be reached by growing InAs QDs on InP substrates. The influence of the growth conditions on the QD properties is investigated and optimized to achieve long wavelength emission. The optical QD properties are analyzed by photoluminescence (PL). Furthermore, the structural properties are examined.

HL 44.42 Tue 18:00 P3

Einfluss von höherer Gate-Spannung und Lichteinfluss auf die Ladespektren von InAs-Quantenpunkt-Proben mit ITO-Gates — •Patrick Labud, Arne Ludwig, Dirk Reuter und Andreas Dirk Wieck — Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, D-44780 Bochum

Die Ladespektroskopie an InAs-Quantenpunkten (QDs) findet ihren Anfang im Jahre 1994, als Drexler et al. [1] zum ersten Mal mittels Kapazitäts-Spannungs-Messungen (C(V)-Messungen) das gezielte Beladen von QDs mit einzelnen Elektronen nachweisen konnten. Anhand der Resultate wurde eine schalenartige Energieniveaustruktur nachgewiesen, weshalb man bei QDs auch von „künstlichen Atomen“ spricht. Durch die Herstellung von transparenten, leitfähigen ITO(Indiumzinnoxid)-Gates auf die Oberfläche von QD-Halbleiterproben kann die Ladespektroskopie um optische Untersuchungen erweitert werden. In diesem Beitrag wird der Einfluss höherer Gate-Spannungen sowie der Lichteinfluss auf die Barrierenhöhe des Schottky-Kontaktes untersucht.

[1] H. Drexler, D. Leonard, W. Hansen, J. P. Kotthaus, P. M. Petroff, *Spectroscopy of Quantum Levels in Charge-Tunable InGaAs Quantum Dots*, Phys. Rev. Lett. **73**, 2252-2255 (1994).

HL 44.43 Tue 18:00 P3

In-situ TEM mechanical testing of InAs nanowires — •Marat Mukhametshin[1], Vadim Migunov[1], Zi-An Li[1], Marina Spasova[1], Andrey Lysov[2], Werner Prost[2], Ingo Regolin[2], Franz-Josef Tegude[2], and Michael Farle[1] — [1]Fakultät für Physik and CeNIDE — [2]Fakultät für Ingenieurwissenschaften and CeNIDE University Duisburg-Essen, 47048 Duisburg, Germany

Recently, it became possible to measure the elastic properties of nanostructures by in-situ Transmission Electron Microscopy (TEM). The characteristic elastic quantities have already been implemented by several methods, such as electromechanical resonance, nanoindentation, tensile stress, bending and buckling testing [1]. In this study we used the "bending method" on InAs nanowires to obtain the bending modulus as the combination of shear and Young's modules by directly imaging the bending curvature in the TEM. The Metal Organic Chemical Vapor Deposition method was used to grow InAs nanowires on InAs (100) substrate from catalyst Au nanoparticles. Scratched and dispersed nanowires were preliminary aligned on standard TEM-grids using dielectrophoresis. A special Atomic Force Microscope in a TEM

(AFM-TEM) sample holder was used to study the dependence of the mechanical properties of the nanowires on their diameter, growth direction, atomic structure and the presence of defects.

[1] Y. Zhu, C. Ke, H.D. Espinosa, Exp. Mech., 47, 7-24 (2007)

HL 44.44 Tue 18:00 P3

Homo- and heteroepitaxial GaP(100) surfaces in process gas ambients — Henning Döscher, Oliver Supplie, •Peter Kleinschmidt, Anja Dobrich, Sebastian Brückner, Christian Höhn, Antonio Müller, Claas Löbbel, and Thomas Hannappel — Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

Phosphorus based III-V semiconductors such as GaP and InP are commonly grown by metalorganic vapor phase epitaxy, where the process gas ambient has a crucial influence on the surface structure: P-rich surfaces feature hydrogen-stabilized and buckled P-dimers, a reconstruction with local p(2×2) and c(4×2) symmetries, and a flipping mechanism changing the orientation of individual dimers. A mixed dimer configuration is typical for III-rich surfaces, but only for GaP(100) in a nitrogen ambient an additional intermediate reconstruction was also observed. Heteroepitaxial growth on Si(100) introduces anti-phase disorder in GaP films, which can be observed by domains of mutually perpendicular dimer orientation on the surfaces.

HL 44.45 Tue 18:00 P3

Development of porous structures in GaSb by ion irradiation — •Tobias Steinbach, Carolin C. Jacobi, and Werner Wesch — Institute of Solid State Physics, Friedrich Schiller University Jena

Ion irradiation of GaSb causes not only defect formation but also leads to the formation of a porous structure. To study the behaviour of this structural modification, GaSb was irradiated with 6 MeV I and two different irradiation procedures: (i) continuous irradiation of samples followed by surface profilometry analysis in air, i.e. step height measurements, and (ii) stepwise irradiation of samples with measurements of the step height in air between subsequent irradiations. Samples irradiated continuously, show a moderate increase of the step height with increasing ion fluence (up to 1.5 x 10^{14} cm^{-2}) followed by a much steeper increase for higher fluences up to a step height of 32 μm. This swelling is induced by the formation of voids, and the two different slopes can be explained by a change from isolated voids to a rod like structure (SEM investigations). For samples irradiated according to procedure (ii), the step height shows the same behaviour up to 1.5 x 10^{14} cm^{-2} but then decreases with further irradiation. The latter effect is caused by an orientation of the rod like structure perpendicular to the ion beam and occurs only if the sample was taken out of the vacuum chamber and then irradiated once more. We investigated e.g. the influence of gas, oxygen, time and pressure but the reason for the change of the behaviour of GaSb, which leads to this effect, is still an open question.

HL 44.46 Tue 18:00 P3

Lithography Optimization on HgTe — •Luis Maier, Mathias J. Mühlbauer, Bruno Krefft, Jiango Yang, Hartmut Buhmann, and Laurens W. Molenkamp — Physikalisches Institut (EP3), Universität Würzburg, 97074 Würzburg

Mercury telluride (HgTe) has become more and more important in recent years due to its topological insulator properties [1,2]. However lithographical processing is still challenging because HgTe cannot endure temperatures over 100° C and in addition mercury forms numerous alloys with various elements. Here, we present recent developments which helped to improve the fabrication of HgTe nanostructures.

Titanium (Ti) etch masks are commonly used for lithographical processes. Unfortunately, Ti reacts as well with Hg and thus influences the sample quality and the efficiency of gate electrodes. To address this problem we introduced in an additional process step a 10 nm thick SiO2 layer to separate the Ti from HgCdTe top layer. Furthermore, thermal indium bonding has been used till recently to provide ohmic contact to the buried two-dimensional electron gas in HgTe quantum well structures. This process is disadvantageous because In contact require a lot of space and the contacting depth is uncontrollable which prevents the use of back gates. A process for evaporated Gold-Germanium contacts has been developed which gives a certain control of the doping depth and additionally can be used with ultrasonic bonding which reduces the required size of the bonding pads by a factor of 3.

[1] M. König et al., Science, 318, 766, (2007)
[2] A.Roth et al., Science 325, 294 (2009)

HL 44.47 Tue 18:00 P3

Das Vorzeichen des elektrischen Feldgradienten in Halbleitern mit großer Bandlücke — •Patrick Kessler[1], Valentin Germic[1], Sergio M.C. Miranda[2], Katharina Lorenz[2], Reiner Vianden[1] und ISOLDE Collaboration[3] — [1]Helmholtz-Institut für Strahlen- und Kernphysik, Universität Bonn, Deutschland — [2]Instituto Tecnológico e Nuclear, P-2686-953 Sacavém, Portugal — [3]CERN, Genf, Schweiz

Die genaue Kenntnis des elektrischen Feldgradienten (EFG) und insbesondere dessen Vorzeichen sind Voraussetzungen für detaillierte theoretische Berechnungen von Kristalleigenschaften.

Mit der Methode der gestörten $\beta - \gamma$ Winkelkorrelation kann die Stärke und das Vorzeichen des EFG bestimmt werden. Dieser wurde mit den Sonden ^{115}Cd und ^{111}Ag in den Halbleitern AlN, GaN und ZnO gemessen. Die Isotope wurden am ISOLDE Experiment des CERN in Genf im Rahmen des Projekts IS481 hergestellt und in die Proben implantiert.

HL 44.48 Tue 18:00 P3

Effects of N and N/Li doping on ZnS epilayers grown on GaP — •Gunther Haas, Udo Römer, Stefan Lautenschläger, Sebastian Eisermann, Melanie Pinnisch, Andreas Laufer, and Bruno K. Meyer — I. Physics Institute, Justus-Liebig-University Giessen, Heinrich-Buff-Ring 16, 35392 Giessen, Germany

High quality ZnS epilayers have been grown on GaP(100) by chemical vapor deposition using metallic zinc and hydrogen sulfide as source materials. An additional ammonia flow was applied to the growth process, with the purpose of N-doping. The co-doping of N and Li was realized due to the evaporation of lithium amide. To clarify the presence of N and Li in the ZnS layers a secondary ion mass spectrometer was used. In addition to that, we analyzed the effects of the dopants on the properties of the ZnS films by investigating the films with X-ray diffraction (XRD), low temperature photoluminescence (PL) and Raman spectroscopy.

HL 44.49 Tue 18:00 P3

Group VII point defects in ZnSe — •Leonardo S. dos Santos, Eva Rauls, and Wolf Gero Schmidt — Theoretische Physik, Universität Paderborn, Germany

Chlorine is one of the best known n-dopants in ZnSe. A recent work [Yamamoto et al., Phys. Rev. Lett. **103**, 053601 (2009)] has shown that independent ZnSe quantum wells doped with fluorine can emit indistinguishable photons, with possible applications in quantum computing. We have used Density Functional Theory calculations to study Cl and F point defects in ZnSe. The use of hybrid functionals for the treatment of electron exchange and correlation leads to significant changes in the defect formation energies, when compared to the use of local functionals. Our results for Cl-doped ZnSe show that Cl atoms are found primarily in the Se-substitutional position, and that the main compensating centers are the zinc vacancy and related complexes, in qualitative agreement with earlier results.

HL 44.50 Tue 18:00 P3

Band Anticrossing in $ZnSe_xTe_{1-x}$ and ZnS_xTe_{1-x} Alloys — Tobias Bertram[1], •Christian Karcher[1], Henning Klaer[2], Sebastian Klembt[2], Carsten Kruse[2], Detlef Hommel[2], and Wolfram Heimbrodt[1] — [1]Department of Physics and Material Sciences Centre, Philipps University of Marburg, Germany — [2]Institute of Solid State Physics, University of Bremen, Germany

The goal of this research is to understand the band forming in ZnSeTe and ZnSTe semiconductors. The Band Anticrossing Model (BAC) was already succesfully applied to explain the band formation in GaNAs. One can compare the chemical properties of ZnSeTe and ZnSTe with those of GaNAs. The key difference being while the electronegativity of Nitrate is almost double that of Arsenic, Tellurium's is only slightly smaller than that of Selenium or Sulphur. Similar to GaNAs the localized Se and S states lie above the ZnTe conduction band. The BAC predicts a repulsion of the localized impurity states and the ZnTe conduction band, causing it to split into a so-called E_-- and E_+-band. The higher Se or S contents in the ZnTe host, the stronger the repulsion of the E_--band, leading to a shrinking of the bandgap energy. This behaviour can also be fitted by introducing a bowing parameter into the Virtual Crystal Approximation. ZnTe incorporated with varying contents of Se and S is characterized by various optical methods. Photoluminescence, photoreflectance and absorption spectroscopy measurements are used to fully determine both the emission

and absorption characteristics of the system and by that help to gain further insight into the way the bands are formed.

HL 44.51 Tue 18:00 P3

Influence of the Mn-concentration on the magnetotransport properties of Cl-doped ZnMnSe — •Christian H. Will[1], Matthias T. Elm[1], Jörg Teubert[1], Peter J. Klar[1], and Michael Hetterich[2] — [1]1. Physikalisches Institut, Justus-Liebig-Universität, Heinrich-Buff-Ring 16, 35392 Giessen — [2]Institut für Angewandte Physik, Universität Karlsruhe, Wolfgang-Gaede-Str. 1, 76131 Karlsruhe

The incorporation of manganese ions in I_{1-x}-Mn_x-VI compounds provides a large localized magnetic moment due to their half-filled inner 3d-shell. Because manganese forms isovalent impurities, it does not affect the carrier concentration. By co-doping with Cl, the carrier concentration can therefore be tuned independently from the Mn content. In order to investigate the influence of the magnetic moment on the transport properties, ZnMnSe:Cl samples were grown by molecular beam epitaxy on undoped GaAs substrates. The samples belong to two different series. Within the first series, the amount of Cl dopants varies by a magnitude of about 10, while the Mn concentration is retained at $x \approx 6\%$. In contrast, the Mn concentration of the samples in the second series alters from 0% to 2%, while the quantity of the carrier concentration is kept constant. The magnetotransport measurements were performed in a temperature range from 1.6 K to 285 K in fields up to 10 T and the results will be discussed.

HL 44.52 Tue 18:00 P3

Tuning the Two-Dimenional Hole Gas Density in CdMnTe Quantum Wells by Near-surface Doping and Photoexcitation — •Franziska Fricke[1], Christian Kehl[1], Georgy Astakhov[1], Jean Geurts[1], Wolfgang Ossau[1], Yuri Kusrayev[2], Kyrill Kavokin[2], Tomek Wojtowicz[3], and Grzegorz Karczewski[3] — [1]Universität Würzburg, Phys. Inst., EP3, 97074 Würzburg, Germany — [2]Ioffe Institute, RAS, 194021 St. Petersburg, Russia — [3]Institute of Physics, PAN, 02668 Warsaw, Poland

P-doped CdMnTe quantum wells are known to exhibit a trend towards ferromagnetism, induced by the two-dimensional gas of heavy holes (2DHG). One way to supply a 2DHG to the quantum well is p-type doping from surface states by tunneling through a very thin capping layer. Tuning of the 2DHG density is achieved by variation the cap layer thickness and by photogeneration of charge carriers.

We present photoluminescence (PL) and magneto-PL studies on CdMnTe/CdMgTe quantum wells using resonant quantum well excitation and above-barrier excitation. The 2DHG is characterized essentially by the intensity and spectral position of the positively charged exciton (trion X^+) with respect to the neutral exciton (X^0). We describe the observed 2DHG behaviour consistently by a model based on specific tunneling times of electrons and holes, which depend on the cap thickness and the power and photon energy of the optical excitation radiation.

HL 44.53 Tue 18:00 P3

Isostructural and heterostructural MgZnO and CdZnO alloys — •André Schleife, Claudia Rödl, and Friedhelm Bechstedt — Institut für Festkörpertheorie und -optik and European Theoretical Spectroscopy Facility, Friedrich-Schiller-Universität Jena, 07743 Jena, Germany

One important goal of materials design is to purposefully tailor the fundamental band gap. Recently, group-II oxides such as MgO, ZnO, and CdO are discussed to possibly supersede the nitrides for certain applications, e.g. in optoelectronics. Since the band gaps of the oxides cover a large spectral range from 1.8 eV (CdO) up to 7.7 eV (MgO), their alloys seem to be promising – unless the different equilibrium crystal structures of the end components (rocksalt-MgO and -CdO vs. wurtzite-ZnO) prevent their application.

By employing three different cluster statistics within a cluster-expansion approach we investigate the impact of different growth conditions on the composition of isostructural and heterostructural $Mg_xZn_{1-x}O$ and $Cd_xZn_{1-x}O$ alloys. Our total-energy calculations are based on density-functional theory using a generalized-gradient approximation for exchange and correlation.

We also compute quasiparticle energies using the HSE03+G_0W_0 approach. This allows us to derive the bowings of fundamental band gaps, which reveal a strongly nonlinear behavior. Using the solution of the Bethe-Salpeter equation for the optical polarization function we investigate the influence of the preparation conditions on the peaks related to bound excitonic states at the absorption edge.

HL 44.54 Tue 18:00 P3

Hydrothermal growth of ZnO nanorods for optoelectronic and photovoltaic applications — •Marco Braun[1], Jonas Conradt[1,2], Janos Sartor[1], Dirk Silber[1], Manuel Reinhard[3], Alexander Colsmann[3], Uli Lemmer[3], and Heinz Kalt[1,2] — [1]Karlsruher Institut für Technologie (KIT), Institut für Angewandte Physik, 76128 Karlsruhe, Germany — [2]Center for Functional Nanostructures (CFN) at KIT — [3]Lichttechnisches Institut at KIT

Incorporating low-dimensional nanostructured, wide-band gap semiconductors, such as zinc oxide (ZnO) nanorods, into optoelectronic devices is a promising approach in order to realize UV light-emitting diodes. The nanorod structure can help to improve guiding and outcoupling of light and device efficiency. We present results on the growth of ZnO nanorods on various substrates using low-temperature, hydrothermal growth. An alternative high-temperature growth method is used to produce longer ZnO nanorods, e.g. on silicon substrates. The nanostructures are characterized by scanning electron microscopy and photoluminescence spectroscopy. We also present a simple method for electrical contacting and first results of electroluminescence measurements.

HL 44.55 Tue 18:00 P3

Investigation of growth catalysts for ZnO nanopillar growth — •Manfred Madel, Ingo Tischer, Benjamin Neuschl, Tobias Meisch, Martin Feneberg, Uwe Röder, and Klaus Thonke — Institut für Quantenmaterie / Gruppe Halbleiterphysik, Universität Ulm

ZnO nanopillars were grown in hexagonal and cubic arrangements employing self-assembling polystyrene (PS) spheres to pre-pattern a-plane sapphire substrates on which gold, silver or a metal free zinc oxide seedlayer were deposited. A cubic arrangement of the PS spheres is achieved with a spin coating method. To remove the catalyst regions not protected by the PS spheres we apply wet-chemical etching. In a CVD growth process ZnO nanopillars with diameters between 200 and 500 nm and lengths up to 5 μm are grown in hexagonal and cubic arrangements. The influence of growth catalysts on growth and crystal quality is investigated and compared by cathodoluminescence, photoluminescence, energy dispersive X-ray spectroscopy and high resolution X-ray diffraction measurements.

HL 44.56 Tue 18:00 P3

vapor phase growth of ZnO single crystals — •xi zhang[1], frank herklotz[1], ellen hieckmann[1], jörg weber[1], and peer schmidt[2] — [1]Institute für Angewandte Physik, Technische Universität Dresden, 01062, Dresden, Germany — [2]Institute für Anorganische Chemie, Technische Universität Dresden, 01062, Dresden, Germany

Zinc oxide is a promising wide band gap semiconductor for future optoelectronic devices. Today ZnO bulk single crystals are grown by three different techniques: hydrothermally, from the melt and by chemical vapor transport. For our studies we employed in addition a simple and low cost vapor phase method which gives us good quality crystals and flexibility in crystal doping. The as-grown single crystals were characterized by resistivity measurements, scanning electron microscopy, electron backscatter diffraction and low temperature photoluminescence spectroscopy. The biggest crystals so far are c-axis oriented needles with maximum length of 40 mm and maximum diameter of 1 mm. The needle-shaped crystals are n-type with main donors due to Al, Ga and In impurities. The growth conditions have a strong influence on the optical properties of as-grown crystals.

This work was supported by the European Regional Development Fund and the Free State of Saxony. SAB project 14253/2423.

HL 44.57 Tue 18:00 P3

Time-resolved photoluminescence spectroscopy on ZnO based films grown by molecular beam epitaxy — •Manuel H. W. Bader, Marcel Ruth, Christina A. Fobbe, and Cedrik Meier — University of Paderborn, Experimental Physics & CeOPP, Warburger Str. 100, 33098 Paderborn

Due to its unique properties such as the large direct bandgap of 3.37 eV and its high exciton binding energy of 60 meV, zinc oxide (ZnO) is a very promising semiconductor for optoelectronic and photonic applications even at room temperature. By adding cadmium (Cd) or magnesium (Mg) the bandgap can be tuned between 2.5 eV and 4.3 eV.

Especially quantum wells and multi-quantum wells can serve as light

emitting sources inside photonic devices. Therefore, thin ZnO and (Zn,Mg)O films have been grown in a plasma assisted molecular beam epitaxy system using silicon (111), sapphire (0001) and ZnO (0001) substrates. Growth conditions were systematically studied using in-situ reflection high energy electron diffraction (RHEED) and ex-situ atomic force microscopy (AFM), x-ray diffraction (XRD) and photoluminescence (PL).

Recombination dynamics and binding energies are studied using time resolved photoluminescence spectroscopy in the temperature range between T=7 K and 300 K.

HL 44.58 Tue 18:00 P3

Donor-acceptor pair recombination in ZnO — •Marko Stölzel, Alexander Müller, Stefan Müller, Gabriele Benndorf, Michael Lorenz, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Institut für Exp. Physik II, Abteilung Halbleiterphysik, Linnéstr. 5, 04103 Leipzig

ZnO is due to its material properties an interesting semiconductor for electronic and optoelectronic applications. However, the difficulties in growing stable p-type ZnO have inhibited the commercial fabrication of devices such as LEDs. Reported acceptor activation energies are usually well above 100 meV. Therefore, only a small fraction of such acceptors would be ionized at room temperature in p-type ZnO.

In this study we report on a donor-acceptor pair (DAP) recombination at 3.325 eV at 2 K found in a nominally undoped ZnO film grown by pulsed-laser deposition on a ZnO:Al buffer layer on a-sapphire.

The sample has been investigated by temperature-dependent time-integrated and time-resolved photoluminescence (PL) as well as electrical investigations. The PL measurements show a clear shift of the DAP recombination to higher energies with increasing excitation power. The transients exhibit a clear non-exponential behavior typical for DAP recombination and were described by the model of Thomas et al. [1] yielding the donor concentration, the Bohr radius of the donor and the pair distance. The determined donor concentration is in good agreement with that obtained from electrical measurements. From that we deduce an acceptor binding energy between 60 and 80 meV.

[1] D. G. Thomas et al. Phys. Rev. **140**, A202 (1965)

HL 44.59 Tue 18:00 P3

Thermal stability of ZnO/ZnCdO/ZnO double heterostructures — Martin Lange, •Anna Reinhardt, Christof P. Dietrich, Gabriele Benndorf, Michael Lorenz, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Semiconductor Physics Group, Linnéstr. 5, D-04103 Leipzig, Germany

Band gap engineering is essential for the fabrication of efficient optoelectronic devices, which are based on heterostructures. For ZnO-based heterostructures, a material with a reduced bandgap is e.g. achieved by incorporation of Cd in ZnO.[1] As in the device fabrication, the behavior of the alloy during post-growth thermal processing is an important issue we studied the thermal stability of ZnO/ZnCdO/ZnO double heterostructures (Cd-DHS). The samples were grown by a pulsed laser deposition process on *a*-plane sapphire substrates using ZnO and CdO targets.[2] The Cd-DHS were annealed in air at temperatures from 620 °C to 970 °C to study their thermal stability.

Luminescence features of ZnO and ZnCdO where observed for the as-grown samples as well as for the annealed samples. Due to the annealing the ZnCdO-related luminescence exhibited a monotonic blue-shift with increasing annealing temperature. The underlying diffusion process, which explains the blue-shift, was investigated to determine the diffusion coefficient for the different annealing temperatures. The activation enthalpy of the diffusion coefficient was found to be between 2.1 eV and 3.5 eV, depending on the growth conditions.

[1] S. Sadofev *et al.*, Appl. Phys. Lett. **89**, 201907 (2006)
[2] M. Lange *et al.*, J. Appl. Phys. **107**, 093530 (2010)

HL 44.60 Tue 18:00 P3

Defects in ZnO thin films studied by photo-capacitance measurements — •Robert Karsthof, Matthias Schmidt, Holger v. Wenckstern, Rainer Pickenhain, and Marius Grundmann — Universtity of Leipzig, Institute for Experimental Physics II, Linnéstraße 5, D-04103 Leipzig

In zinc oxide (ZnO) extensive knowledge on localized electronic states in the vicinity of the conduction band edge exists whereas the number of reported hydrogenic acceptor states or deep levels in the midgap region is scarce. One reason is that capacitance spectroscopic methods commonly measure the thermal emission rate of trapped charge carriers. This works well for levels within 1 eV from the respective band edge at experimentally accessible temperatures and measurement times. In this study we investigated electronic states in the midgap and the vicinity of the valence band of pulsed laser deposited ZnO thin films by means of capacitance spectroscopy with additional optical excitation. The samples were thermally annealed in 700 mbar oxygen and nitrogen atmosphere as well as in vacuum at approx. 700 °C. Two states in the vicinity of the valence band have been detected of which at least one is generated by annealing the samples under low oxygen partial pressures. The photo-ionisation cross-section of the latter one was determined. A midgap level with a threshold photo-ionisation energy of approx. 1.7 eV was detected in every investigated sample. Concentration profiles of the investigated traps have been obtained from capacitance-voltage measurements conducted in the dark as well as under monochromatic excitation.

HL 44.61 Tue 18:00 P3

Back-illuminated visible-blind and wavelength selective metal-semiconductor-metal photodetectors based on MgZnO-heterostructures — •Zhipeng Zhang, Holger von Wenckstern, Jörg Lenzner, Michael Lorenz, Holger Hochmuth, and Marius Grundmann — Universität Leipzig, Fakultät für Physik und Geowissenschaften, Institut für Experimentelle Physik II, Linnéstraße 5, 04103, Leipzig

We report on the utilization of $Mg_{x_1}Zn_{1-x_1}O/Mg_{x_2}Zn_{1-x_2}O$ heterostructure having two different Mg-content ($x_1 < x_2$) enabling the construction of wavelength-selective backside-illuminated photodetectors. For that, the $Mg_{x_2}Zn_{1-x_2}O$-layer is heteroepitaxially grown by pulsed-laser deposition on a both-side polished a-plane sapphire substrate, and acts as an integrated optical passive filter blocking high energy radiation. Subsequently the $Mg_{x_1}Zn_{1-x_1}O$-layer, being the active layer of the devices is deposited. The width of bandpass of the devices is given by the bandgap difference of the two MgZnO-layers, and the center of bandpass can be shifted by using different combination of x_1 and x_2. The Schottky contacts of the interdigital metal-semiconductor-metal (MSM) structure were fabricated by reactive dc-sputtering of Pd and Pt with Pd- and Pt-capping [1], respectively.

[1]: H. v. Wenckstern *et al.*, Mater. Rec. Soc. Symp. Proc., **1201**, H04-02 (2010)

HL 44.62 Tue 18:00 P3

Investigation of the band structure of $Zn_xMg_{1-x}O$ alloys — •Christian Franz, Michael Czerner, Marcel Giar, Markus Heinemann, and Christian Heiliger — I. Physikalisches Institut, Justus Liebig University Giessen, D-35392, Germany

We investigate the electronic structure of $Zn_xMg_{1-x}O$ alloys as a function of composition *ab initio* by means of density functional theory. Thereby, we model the alloys by using the coherent potential approximation (CPA) [1] implemented in a Korringa-Kohn-Rostoker Green's function method. Within the CPA the band structure itself is not well defined but we can analyze the Bloch spectral functions. Out of these spectral functions we extract effective masses, the positions of band edges, and the band gap. All these quantities are discussed with respect to their dependence of composition.

[1] Soven, P.,*Coherent-Potential Model of Substitutional Disordered Alloys* , Physical Review 156,(1967)

HL 44.63 Tue 18:00 P3

Microstructuring and characterization of Cu_2O/ZnO heterostructures — •Sören Zint, Julian Benz, Achim Kronenberger, Daniel Reppin, Philipp Hering, Torsten Henning, Peter J. Klar, and Bruno K. Meyer — I. Physikalisches Institut, Justus-Liebig-Universität, Heinrich-Buff-Ring 16, 35392 Giessen

Cuprous oxide (Cu_2O) is a promising candidate for photovoltaic applications due to its direct band gap in the visible spectral range. Moreover Cu_2O is a non toxic and sustainable material. Thin Cu_2O films can be deposited on different substrates by sputtering. Since the production of n-type Cu_2O is a difficult task, ZnO can be employed for fabricating a p-n-junction. We report on the growth of lateral Cu_2O/ZnO heterostructures and current-voltage measurements of these systems. We present a model for explaining the influence of the interface cross-section distribution on the current-voltage characteristics.

HL 44.64 Tue 18:00 P3

***Ab initio* investigations of Mg diffusion in ZnMgO** — •Marcel Giar and Christian Heiliger — I. Physikalisches Institut, Justus-Liebig-Universität, D-35392 Giessen, Germany

We present *ab initio* calculations of possible diffusion paths for a single Mg atom in a ZnMgO supercell. Simple models are selected for the diffusion paths. We further estimate the energetic barrier by assuming that thermal energy at room temperature and elevated temperature suffices to activate the diffusion within the structure.

HL 44.65 Tue 18:00 P3

Preparation of donor doped ZnO_xS_{1-x} thin films — •Achim Kronenberger, Philipp Schurig, Andreas Laufer, Hauke Metelmann, Jan E. Stehr, Jan Philipps, Benedikt Kramm, Angelika Polity, Detlev M. Hofmann, and Bruno K. Meyer — I. Physikalisches Institut, Justus-Liebig-Universität Giessen, Heinrich-Buff-Ring 16, 35392 Giessen, Germany

It is well known that ZnO can easily be doped n-type which is commonly realized by incorporating group-III elements on a Zn lattice place. In contrast to that there are rather few publications reporting successful n-type doping of ZnS. The ternary material system ZnO_xS_{1-x} can be prepared without any miscibility gap by radio frequency sputtering. This offers the possibility to study the electrical activity of the shallow donor dopants over the complete composition range. In our work ZnO_xS_{1-x} thin films were deposited from a ceramic ZnS target by radio frequency sputtering on glass, sapphire and semiconductor substrates. Through reactive sputtering with oxygen gas the film composition can be adjusted to the wanted oxygen/sulphur ratio. As dopants Al, F and H were incorporated by using additional target material or reactive gas, respectively.

HL 44.66 Tue 18:00 P3

An EPR investigation of the nitrogen center in ZnO — •Jan E. Stehr, Detlev M. Hofmann, and Bruno K. Meyer — 1st Physics Institute, Justus-Liebig-University Gießen, Heinrich-Buff-Ring 16, 35392 Gießen, Germany

ZnO with the direct band gap of 3.36 eV at room-temperature is a promising material for UV light emitting devices. Therefore it is necessary to have n-type conducting ZnO as well as p-type conducting ZnO. Since ZnO is an intrinsic n-type material, p-type conductivity is the major challenge. In the last years it turned out that nitrogen is the most promising candidate.

We investigated an electron irradiated Eagle Picher ZnO bulk crystal with the method of Electron Paramagnetic Resonance (EPR). After illumination with light the well known 3-line EPR spectrum of nitrogen with I=1 in ZnO shows up [1]. We tracked the angular dependency of the 3 lines and the 6 *forbidden* EPR transitions of nitrogen. Photon-irradiation with energies higher than 2.2 eV leads to the creation of the EPR-signal and with energies of 0.7 eV it was also possible to quench it. Also the time-dependency of the EPR-signal was measured to get information on its creation- and the decay-behavior.

[1] N. Y. Garces et al., Appl. Phys. Lett. 80, 1334 (2002)

HL 44.67 Tue 18:00 P3

Electric properties of ZnO thin films before and after ion irradiation — •Florian Kuhl, Markus Piechotka, Martin Fischer, Torsten Henning, and Peter J. Klar — 1. Physikalisches Institut, Justus-Liebig-Universität, Heinrich-Buff-Ring 16, 35392 Giessen

ZnO doped with Al (AZO) is a transparent conducting oxide (TCO) and arouses interest for spacecraft applications, for example as electrode or covering layer in solar cells. In space environment this material has to resist radiation. We exposed AZO thin films to beams of Ar^+-ions to simulate the particle irradiaton in space environment.

Before and after irradiaton we characterized the surface morphology and the electrical properties of the thin films and compared them. The electrical properties, i.e. the carrier concentration and the mobility were measured in the van-der-Pauw geometry at temperatures from 1.5 K to 285 K. To investigate the surface morphology we used SEM and optical microscopy.

We found out that there are changes in electrical properties at an acceleration voltage of 500 V. With lower acceleration voltages we could not find significant changes of the electrical properties.

HL 44.68 Tue 18:00 P3

Influence of nitrogen on optical properties of zinc oxide using Raman spectroscopy — •Christian Reindl, Julian Benz, Thomas Sander, Stefan Lautenschläger, Sebastian Eisermann, Peter J. Klar, and Bruno K. Meyer — I. Physikalisches Institut, Justus-Liebig-Universität, Heinrich-Buff-Ring 16, 35392 Gießen

The wide bandgap semiconductor zinc oxide (ZnO) is an interesting material for the production of blue and UV optoelectronic devices. P-type doping remains an obstacle for fabricating devices completely based on ZnO. Since nitrogen is a promising candidate for p-type doping ZnO, thin ZnO:N layers produced by low temperature CVD using ammonia as precursor for nitrogen were investigated. We studied the influence of nitrogen on the optical properties of ZnO by Raman spectroscopy. Numerous modes related to nitrogen were found in the Raman spectra. We investigated angle dependence and the scaling of these modes with the N-concentration using green and red lasers.

HL 44.69 Tue 18:00 P3

The Role of Power-Law Correlated Disorder in the Anderson Metal-Insulator Transition — •Alexander Croy[1], Philipp Cain[2], and Michael Schreiber[2] — [1]Max-Planck-Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany — [2]Institut für Physik, Technische Universität, 09107 Chemnitz, Germany

The Anderson Model of localization provides a paradigmatic description of a metal-insulator transition (MIT). A systematic variation of the effective disorder of the energy potential in a three dimensional (3D) sample leads to a change of the electronic wave function from extended to localized behavior. This MIT is characterized by a set of critical parameters,e.g., universal exponents, which depend on the type of disorder.

Here we study the case of long-ranged power-law correlated disorder. In one dimension we compare our numerical results with analytical predictions. In 3D the influence of long-range correlations on the MIT is still largely unexplored. We present numerical simulations for the density of states and the localization length for 1D and 3D systems using standard transfer matrix calculations and finite size scaling of the largest inverse Lyapunov exponent. Further we discuss the phase diagram of the MIT and the influence of the correlations on the critical exponents.

HL 44.70 Tue 18:00 P3

Disorder Induced Metal-Insulator Transition in Crystalline $Ge_1Sb_2Te_4$ — •Hanno Volker[1], Theo Siegrist[1,2], Peter Jost[1], Michael Woda[1], Philipp Merkelbach[1], Carl Schlockermann[1], and Matthias Wuttig[1] — [1]1st Institute of Physics (IA), RWTH Aachen, 52056 Aachen, Germany — [2]Department of Chemical and Biochemical Engineering, FSU, Tallahassee, FL 32310

Localization of charge carriers in crystalline solids has been the subject of numerous investigations over more than half a century. Materials showing a metal to insulator transition (MIT) without a structural change are therefore of great interest. Concepts based on electron correlation (Mott) or disorder (Anderson) are often invoked to explain such an MIT, but a clear distinction between the two mechanisms is difficult.

In this study [1] we report the observation of an MIT in crystalline $Ge_1Sb_2Te_4$ which is caused by disorder-induced localization in the 3-dimensional solid. A combination of X-ray diffraction experiments as well as optical (FT-IR) and electrical measurements reveals that the observed MIT is an intra-grain effect. The Hall carrier density barely changes during the MIT and is much higher than predicted by the Mott criterion. Therefore, the MIT is not of the Mott type, but driven by disorder.

[1] Siegrist, T. *et al.* Disorder Induced Localization in Crystalline Phase Change Materials. *Accepted for publication in Nature Mater.*

HL 44.71 Tue 18:00 P3

Statistical analysis of contact resistance between P3HT and several electrode materials on flexible substrates — •Arne Hendel, Miriam Hehn, and Veit Wagner — Jacobs University Bremen, School of Engineering and Science, Campus Ring 1, 28759 Bremen, Germany

Finite contact resistance in organic field-effect transistors is one of the major obstacles towards higher switching frequencies. In this work optimal contact materials / treatments for the organic semiconductor poly(3-hexylthiophen) (P3HT) are identified. Considered candidates are sputtered or printed Copper, Gold and Silver structures. For proper comparison the preparation of many devices (>50) and statistical analysis was found to be essential to overcome the finite sample to sample variation typically observed in organic field effect transistors

(OFETs). To avoid dominating influences of adsorbates on the work functions of the different metals, ozone cleaning has been optionally applied before spin-coating the P3HT layer. The identified contact resistances were further investigated by potential mapping of the transistor channel enabled by additionally patterned sense fingers. This approach allows to determine the relative weight of source and drain contribution to the total contact resistance.

HL 44.72 Tue 18:00 P3

Contact degradation in wet-chemically produced high mobility semiconductor devices — •Mark Nikolka, Marlis Ortel, and Veit Wagner — School of Engineering and Science, Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

Novel wet chemical processing techniques have recently enabled to produce very high mobility devices, e.g. diodes or field-effect transistors (FETs). Yet, for high mobility devices effects start playing a role which previously could be neglected. One of these effects is contact degradation due to high current densities which eventually renders the device useless.

Therefore, a study was done on high mobility ($\mu > 1\ cm^2/Vs$) FETs made from a metal oxide-based semiconductor with gold as electrode material. The investigated devices had wide electrodes with a typical cross sectional area of 20 um x 30 nm, i.e. the electrodes were wider than the channel length of the transistor. Nevertheless these devices showed strong effects of contact degradation even after recording a single electrical device characteristic lasting less than 60 seconds. Those effects hence, could be related to high current densities present in the FET electrode finger structure. Furthermore, it was found that different types of damages occurred at the source and the drain contact, respectively. This difference cannot be explained by simple electromigration just in the elctrodes but has to be correlated to the transistor channel as well. A corresponding, more complex model is presented which explains the experimental findings.

HL 44.73 Tue 18:00 P3

Optical spectroscopy study of c(4x2) Ge (001)-surfaces, covered with atomic Au wires — Utz Bass[1], Eugen Speiser[2], Sebastian Meyer[1], Jörg Schäfer[1], Norbert Esser[2], and •Jean Geurts[1] — [1]Universität Würzburg, Physikalisches Institut, Am Hubland, 97074 Würzburg — [2]ISAS, Albert-Einstein-Straße 9, 12489 Berlin

Novel quasi-1D systems like e.g. atomic gold chains on a c(4x2) reconstructed Ge(001)-surfaces enable the investigation of 1D-effects like the possible occurrence of the Luttinger- to Fermi liquid transition. As there is a crucial interplay of the lattice vibrations and the electrical and structural properties on such sensitive systems, phonon dynamics are in the focus of this work. The phonons were addressed by Raman spectroscopy and reveal a clear change from the Ge-oxide layer to the final surface with Au-nano wires. Thermally deoxidizing the Ge-surface under UHV leads to a distinct low-frequency vibration around 65cm-1. Its frequency range and its persistence after Gold deposition in the submonolayer range indicate that this signal is surface related. Additionally, the surface-induced anisotropy of the optical reflectance was complementary investigated by Reflectance-Anisotropy-Spectroscopy (RAS) and IR-ellipsometry.

HL 44.74 Tue 18:00 P3

Detailed analysis of hydrogen termination of MOVPE prepared Si(100) surfaces — Sebastian Brückner, Anja Dobrich, •Claas Löbbel, Peter Kleinschmidt, Henning Döscher, and Thomas Hannappel — Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

Hydrogen is usually present as carrier gas and by-product from precursors during the preparation of Si(100) in the MOVPE environment. The step structure of the silicon surface might be strongly affected by hydrogen. For a detailed analysis of hydrogen at the Si(100) surface, we applied reflectance anisotropy spectroscopy (RAS) for in situ monitoring and used various surface sensitive UHV-based techniques accessed by a contamination free MOVPE to UHV transfer system.

At Si(100), RAS measures characteristic spectra for the clean and hydrogen terminated surface, which enabled us to study H adsorption and desorption during preparation. Fourier-transform infrared (FTIR) spectroscopy in an attenuated total reflection (ATR) configuration enabled surface sensitive measurements of the silicon hydrogen bonds. Tip induced H desorption by scanning tunneling microscopy (STM) evidenced the complete H termination of the surface.

Correlation between these results led to the conclusion that the surface is hydrogen free at high temperatures of T > 900°C in H_2 ambient and monohydride terminated after cool down in H_2.

HL 44.75 Tue 18:00 P3

Density-Functional Investigation of Gallium Phosphide- Silicon Interface — •Gabi Steinbach[1], Michael Schreiber[1], Sibylle Gemming[1,2], Henning Döscher[3], and Thomas Hannappel[3] — [1]Institut für Physik, Technische Universität Chemnitz, D-09107 Chemnitz, Germany — [2]Institute of Ion Beam Physics and Materials Research, HZ Dresden-Rossendorf, Postfach 51 01 19, D-01314 Dresden, Germany — [3]Helmholtz Center Berlin for Materials and Energy, Hahn-Meitner-Platz 1, D-14109 Berlin, Germany

Gallium phosphide is an established compound semiconductor in the optoelectronic industry with an indirect band gap of 2.26 eV. Used as substrate for GaAsP LEDs or active LED material itself, GaP thin films on cheaper silicon substrates promise a high application potential for LED engineering. The present study addresses the material discontinuities occuring at the boundaries of a GaP thin functional layer on a silicon substrate. Density-functional calculations have been performed with the pseudopotential plane-wave code ABINIT [1]. At the ideally flat GaP(001)|Si(001) interface both the Ga-rich and the P-rich terminations of the GaP layer are studied along with partially Si-occupied boundary layers. Substantially negative values of the work of separation for all investigated interfaces indicate the high stability and the low remanent stresses at the GaP-Si interface. Extended studies contain steps along the <110> direction with the aim to distinguish point-defects and line-defects as origin of the experimentally observed anti-phase boundaries. [1] www.abinit.org.

HL 44.76 Tue 18:00 P3

Raman study of band-bending at ZnSe/GaAs(001) interfaces — Utz Bass, Alex Frey, Suddhasatta Mahapatra, Claus Schumacher, Karl Brunner, and •Jean Geurts — Universität Würzburg, Physikalisches Institut, Experimentelle Physik III, Am Hubland, 97074 Würzburg

At heterovalent interfaces thermodynamically induced intermixing of the constituent materials with different numbers of valence electrons usually causes large variations in band offsets and local doping density, depending on the spatial arrangement of atoms at the interface. We varied the interface stoichiometry of n-doped ZnSe / GaAs (001) heterostructures by the predeposition of different amounts of Zn or Se on n-GaAs prior to n-ZnSe layer growth by MBE. The induced changes in band bending were optically analysed by Raman spectroscopy from coupled Plasmon-LO-Phonon modes and by Far-Infrared reflectance spectroscopy for calibration. We detect a depletion layer of about 50 nm at the heterointerface, which partially shifts from the GaAs into the ZnSe with Se predeposition. Together with data from electrical transport across the interface and capacitance-voltage profiling, our results are explained consistently by a 550 mV potential barrier in the conduction band at a Zn-rich n-ZnSe / n-GaAs interface, which is tuned down to about 70 mV by increasing Se predeposition. In addition, PL signatures for excitation above and below the ZnSe band gap are presented.

HL 44.77 Tue 18:00 P3

Electro-forming – the initial step to resistance switching in vacancy-doped metal-$SrTiO_3$-metal structures — •Florian Hanzig, Juliane Seibt, Ralph Strohmeyer, Hartmut Stöcker, Barbara Abendroth, and Dirk C. Meyer — TU Bergakademie Freiberg, Institut für Experimentelle Physik, Leipziger Straße 23, 09596 Freiberg

Strontium titanate is a widely-used model oxide for solids which crystallize in the perovskite-type of structure. With its large bandgap energy, high dielectric constant and its mixed ionic and electronic conductivity, $SrTiO_3$ is a candidate material for future metal-insulator-metal (MIM) structures in resistive switching memory cells. Here, strontium titanate single crystals doped with oxygen vacancies induced by high temperature vacuum annealing were used. The essential step to enable resistive switching is the electro-forming of the structures by dedicated current-voltage programs. Therefore, the longtime current behaviour of such MIM stacks was investigated. A degradation of the electrical resistance led to a minimum resistivity after a characteristic forming time. During continued formation the resistivity increases up to a failure of the system. A model related to oxygen vacancy diffusion and the introduction of novel structural phases near the surface is proposed.

HL 44.78 Tue 18:00 P3

Investigation of morphological changes of $SrTiO_3$ surfaces induced by annealing and ion bombardment — •Ralph Strohmeyer, Juliane Seibt, Florian Hanzig, Tina Nestler, Mandy Koitzsch, Hartmut Stöcker, Barbara Abendroth, and Dirk C. Meyer — TU Bergakademie Freiberg, Institut für Experimentelle Physik, Leipziger Straße 23, 09596 Freiberg

Strontium titanate is a promising oxide semiconductor in which oxygen vacancies act as intrinsic donors. In order to produce n-doped layers, several approaches to modify the crystal surface are possible. Different methods of vacuum annealing and ion implantation are commonly used. Here, we use atomic force microscopy to study $SrTiO_3$ single crystal surfaces that were modified according to these known methods to investigate whether the surface structure is changed during the process and if the electrical properties correlate with these changes. Based on the morphology of the untreated surface, which shows a terrace structure with step heights equal to the dimensions of the cubic $SrTiO_3$ unit cell, the exposure to heat leads to a formation of 'bubble-like' structures and possibly even local melting and recrystallization. The kind of restructuring strongly depends on temperature and exposure time. The implantation of different ions (i.e. of Ar, O and H) is found to have a comparatively weaker impact on the surface morphology.

HL 44.79 Tue 18:00 P3

Strontium titanate surface and bulk modifications due to vacuum annealing — •Juliane Seibt, Florian Hanzig, Ralph Strohmeyer, Hartmut Stöcker, Barbara Abendroth, and Dirk C. Meyer — TU Bergakademie Freiberg, Institut für Experimentelle Physik, Leipziger Straße 23, 09596 Freiberg

Vacuum annealing is a widely used method to increase the electric conductivity of $SrTiO_3$ single crystals. The induced oxygen vacancies act as intrinsic donors and lead to n-type conductivity. Apart from the changed electric properties, however, also structural modifications arise from this treatment. Here, we try to summarize all such changes originating from the in-vacuum heat-treatment. Used characterization methods include atomic force microscopy, transmission electron microscopy, X-ray diffraction, ellipsometry, infrared and photoluminescence spectroscopy. Beside the expected variation of bulk properties, especially surface modifications could be detected. The intrinsic number of near-surface dislocations in the samples was reduced by vacuum annealing but the surface roughness increased due to a self-organized restructuring process. Furthermore, the photoluminescence spectra revealed dependencies on exposure time and surrounding atmosphere. The influence of adsorbed or intrinsic surface layers on the observed behaviour will be discussed.

HL 44.80 Tue 18:00 P3

Cubic-tetragonal phase transition at elevated temperatures and resistivity hysteresis of surface vacuum annealed $SrTiO_3$ — •Tina Nestler[1], Kay Potzger[2], Hartmut Stöcker[1], Barbara Abendroth[1], Ralf Strohmeyer[1], Robert Zierer[1], and Dirk C. Meyer[1] — [1]TU Bergakademie Freiberg, Institut für Experimentelle Physik, 09596 Freiberg, Germany — [2]Forschungszentrum Dresden-Rossendorf e.V., Institut für Ionenstrahlphysik und Materialforschung, Bautzner Landstraße 128, 01328 Dresden, Germany

Electrical properties of $SrTiO_3$ single crystal samples treated by an anisotropic surface annealing technique under reducing conditions have been investigated in the temperature range of 35 K–300 K. Optical and atomic force microscopy shows that annealing gives rise to the formation of colored dendritic structures and polycrystallization. Hall and resistivity measurements show metallic behavior due to oxygen vacancy doping. Additionally, the temperature dependent resistivities indicate the cubic-tetragonal phase transition, which has not been reported to our knowledge before. Furthermore, the transition occurred up to 53 K above the known bulk transition temperature T_C at 105 K with a hysteresis up to a temperature of 220 K. Both phenomena possibly arise from dislocations and associated strains introduced by surface annealing that are assumed to lower the free energy of the tetragonal phase and simultaneously pin tetragonal domains. Thus, microregions of the tetragonal phase persist above T_C causing the hysteresis in resistivity up to ∼3 %. This possibly provides new chances for future oxide based non-volatile data storage devices.

HL 44.81 Tue 18:00 P3

Valence Change of $SrTiO_3$ in a DC Electric Field due to Oxygen Redistribution — •Hartmut Stöcker[1], Tilmann Leisegang[2], Matthias Zschornak[1], Juliane Seibt[1], Florian Hanzig[1], and Dirk C. Meyer[1] — [1]TU Bergakademie Freiberg, Institut für Experimentelle Physik, Leipziger Str. 23, 09596 Freiberg — [2]Forschungszentrum Dresden-Rossendorf, Bautzner Landstr. 400, 01328 Dresden

Strontium titanate is an oxidic semiconductor and crystallizes in the perovskite-type of structure, however, several methods have been shown to induce distortions of this perfect cubic lattice. One of the key parameters is the oxygen stoichiometry that on the one hand acts as doping and has great influence on the electric conductivity but on the other hand also couples to the crystal structure. Since oxygen ions and vacancies are electrically charged, external electric fields make it possible to redistribute oxygen and to study accompanying structural modifications. Therefore, $SrTiO_3$ (001) wafers have been investigated *in situ* by fluorescence X-ray absorption near edge structure (XANES) analysis in grazing incidence geometry. The XANES spectra show a clear shift of the Ti-K absorption edge energy depending on the polarity of the applied static electric field. The shift can be attributed to a change of the Ti valence state due to diffusion of oxygen in the near-surface region. No shift was observed for the Sr-K absorption edge energy. A controlled switching of the Ti valance may give rise to a variety of interesting applications.

HL 44.82 Tue 18:00 P3

Electrical and Optical Characterisation of ta-C/Silicon MASS Diodes — •Julian Alexander Amani, Marc Brötzmann, Ulrich Vetter, and Hans Hofsäss — Georg-August-Universität Göttingen, II. Physikalisches Institut, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

The metal - amorphous semiconductor - semiconductor (MASS) system metal/ta-C/silicon forms heterojunctions, which exhibit a pronounced rectifying behaviour, low saturation current and low parasitic currents. The conduction in this system is well described by a serial arrangement of an ideal Schottky diode and a Frenkel-Poole resistance which is dominant at forward bias [1,2].

In this work ta-C based MASS diodes were produced via mass separated ion beam deposition of carbon on p-type silicon substrates. To facilitate photoconductivity measurements of the heterostructures ITO was used as gate contact.

We present electrical characterizations of those structures with I-V and C-V measurements. Time and wavelength resolved photoconductivity measurements were performed in order to find the energetic distribution of defect states in the ta-C band gap.

[1] M. Brötzmann et al., JAP 106, 063704 (2009)
[2] M. Brötzmann et al., PSS C 7, 256 (2009)

HL 44.83 Tue 18:00 P3

The study of Landé g-factor and effective mass of electrons in GaAs/AlGaAs quantum wells — •feng liu[1], alexander schwan[1], gregor bartsch[1], dmitri yakovlev[1], k biermann[2], r hey[2], p.v. antos[2], and manfred bayer[1] — [1]Experimental Physics 2, TU Dortmund University, D-44221 Dortmund, Germany — [2]Paul-Drude-Institute für Festkörperelektronik, 10117 Berlin, Germany

The Landé g-factor is a quantity which characterizes energy levels of electrons in magnetic field. The g-factor is important because the behavior of electron spins can be manipulated by controlling the electron g-factor. In our work, the influence of the spin-orbital splitting in the conduction band in GaAs quantum wells (QWs) on electron g-factor was studied. The g-factor of free electrons in GaAs/AlGaAs QWs with and without spin-orbit splitting in the conduction band was measured using time-resolved Kerr rotation technique and compared. It was found that the spin-orbit splitting of the conduction band only slightly influence the electron g-factor. Additionally, the effective mass of free electrons is also measured using optically detected cyclotron resonance technique and internal transitions of trions were observed.

HL 44.84 Tue 18:00 P3

Reducing the dislocation density of GaAs on Si(001) using InAs quantum dots — •Martin Etter, Michael Wiesner, Wolfgang-Michael Schulz, Robert Rossbach, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und funktionelle Grenzflächen, Universität Stuttgart, Allmandring 3, 70569 Stuttgart, Germany

In order to integrate optoelectronics with standard Si microelectronics, several attempts were made to grow GaAs on Si by using buffer layers of Ge/GeSi/Si or graded GaAsP or InGaP layers or the use of

strained-layer superlattices consisting of InGaAs, GaAsP or AlGaAs layers to overcome the large lattice mismatch and the different thermal expansion coefficient. A novel approach is the implementation of InAs quantum dots, which have the ability to suppress the dislocations which propagate to the GaAs surface due to their high strain field. In our work we characterize GaAs/Si-samples including different numbers of InAs quantum dot layers with a maximum GaAs layer thickness of 1 μm. Characterization is done by X-ray diffraction measurements, scanning electron microscopy (SEM), atomic force microscopy, respectively photoluminescence spectroscopy were perfomed to characterize the GaAs layers. Thereby SEM pictures show clearly the improvement of the GaAs surface compared to the other approaches. Furthermore, the influence on the quality of optoelectronic structures is shown.

HL 44.85 Tue 18:00 P3

Device Simulation of ZnO/Cu_2O Heterojunction Solar Cells — •Philipp Hering and Bruno. K. Meyer — 1. phys. Inst., Justus-Liebig-Universität, Heinrich-Buff-Ring 16, 35392 Giessen, Germany

Cuprous oxide thin films constitute despite the relatively large band gap (2.17 eV) a very promising absorber material for sustainable low cost photovoltaic application due to the high absorption coefficient and great abundance. A model was developed to describe the illuminated operation of the heterojunction zinc oxide forms with cuprous oxide, taking full account of interface recombination. Numerical analysis was performed, providing insight into the impact of the conduction band discontinuity, interface states and doping on power conversion efficiency

HL 44.86 Tue 18:00 P3

Determination of the band offset for the heterostructure ZnO/Cu_2O and ZnS/Cu_2O via X-Ray Photoelectron Spektroscopy (XPS) — •Benedikt Kramm, Andreas Laufer, Achim Kronenberger, Swen Graubner, Daniel Reppin, Alba Seibert, Philipp Schurig, Angelika Polity, and Bruno K. Meyer — 1. Physikalisches Institut, Justus-Liebig-Universität, Heinrich-Buff-Ring 16, 35392 Gießen, Germany

ZnO and Cu_2O are direct band-gap semiconductors. Both are promising materials for electronic devices like diodes, transistors or solar cells. Important is, that ZnO and Cu_2O contain only non toxic und sustainable elements. Due to a band-gap energy of 2.1 eV for Cu_2O a high absorption in the visible light spectrum could be obtained which is suitable for solar cells. We produced a heterojunction of intrinsic p-type Cu_2O and hydrogen doped n-type ZnO or ZnS on sapphire using sputter deposition. Investigating the energy band structure of the thin film heterojunction ZnO/Cu_2O via XPS yield to be a type II alignment with a valence-band offset between $2.4-2.7$ eV. Furthermore the band offset between ZnS and Cu_2O, using ZnS as a buffer-layer for the heterostructure ZnO/ZnS/Cu_2O, was explored. For the band offset structure of the whole system the band offset values for ZnS/ZnO, determined by Persson [1], have been used.

[1] Perrson et al. Strong Valance-Band Offset Bowing of $ZnO_{1-x}S_x$ Enhances p-Type Nitrogen Doping of ZnO-like Alloys, *Phys. Rev. Lett.*, Okt 2006, **97**(14):146403

HL 44.87 Tue 18:00 P3

Photoluminescence studies of top-down $Zn_{1-x}Mg_xO$/ZnO quantum square samples with different dimensions — •Martin Fischer[1], Markus Piechotka[1], Torsten Henning[1], Alexej Chernikov[3], Bernhard Laumer[2], Sangam Chatterjee[3], Peter J. Klar[1], Martin Eickhoff[1], and Bruno K. Meyer[1] — [1]I. Physikalisches Institut, Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, 35392 Gießen — [2]Walter-Schottky-Institut, Technische Universität München, Am Coulombwall 3, 85748 Garching — [3]Fachbereich Physik, Philipps-Universität Marburg, Renthof 5, 35032 Marburg

Quantum square structures with lateral lengths from 100 nm to 4 μm were prepared from PAMBE-grown $Zn_{1-x}Mg_xO$/ZnO single quantum well samples with 10 nm well width and a Mg content of 0.16 by using electron beam lithography followed by ion-beam etching. Low temperature photoluminescence spectroscopy studies were done on groups of several squares. We also investigated single squares in time-dependent photoluminescence spectroscopy. We report the influence of strain relaxation in quantum squares of different dimensions on the excitonic transitions. The lateral dimension of the quantum squares allows one to exclude additional lateral quantum confinement effects in the samples.

HL 44.88 Tue 18:00 P3

Spectroscopic ellipsometry for process control in PLD growth — •Jan Lorbeer, Tammo Böntgen, Jan Zippel, Rüdiger Schmidt-Grund, Michael Lorenz, and Marius Grundmann — Universtät Leipzig, Institut für Experimentelle Physik II, Linnéstr. 5

We present detailed measurements of the surface condition of typical substrates and the dynamics of growth processes in heterostuctures. Process control is a vital part of modern thin film synthesis. We have used in situ spectroscopic ellipsomety (SE) to gain inside into the growth process of several oxidic compounds. Surface quality plays an important role for epitaxial growth as it determines the possible relations between the substrate and the epilayer. Thus in situ control of the surface condition is of importance. This is especially true when special growth conditions lead to surface reconstruction or the formation of oxide layers. We have investigated the surface of severals typical substrates (e.g. Si, GaAs, ZnO). Si and GaAs both exhibit the growth of an oxide layer when exposed to high oxygen partial pressure during heating. When heated under vacuum conditions on the other hand the a reduction of the Si oxide layer thickness was observed. ZnO is also prone to oxygen loss in low pressure conditions, leading to a reduction of the ZnO surface. We observed a change of the surface of single crystal ZnO substrates when heated in vacuum conditions. These results are compared to RHEED measurement of the same sample. This work was supported by Deutsche Forschungsgemeinschaft in the framework of Sonderforschungsbereich 762 "Functionality of Oxidic Interfaces".

HL 44.89 Tue 18:00 P3

Combinatorial growth of ZnO resonators — •Helena Hilmer[1], Tom Michalsky[1], Chris Sturm[1], Rüdiger Schmidt-Grund[1], Jesús Zúñiga-Pérez[2], Renate Fechner[3], Frank Frost[3], and Marius Grundmann[1] — [1]Universität Leipzig, Inst. für Exp. Physik II, Linnéstr. 5, 04103 Leipzig — [2]CRHEA, Rue Bernard Grégory, 06560 Valbonne, France — [3]IOM e.V., Permoserstr. 15, 04318 Leipzig

We report on the growth of planar microresonators, which consist of two all-oxide Bragg reflectors surrounding either a MgZnO/ZnO quantum well (QW) structure or a ZnO bulk cavity as active medium. For the growth of such resonators, there is a competition between a high-quality photonic structure and a homogeneous electronic system. In order to improve both simultaneously we use a combination of different preparation techniques as pulsed laser deposition (PLD), molecular beam epitaxy (MBE) and ion beam smoothing (IBS).

ZnO bulk cavities, grown intentionally rough, yield good electronic properties. By applying IBS on these structures we have improved the photonic properties. Clearly, two polariton branches can be seen, which are related to the A-/B- (coupling strength $V_{A,B} \cong 15\,\mathrm{meV}$) and the C-exciton ($V_C \cong 60\,\mathrm{meV}$) at $T = 10\,\mathrm{K}$, indicating both, high photonic and electronic quality.

For the QW-cavity, we have found an influence of the resonator on the QW-exciton lifetime, i.e. resonator is in the weak coupling regime. For the enhancement of the oscillator strength, multiple QW-cavities have been grown by a combination of PLD and MBE showing smooth layers together with good electronic properties.

HL 44.90 Tue 18:00 P3

Cavity-photon mode dispersion in 1D confined optically anisotropic microresonators — •Chris Sturm, Helena Hilmer, Rüdiger Schmidt-Grund, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Linnéstraße 5, 04103 Leipzig

Microresonators with an anisotropic cavity medium, e.g. GaN and ZnO, became more important in the last years. These structures allow the realization of devices operating in the UV spectral range (e.g. blue LEDs) and the observation of a strong exciton-photon coupling at room temperature and above. For a precise description and understanding of the coupled particles the properties of the involved photons (especially their dispersion) have to be known.

Here we present an approach to the calculation of the cavity-photon dispersion which takes into account the optical anisotropy of the cavity medium as well as the number of layer pairs of the Bragg reflectors which are used as mirrors for the microresonator. Thereby we found, that even for a uniaxial c-plane oriented cavity with a birefringence of 3% (similar to that of ZnO), the influence of the anisotropy on the TE-TM splitting is in the same order of magnitude as the splitting itself. Therefore the anisotropy of the cavity medium cannot be neglected. Furthermore, we applied this model to a ZnO-based microresonator

which yields good agreement with the experimentally observed dispersion of the cavity-photon mode.

HL 44.91 Tue 18:00 P3

Electrical and structural properties of the ZnO/$BaTiO_3$ interface — •Peter Schwinkendorf, Kerstin Brachwitz, Tammo Böntgen, Jan Zippel, Holger Hochmuth, Michael Lorenz, and Marius Grundmann — Fakultät für Physik und Geowissenschaften, Institut für Experimentelle Physik II, Universität Leipzig

Semiconductor/ferroelectric heterostructures are important for the realisation of new microelectronic applications such as the ferroelectric field-effect transistor[1]. To develop corresponding technologies up to commercial relevance there are several problems left to be solved. In particular, the interface semiconductor/ferroelectric seems to be the major key to further progress.
ZnO/$BaTiO_3$(BTO) heterostructures were grown by pulsed laser deposition on $SrRuO_3$(SRO) covered $SrTiO_3$(100) substrates. X-Ray diffraction measurements revealed the orientation of the SRO layer to be (100) and that of BTO to be (001), respectively. The surface morphology of the particular layers was studied by atomic force microscopy. The interfaces are smooth exhibiting RMS values of about 1 nm. For electrical measurements ohmic top Au-contacts were fabricated by dc-sputtering. The conducting SRO layer ($\varrho = 3.3\times10^{-6}\,\Omega$m) serves as ohmic back-contact. Due to this design the structures are considered to be of MIS type. Current-voltage measurements indicate charging effects at the ZnO/BTO interface. To further investigate these charging effects, capacitance-voltage- and admittance-spectroscopy were performed.
[1] M. Brandt *et al.*, J. Vac. Sci. Technol. B, Vol. 27, 1789 (2009)

HL 44.92 Tue 18:00 P3

Growth induced structural defects in $BaTiO_3$3-ZnO-heterostructures — •Christian Kranert, Tammo Böntgen, Rüdiger Schmidt-Grund, Michael Lorenz, and Marius Grundmann — Universität Leipzig, Semiconductor Physics Group, Institut für Experimentelle Physik II, Leipzig, Germany

The coupling of the switchable and non-switchable polarization of ferroelectric ($BaTiO_3$) and pyroelectric (ZnO) materials, respectively, in heterostructures results in new physical effects which can be used for modulators, sensors and memories. Their fabrication requires epitaxial growth processes. We present investigations on the crystal structure of $BaTiO_3$-ZnO-heterostructures grown by pulsed laser depostion using X-Ray diffraction and Raman spectroscopy. The latter was carried out with an excitation wavelength of 325 nm in the absorption regime allowing to study the Raman spectra of ultra-thin (< 10 nm) $BaTiO_3$ layers.

We show that the orientiation of $BaTiO_3$ grown on ZnO can be switched between (001) and (111) by variation of the growth parameters for a certain range of the layer thickness. Especially the (111)-oriented $BaTiO_3$ layers exhibit the assembly of a hexagonal impurity phase. Different rotation domains were observed in the top layer ($BaTiO_3$ on ZnO or vice versa) in agreement with a recent group-theoretical treatment [1].

[1] M. Grundmann et al., Phys. Rev. Lett. **105**, 146102 (2010)

HL 44.93 Tue 18:00 P3

Plasma-oxidation of Ge(100)-surfaces characterized by MIES, UPS and XPS — •Lienhard Wegewitz[1], Sebastian Dahle[1], Oliver Höfft[2], Wolfgang Viöl[3], Frank Endres[2], and Wolfgang Maus-Friedrichs[1] — [1]Institut für Energieforschung und Physikalische Technologien, Technische Universität Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld, Germany — [2]Institut für Mechanische Verfahrenstechnik, Technische Universität Clausthal, Arnold-Sommerfeld-Str. 6, 38678 Clausthal-Zellerfeld, Germany — [3]HAWK Göttingen, Fakultät Naturwissenschaften und Technik, Von-Ossietzky-Str. 99, 37085 Göttingen, Germany

Cleaning and passivation of Germanium surfaces is of tremendous technological interest. Germanium has various applications, for example in complementary metal-oxide-semiconductor elements. It turned out to be difficult to prepare contamination free Germanium surfaces by methods of wet chemistry. Several attempts have been made preparing such surfaces by different plasma treatments. We report cleaning and passivation of Ge(100)-surfaces by dielectric barrier discharge plasma at ambient temperature in oxygen and in air studied by Metastable Induced Electron Spectroscopy (MIES) and Photoelectron Spectroscopy (UPS(He I) and XPS). The plasma treatment is carried out in a special high-vacuum chamber which operates up to ambient pressure and is directly connected to the ultra-high vacuum chamber including the analysis equipment. In summary the air plasma treatment as well as the oxygen plasma treatment result in contamination free GeO_2 covered surfaces.

HL 44.94 Tue 18:00 P3

Soft landing Indium ion beams produced by a variable energy focused ion beam system — •Yu-Ying Hu, Dirk Reuter, and Andreas D. Wieck — Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, D-44780 Bochum, Germany

A focused ion beam (FIB) system under conventional operation employs 30 keV ions for micro-fabrication. In this work, the landing energy of ions can be tuned by applying positive voltages on the substrate, i.e. employing a retarding mode: the substrate potential decelerates the 30 keV ions, generating ions with various landing energies given by the difference between the accelerating and the decelerating voltage. The decelerating voltage to be operated on the GaAs substrate is at maximum 30 kV, i.e. soft landing is possible. In this study, we employ ion beams with very low landing energies of a few tens to few hundreds of eV which yields implantation depths in the range of only a few nm according to simulations. An Indium liquid metal ion source is produced for this experiment. The ion-induced damage is reduced due to low landing energy, which is observed through secondary electron images after ion sputtering. Above 29.76 kV decelerating voltage, no ion sputtering trace can be seen on the substrate. The adaptive objective lens voltage has to be reduced to focus the soft landing ion beam. Nevertheless, the diameter of the low energy beam is several μm, i.e., roughly 30 times larger as without a retarding voltage.

HL 44.95 Tue 18:00 P3

Copper oxide films prepared by rf sputter deposition — •Ekachai Chongsereecharoen, Achim Kronenberger, Angelika Polity, and Bruno K. Meyer — I. Physikalisches Institut, Justus-Liebig-Universität Giessen, Heinrich-Buff-Ring 16, 35392 Giessen, Germany

Cuprite (Cu_2O) and tenorite (CuO) are two well known phases of copper oxide. A metastable copper oxide, paramelaconite (Cu_4O_3), is another phase of copper oxide which has been rarely studied. CuO is p-type semiconductor which has many application such as solar cells, sensors and lithium ion Batteries. In this study CuO and Cu_4O_3 films were prepared on glass substrates by reactive rf sputter deposition. The structural properties were characterized by x-ray diffraction. The results show that with varying deposition conditions (sputtering power and oxygen flow rate), the formation of CuO and Cu_4O_3 phase is controllable. The optical and electrical properties of the sputtered films were investigated by optical spectroscopy and Hall effect measurement respectively. The properties of the films depend on the phase of the prepared films and deposition conditions.

HL 44.96 Tue 18:00 P3

Quantification of Impurities in Cu2O — •Hauke Metelmann[1], Andreas Laufer[1], Daniel Reppin[1], Swen Graubner[1], Angelika Polity[1], Bruno K. Meyer[1], Sebastian Geburt[2], and Carsten Ronning[2] — [1]I. Physikalisches Institut, Justus-Liebig-Universität Giessen, Heinrich-Buff-Ring 16, 35392 Giessen, Germany — [2]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

Cuprous oxide (Cu2O) has suitable properties for thin film solar cell applications. One powerful method to investigate concentrations of impurities is secondary ion mass spectrometry (SIMS). This method stands out due the fact that the chemical identity can be directly determine without considerations of ionisation state or binding energy. The quantification of SIMS data requires the usage of so called relative sensitivity factors (RSFs) which are dependent on the analysed material. While some materials like Si, GaAs, InP or ZnO already have established RSF tables there has been no such reference for Cu2O yet. In the presented work the RSF table for Cu2O has been determined for sputtered Cu2O thin films by using implantation standards. The RSFs of the elements follow systematic trends according to their ionisation potential and their electron affinity so that the RSF value for unmeasured elements can be interpolated or extrapolated by a set of determined RSFs. Finally, these RSFs have been used to investigate impurities in various Cu2O layers.

HL 44.97 Tue 18:00 P3

Strukturelle und elektrische Eigenschaften von PLD-gezüchteten Zinkferrit-Dünnfilmen — •Katja Mexner, Matt-

hias Brandt, Kerstin Brachwitz, Holger Hochmuth, Michael Lorenz und Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Linnéstrasse 5, 04103 Leipzig

Zinkferrit ($ZnFe_2O_4$) ist ein Material, mit einer Curie-Temperatur $T_C > 300\,K$, das durch seine elektrischen und magnetischen Eigenschaften in der Spintronik Anwendungen finden kann. Mittels gepulster Laserabscheidung wurden von stöchiometrischen Targets Zinkferrit-Dünnfilme ($d \approx 200\,nm$) auf (001)-orientierten $SrTiO_3$- und MgO-Substraten hergestellt. Die jeweiligen Gitterfehlpassungen betragen $\Delta a_{SrTiO_3} = 7,5\%$ und $\Delta a_{MgO} = 0,2\%$. Durch Röntgenbeugungsmessungen konnte (001)-orientiertes, epitaktisches Wachstum auf den verwendeten Substraten festgestellt werden. Es zeigte sich, dass die strukturellen und elektrischen Eigenschaften der Dünnfilme deutlich von der Substrattemperatur und weniger vom Sauerstoffpartialdruck während der Abscheidung abhängen. Mit steigender Temperatur sinken das Zn/Fe-Verhältnis und die out-of-plane-Gitterkonstante, die 2Θ–ω-Röntgenreflexe werden schärfer und der spezifische Widerstand nimmt zu. Temperaturabhängige Messungen des spezifischen Widerstandes zeigen einen thermisch aktivierten Leitungsmechanismus in den $ZnFe_2O_4$-Dünnfilmen. Es wurden Aktivierungsenergien von 50 bis 90 meV bestimmt. Magnetfeldabhängige Messungen des Hallwiderstandes bis 2 T zeigen den Einfluss des anomalen Hall-Effekts für $B < 0,5\,T$.

HL 44.98 Tue 18:00 P3

Electrical and structural properties of Zn-Co-O thin films — •Friedrich Schein, Holger Hochmuth, Holger von Wenckstern, Michael Lorenz, and Marius Grundmann — Universität Leipzig, Fakultät für Physik und Geowissenschaften, Institut fürExperimentelle Physik II, Linnéstr. 5, 04103 Leipzig

Considering that virtually all transparent oxide semiconductors (TOSs) are n-type it is of great interest to investigate p-type TOSs. A promising class of such materials are the zinc spinels ZnM_2O_4 (M = Co, Rh, Ir) [1]. They can be fabricated near and at room temperature; for $ZnRh_2O_4$ [2] and $ZnCo_2O_4$ [3] indications for stable p-type conductivity even in amorphous form were reported.

We present structural and electrical properties of zinc-cobalt-oxide thin films grown by pulsed laser deposition. The fabrication parameters like oxygen partial pressure and temperature are optimized in terms of electrical conductivity σ and surface quality. Zn-Co-O thin films deposited at low temperature ($\approx 200°$ C) are polycrystalline and exhibit σ up to 18 S/cm whereas room temperature fabrication reveals X-ray-amorphous films having $\sigma = 6\,S/cm$. Smooth surfaces with rms-roughness less than 0.5 nm have been measured with atomic force microscopy. The presentation includes a discussion of Hall effect measurements indicating p-type conductivity for certain growth conditions. Heterostructures using ZnO as n-type TOS are also shown.

[1] Dekkers *et al.*, Appl. Phys. Lett. **90**, 021903 (2007)
[2] Narushima *et al.*, Adv. Mater. **15**, 1409 (2003)
[3] Kim *et al.*, J. Appl. Phys. **107**, 103538 (2010)

HL 44.99 Tue 18:00 P3

Sputtering of ZnO by a modified Radio-Frequency Ion Thruster (RIT) as Ion-Beam-Sputter-Source — •Martin Becker, Angelika Polity, Davar Feili, and Bruno K. Meyer — I. Physikalisches Institut, Justus-Liebig-Universität Giessen, Heinrich-Buff-Ring 16, 35392 Giessen, Germany

Radio-Frequency-Ion-Thrusters, as designed for propulsion systems (ion extraction and grid system), are also qualified for thin film deposition and surface etching, because they can be used with different gases (inert and reactive) and extraction voltages.

ZnO thin films were deposited on float glass using a 4 inch ceramic ZnO target. The deposition temperature was varied using a heated substrate holder, as well as additional oxygen flow was provided to control the stoichiometry of the films. First investigations on this thin films will be presented.

HL 44.100 Tue 18:00 P3

Electronic structure of ZrS_xSe_{2-x} by density functional theory — •Ailakbar Ghafari[1], Arash Bouchani[2], Mohamed Moustafa[1], Christoph Janowitz[1], Helmut Dwelk[1], and Recardo Manzke[1] — [1]Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, D-12489 Berlin, Germany — [2]Physics Department, Islamic Azad University, Kermanshah Branch, Iran

The electronic properties of the ZrS_xSe_{2-x} (x varies between zero and two) semiconductors have been calculated by density functional theory (using the Wien2K code) employing the full potential Hamiltonian within the Generalized Gradient Approximation (GGA) method. The results obtained for the end members of the series, i.e. ZrS_2 and $ZrSe_2$ reveal that the valence band maximum and conduction band minimum are located at Γ and between Γ and K respectively which is in agreement with our photoemission experimental data. Trends in the electronic structure for the whole substitution series are discussed.

HL 45: Joint Poster Session

Time: Tuesday 18:00–21:00 Location: P1

HL 45.1 Tue 18:00 P1

Investigation of the built-in voltage in organic pin solar cells using electroabsorption spectroscopy — •Ellen Siebert-Henze, Wolfgang Tress, Vadim G. Lyssenko, Susanne I. Hintschich, Karl Leo, and Moritz Riede — Institut für Angewandte Photophysik, Dresden, Deutschland

The built-in voltage of small molecule organic solar cells based on the pin concept is investigated. We use the method of electroabsorption spectroscopy whose principle is the detection of absorption changes due to electrical excitation (Stark effect). A voltage consisting of a DC and an AC part is applied to the sample and the change in absorption is detected using a lock-in amplifier. The variation of the applied DC voltage modifies the DC field across the sample leading to a linear change of the corresponding Stark signal. This supplies information about the built-in voltage of the device which is determined for different combinations of donor materials and hole transport materials (MeO-TPD, BPAPF, alpha-NPD, and ZnPc). In addition, the doping concentration of the hole transport layer is modified and the influence of the consequential change of the work function on the built-in voltage is examined. It is shown that both the short-circuit current as well as the fill factor increase for larger built-in voltages.

HL 45.2 Tue 18:00 P1

Bias stress analysis of P3HT organic Field-effect transistors — •Hippolyte Hirwa and Veit Wagner — School of Engineering, Jacobs University Bremen, Campus Ring 1, D-28759 Bremen, Germany

Understanding and minimizing potentially existing bias stress behavior of organic field effect transistors (OFETs) is crucial for reliable operations of devices. Existing considerable bias stress, i.e. current change upon prolonged operation time, can render otherwise promising approaches useless for real applications. In this contribution we analyze the bias stress in poly (3-hexylthiophen) (P3HT) based field effect transistors. The drain current decay under bias stress can be seen as a change of the total resistance of the device with time. This resistance change is a combination of the contact resistance change and the channel resistance change. The channel resistance channel change is a result of the threshold voltage change and a change of the mobility value. The contact resistance change and the threshold voltage change interpreted as caused by the trapping of carriers into trap levels in both the contact and the channel regions. Encapsulated P3HT layers have been proven to be stable for short time bias stressing but on longer time scales and depending on the environment bias stress effects are evident.

HL 45.3 Tue 18:00 P1

Photoinduced absorption spectroscopy of poly(3-hexylthiophene):fullerene solar cells — •Ralph Huber, Elizabeth von Hauff, and Jürgen Parisi — University of Oldenburg, Department of Physics, Energy and Semiconductor Research Laboratory, Carl-von-Ossietzky Str. 9-11, 26129 Oldenburg, Germany

Photoinduced absorption (PIA) spectroscopy is a versatile tool in the study of excited states in organic thin films and devices. PIA is a pump-probe method which uses a modulated or pulsed light beam of

a specific wavelength to excite the semiconductor (pump beam). Via a white light source the sample is illuminated additionally to measure its absorption in a reflective or transmittive manner (probe beam). The change in absorption for different wavelengths can be used to identify excited states like excitons or free charge carriers.

In this study we employed steady state PIA to investigate poly(3-hexylthiophene):fullerene organic solar cells. The results of PIA measurements on the solar cells is presented.

HL 45.4 Tue 18:00 P1

Lock-In Thermography Investigation of Polymer Solar Cells and Modules — •Maik Bärenklau, Roland Rösch, Burhan Muhsin, Marco Seeland, Gerhard Gobsch, and Harald Hoppe — Institute of Physics, Ilmenau University of Technology, Ilmenau, Germany

Since polymer-fullerene solar cells and modules are typically designed in a multilayer architecture, local defects such as shunts and short-circuits in the device can cause the breakdown of the whole cell or module. Further more, highly resistive series connection can be a major cause for efficiency loss in solar modules. For screening and characterization of such processing imperfections, we apply lock-in thermography (LIT), a highly sensitive thermographic imaging method. We show that LIT is a useful tool for non-destructive qualitity control of large area polymer solar cells and modules that allows detection of local defects with high heat dissipation and also to test the quality of encapsulation.

HL 45.5 Tue 18:00 P1

Electric field induced exciton and charge transfer dissociation — •Sebastian Schwab[1], Julia Kern[1], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Faculty of Physics and Astronomy, Julius-Maximilians-University of Würzburg, D-97074 Würzburg — [2]ZAE Bayern, Div. Functional Materials for Energy Technology, D-97074 Würzburg

The enormous potential of organic opto–electronic devices such as organic light emitting diodes and solar cells is still limited due to a lack of understanding of underlying processes and energetics. A deeper comprehension of the processes governing exciton and charge transfer dissociation as well as the parameters influencing them is crucial to reduce existing uncertainties. Therefore we studied the field induced quenching of photoluminescence of various materials such as MDMO–PPV. An applied electric field dissociates the singlet respectively charge transfer excitons, generated by laser illumination, into electron–hole pairs which corresponds to a reduction of radiative recombination and therefore of photoluminescence signal. We discussed our experimental results in view of the Braun–Onsager–Model of electric field assisted dissociation.

HL 45.6 Tue 18:00 P1

Enhancement of the photocurrent in Diindenoperylene based organic photovoltaic cells — •A. Steindamm[1], A.K. Topczak[1], A. Riecke[1], and J. Pflaum[1,2] — [1]Inst. Exp. Phys. VI, Würzburg University, 97074 Würzburg — [2]ZAE Bayern, 97074 Würzburg

The organic semiconductor Diindenoperylene (DIP) has shown its good potential as donor material for highly efficient organic photovoltaic cells (OPVCs). In combination with C_{60} as acceptor high open circuit voltages (V_{OC}) of 0.9 eV and a high fill factor above 70 percent have been observed. The latter can be explained by the high crystallinity of DIP thin films leading to exciton diffusion lengths of up to 100 nm [1], resulting in a high charge collection efficiency. One challenge in DIP based OPVCs is the comparably low photocurrent, which is mainly caused by rather poor light absorption due to the upright stacking of DIP molecules and the related transition dipole orientation perpendicular to the electric field vector of incoming light. Therefore we addressed the enhancement of the photocurrent in DIP/C_{60} cells by various approaches: First, we performed studies on excitonic transport by photoluminescence (PL)-quenching. Second, different exciton blocking layers (EBL) like Batho-Phenanthroline (BPhen) or 1,4,5,8-Naphthalene-Tetracaboxylic Acid Dianhydride (NDTCA) were employed for minimizing the recombination losses at the organic-metal interface. Finally, metallic nanostructures were implemented for improving the light absorption of DIP. Financial support by DFG (project PF385/4) is gratefully acknowledged.

[1] D. Kurrle and J. Pflaum, Appl. Phys. Lett. 92 (2008) 133306

HL 45.7 Tue 18:00 P1

Characterization Of Pentacene-Based Organic Field-Effect Transistors With SAM-Functionalized Gates — •Nis Hauke Hansen[1], Sebastian Röding[1], and Jens Pflaum[1,2] — [1]Inst. Exp. Phys. VI, Julius-Maximilians-University, 97074 Würzburg — [2]ZAE Bayern, 97074 Würzburg

In order to design low-voltage organic thin film transistors, ultrathin self-assembled monolayer (SAM) gate dielectrics have been proven of promising technological potential [1]. Alkylphosphor-SAMs chemically bound on aluminumoxide allow for high capacitances in combination with superior insulation characteristics. In this contribution we discuss the influence of SAM gate dielectrics on the growth and the performance of pentacene (PEN) thin film transistors (TFTs). Current-voltage (IV) measurements of vacuum deposited PEN TFTs have been performed showing high mobilities and low operating voltages. The structural properties of the films are determined by x-ray diffraction (XRD) and atomic force microscopy (AFM). The SAM thickness and surface roughness have been analysed by x-ray reflectivity (XRR) and multidimensional modeling by the Parratt-algorithm. Combining this data we develop a correlation between the roughness of the substrate and the structural and electrical PEN properties. In addition, by temperature dependent measurements we determine the dominant transport mechanisms in PEN TFTs at different temperature ranges. Financial support by BMBF (project GREKOS) is gratefully acknowledged.

[1] H. Klauk, et al., Nature 445 (2007) 745

HL 45.8 Tue 18:00 P1

Temperature dependent studies of the recombination process in organic bilayer solar cells — •Thiemo Gerbich[1], Alexander Foertig[1], David Cheyns[2], Paul Heremans[2], Carsten Deibel[1], and Vladimir Dyakonov[1,3] — [1]Experimental Physics VI, Physical Institute, Julius-Maximilians-University of Würzburg, Am Hubland, D-97074 Würzburg — [2]IMEC v.z.w., Kapeldreef 75, 3001 Leuven, Belgium — [3]Bavarian Centre for Applied Energy Research (ZAE Bayern e.V.), Am Hubland, D-97074 Würzburg, Germany

In spite of organic solar cells having reached more than 8 % power conversion efficiencies recently, fundamental processes such as the recombination dynamics are still not fully understood. Therefore we investigated evaporated copper phthalocyanine (CuPC):C60 bilayer devices with a well defined donor-acceptor interface. The technique of Transient Photovoltage (TPV) and Photocurrent (TPC) was used to study the recombination dynamics in dependence of temperature and active layer thickness. We found recombination orders higher than two, and discuss the relevant fundamental contributions of internal processes.

HL 45.9 Tue 18:00 P1

Theoretical investigations of the optical properties of (Mn-, Fe-, Co-, Ni-, Cu-, Zn-) phthalocyanines — •Davoud Pouladsaz and Michael Schreiber — Institut für Physik, Technische Universität Chemnitz

Phthalocyanines have attracted considerable attention due to their wide range of applications that stem from their electronic, optical, and structural properties. The optical properties of metal-phthalocyanine complexes are determined by the energetics of the frontier orbitals and their dependence on the deformation in the relaxed excited state. In the present work, the geometry of (Mn-, Fe-, Co-, Ni-, Cu-, Zn-) phthalocyanines has been optimized with density functional methods and the deformation in the relaxed excited geometries has been obtained from time-dependent density functional theory, which leads us to calculate the PL gap and the PL lineshape of each molecule. From randomized starting geometries and stability analysis including the calculation of vibrational modes, it was found that the minimum of the potential energy surfaces of the excited state of each molecule is also in D_{4h} geometry. We considered the Franck-Condon principle for calculating the couplings between electronic excitations and internal vibrations of each molecule.

HL 45.10 Tue 18:00 P1

Optical properties of pentacene layers on zinc oxide — •Jonatan Helzel, Stephanie Jankowski, Mira El Helou, Gregor Witte, and Wolfram Heimbrodt — Philipps Universität Marburg; Department of Physics and Material Sciences Centre Germany

In comparison to other organic semiconductor pentacene has a high carrier mobility. Pentacene is one of the most promising organic semiconductors for semiconducting devices. Like many other organic semiconductors pentacene is a p-type semiconductor, hence for electronic components as e.g. diodes, an n-type semiconductor is needed. We prepared the p-pentacen films with various thicknesses on n-ZnO sub-

strates by molecular beam deposition. Optical spectroscopy was used to study the properties of these hybrid systems. The samples have been characterized by means of absorption and photoluminescence. The HOMO-LUMO transition as well as the excitonic states have been measured in the temperature range between 10 K and room temperature. At low temperatures a thickness dependent shift was observed for the two Davydov components of the pentacene exciton. Furthermore the exciton binding energies exhibit a thickness and temperature dependence. The reason of this unique behaviour will be discussed. Pentacene and ZnO have very different thermal expansion coefficients. This leads most likely to a tensioning of the thin films and a relaxation for the upper part of the thicker films. Due to the anisotropic expansion of pentacene not only the lattice constants, but also the angle between the molecules changes, while cooling them down.

HL 45.11 Tue 18:00 P1

Single Molecule Current Sensors — •Maximilian Nothaft[1], Steffen Höhla[2], Fedor Jelezko[1], Jens Pflaum[3], and Jörg Wrachtrup[1] — [1]3. Phys. Institut, Univ. Stuttgart, 70550 Stuttgart — [2]Char of Display Technology, Univ. Stuttgart, 70550 Stuttgart — [3]Exp. Phys. VI, Univ. Würzburg and ZAE Bayern, 97074 Würzburg

In this study we present our results on nanometer scale current sensing using photoluminescence quenching of single fluorescent dye molecules. From the quenching degree and internal molecular rate parameters it is possible to calculate the recombination rate and current density within the respective molecular capture radius. One striking aspect of this approach is the feasibility to optically measure the current dynamics by investigating photon correlation properties (FCS) of emitted photons.

Alterations in these properties can be directly related to time-dependent charge carrier densities. Therefore, this method enables a non-invasive determination of current densities in OLED devices at nm spatial resolution under operation.

As an example single Dibenzoterrylene dye molecules were dispersed in an OLED consisting of Poly(phenylene vinylene) (PPV) as host material. Besides determination of current density values, its spatial heterogeneity will be discussed. Additionally, a detailed analysis of current sensing sensitivity will be presented, discussing the resolution, its dependencies on internal molecular rate parameters and possible routes to further improve the measurement process.

HL 45.12 Tue 18:00 P1

Structural properties of thin films of organic charge transfer complexes — •Diana Nanova[1], Sebastian Beck[1], Milan Alt[1], and Michael Kröger[2,3] — [1]Kirchhoff-Institut für Physik, Universität Heidelberg — [2]InnovationLab GmbH, Heidelberg — [3]Institut für Hochfrequenztechnik, TU Braunschweig

Charge transfer (CT) complexes in the presented context are a mixture of two different types of molecules, one with electron accepting properties and one acting as a donor, which induces a charge transfer between the molecules. The band gap as well as the electronic and optical properties of the CT- compound depends on the degree of charge transfer. Mixing two CT-complexes at different concentrations by substituting only the acceptor molecules, might allow adjustment of the band gap and the optical properties in analogy to inorganic III-V semiconductor compounds. These materials could be applied in organic field-effect transistors or organic photovoltaic cells. Due to the importance of thin film deposition techniques for organic electronic devices we studied the growth of CT-compounds, like tetrathiafulvalene, tetracyanquinodimethane and its derivatives by thermal evaporation. The morphology of the films was investigated with atomic force microscopy and X-Ray diffraction on different substrates. To gain information about the electronic structure, we used ultra violet photoelectron spectroscopy and inverse photoelectron spectroscopy. We determined the degree of charge transfer in the complexes with infrared-spectroscopy using the linear relationship between the shift in the excitation energy of the C-N- stretching mode of the acceptor and the charge transfer.

HL 45.13 Tue 18:00 P1

Influence of silanization process on stability of solution processed bottom contact transistors — •Teodor Toader, Claudia Bock, and Ulrich Kunze — Werkstoffe und Nanoelektronik, Ruhr-Universität Bochum, Germany

In this work the influence of the silanization on the stability of solution-processed bottom-contact pentacene transistors using 13,6-N-Sulfinylacetamidopentacene (NSFAAP) [1] as precursor was investigated. The oxide of the devices is modified by trimethylchlorsilane (TMCS). Samples with an untreated oxide act as reference. The devices are stored under dark ambient conditions and nitrogen atmosphere, respectively. A clearly improved transistor performance of the TMCS-treated devices is found. A thirty times smaller sheet resistance of the treated transistors indicates an improved homogeneity of the film and is responsible for the superior device parameters. For transistors stored under dark ambient atmosphere the field-effect mobility decreased within 552 hours by 80% and 70% for untreated and treated transistors, respectively. The degradation of transistors stored under dark nitrogen atmosphere is considerable reduced (25% within 552 hours). The shift of the threshold voltage vs. time demonstrates that the absorption of H_2O on the pentacene layer is the main reason for the reduced stability of devices stored under ambient conditions.

[1] Ali Afzali, *et al.*, J. Am. Chem. Soc. **124** (30), 8812 -8813, (2002).

HL 45.14 Tue 18:00 P1

Time resolved Spectroscopy on different organic polymer/fullerene blends — •Berthold Jaeck[1], Bjoern Gieseking[1], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Experimentelle Physik VI, Julius-Maximilians-Universitaet Wuerzburg, D-97074 Wuerzburg — [2]ZAE Bayern, Div. Functional Materials for Energy Technology, D-97074 Wuerzburg

One main topic for highly efficient organic bulk-heterojunction solar cells is a better understanding of the fundamental physical processes after photo-excitation and hence the optimization of the device design. Many of these processes, e.g. the interfacial charge transfer dynamics and the free charge carrier generation, are occuring on very short time scales in the sub-picosecond regime. Therefore time resolved spectroscopic techniques are of crucial importance.

Using femtosecond transient absorption spectroscopy we investigated the exciton and free charge carrier dynamics of poly(3-hexylthiophene), P3HT and poly[2,3-(4,4-bis-(2-ethylhexyl)-4H-cyclopenta[2,1-b;3,4-b']dithiophene)-alt-4,7-(2,1,3-benzothiadiazole)], PCPDTBT blended with diverse fullerene derivatives. Additionally, picosecond time resolved photoluminescence measurements were carried out, probing radiative decay paths so that a complete picture of these intial processes could be reached. Furthermore, the influences of structural and energetic disorder on these dynamics were examined.

HL 45.15 Tue 18:00 P1

Spectrally Resolved Transient Absorption in Polymer:Fullerene Blend Films — •Andreas Kämpgen[1], Julien Gorenflot[1], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius-Maximilians-University Würzburg, 97074 Würzburg, Germany — [2]Bavarian Centre for Applied Energy Research (ZAE Bayern), 97074 Würzburg, Germany

Bimolecular charge carrier recombination is an efficiency limiting mechanism in organic solar cells. As this fundamental loss process is strongly related to the nanomorphology in blend films of electron donating and electron accepting materials, the study of this mechanism allows to draw conclusions about the impact of spatial (dis)order and phase separation on cell performance. The bimolecular recombination dynamics were investigated by nanosecond transient absorption spectroscopy. Measurements were carried out on blend films of polymers and fullerene derivatives in the temperature range from 30K to 300K. In order to distinguish between different excited species, different probe beam wavelengths were used. The decays were monitored on nanosecond to microsecond timescale and interpreted in terms of morphological as well as energetic trapping of charges.

HL 45.16 Tue 18:00 P1

Structural analysis of homoepitaxial grown surface structures on rubrene single crystals — •T. Schmeiler[1], R. J. Stöhr[2], J. Wrachtrup[2], and J. Pflaum[1,3] — [1]Inst. Exp. Phys. VI,Julius-Maximilians-Universtiy,97074 Würzburg — [2]3rd Phys. Inst.,Stuttgart University,70550 Stuttgart — [3]ZAE Bayern,97074 Würzburg

Self-assembled pyramidal surface structures on 5,6,11,12-tetraphenyltetracen (rubrene) single crystals offer an interesting approach to study exciton transport under spatial confinement [1]. These structures grown by physical vapor deposition could be applicable as organic micro-resonators and e.g. be coupled to single photon sources. Therefore an understanding of structural formation is inevitable. We have used smooth rubrene single crystals as substrates and analyzed the nucleation and growth behavior of homoepitaxially grown rubrene thin films deposited on-top by sublimation in high vacuum. We display different growth phases as a function of substrate temperature T and deposition rate R. Choosing R= 0.25 Å/s a pronounced island growth

was observed. In order to establish a relation between the pyramidal structures and the islands, their evolution was investigated at constant T and R for various film thicknesses. The surface topography was determined by AFM measurements and subsequently analyzed by Fourier transformation. We show a straight connection between the initial islands and the macroscopic pyramidal structures enabling the controlled growth of rubrene structures for opto-electronic applications. Financial support by the DFG (project PF385/4) is gratefully acknowledged.[1] R. Stoehr et al., Appl. Phys. Lett. 96 (2010) 231902

HL 45.17 Tue 18:00 P1

Photoconductive AFM-Measurements to prove the Meyer-Neldel Rule in C_{60} films — •Astrid Wachauer[1], Igor Beinik[1], Markus Kratzer[1], Mujeeb Ullah[2], Helmut Sitter[2], Andrey Kadashchuk[3], and Christian Teichert[1] — [1]Institute of Physics, University of Leoben, Franz Josef Straße 18, A-8700 Leoben, Austria — [2]Institute of Semiconductor and Solid State Physics, Johannes Kepler University of Linz, A-4040 Linz, Austria — [3]Institute of Physics, National Academy of Science of Ukraine, Prospect Nauky 46, 03028 Kyiv, Ukraine

The Meyer-Neldel rule (MNR) provides a link between the activation energy and the pre-exponential factor of a thermally activated process (e.g. electrical transport in organic semiconductors). Recently, it has been demonstrated that the MNR for the temperature dependences of the charge carrier mobility is fulfilled upon varying the charge carrier concentration in organic semiconductors [1]. In this study, we applied Photoconductive Atomic Force Microscopy (PC-AFM) in order to investigate the temperature dependence of the photocurrent in C_{60} thin films under different degrees of illumination. The films were grown on ITO by Hot Wall Epitaxy and measured with PC-AFM in inert atmosphere. The charge carrier concentration was modulated by varying the intensity of the Xe 150W light source. Besides verifying the MNR, we observed a variation in the conductivity of the crystalline C_{60} including almost nonconductive grains. Supported by Austrian Science Fund (FWF) NFN projects S9706-N20, S9707-N20 and P19636.
[1]M. Ullah, et al., Appl. Phys. Lett. 96, 213306 (2010).

HL 45.18 Tue 18:00 P1

Investigation of ZnO interlayer and different substrates for dye-sensitized ZnO/polymer hybrid solar cells — •Julia Waltermann[1], Kay-Michael Günther[1], Stefan Kontermann[2], and Wolfgang Schade[2] — [1]Clausthal University of Technology, EFZN, EnergieCampus, Am Stollen 19, 38640 Goslar — [2]Fraunhofer Heinrich-Hertz-Institute, EnergieCampus, Am Stollen 19, 38640 Goslar

Dye-sensitized solar cells composed of an n-doped ZnO nanowire array and a p-doped polymer layer appears to be a promising candidate for low-cost production of environment-friendly solar cells. Earlier investigations on hybrid devices consisting of a transparent conducting oxide (TCO) substrate, ZnO-nanowires, a ruthenium dye (N719) and a PEDOT:PSS or P3HT layer have exposed that in our setup an additional polycrystalline ZnO layer beneath the ZnO nanowires is needed. It prevents short circuits caused by polymer seeping between the nanowires towards the counter electrode. To find the best combination of substrate material and ZnO deposition technique in this work three different TCO substrates: ITO, FTO or aluminium doped zinc oxide (ZnO:Al) are combined with ZnO layers prepared either by sputtering or by a sol-gel method. The samples are compared regarding surface topography, resistivity and possible build-up Schottky barriers.

HL 45.19 Tue 18:00 P1

ITO-free inverted polymer-fullerene bulk-heterojunction solar cells with different contact configurations — •Sebastian Wilken, Holger Borchert, Elizabeth von Hauff, and Jürgen Parisi — University of Oldenburg, Department of Physics, Energy and Semiconductor Research Laboratory, Carl-von-Ossietzky-Str. 9-11, 26129 Oldenburg, Germany

In order to replace the expensive indium-tin oxide (ITO), commonly used as transparent electrode in organic solar cells, we studied P3HT:PCBM bulk-heterojunction solar cells with an inverted layer sequence. Different concepts were used to obtain both a transparent and a highly conductive anode, e.g. ultra-thin gold layers (∼10 nm) or polymers like PEDOT:PSS in combination with metal grids. We performed transmittance and sheet resistance measurements for various layer thicknesses to acheive a compromise between high transmission in the absorption range of P3HT and good electrical conductivity. Furthermore the impact of electron-selective materials such as solution-processed ZnO nanoparticles on the cathode side was examined. Here we present the photovoltaic performance of the different inverted solar cell structures. The active area of the devices was relatively large, with an area of nearly 1 cm^2.

HL 45.20 Tue 18:00 P1

Solution processed bulk heterojunction solar cells with molecularly doped active layers — •Antonietta De Sio[1], Ali Veysel Tunc[1], Elizabeth von Hauff[1], Felix Deschler[2], Enrico Da Como[2], and Jürgen Parisi[1] — [1]Energy and Semiconductor Research Laboratory, Institute of Physics, Carl von Ossietzky Universität Oldenburg, 26111 Oldenburg, Germany — [2]Photonics and Optoelectronics Group, Department of Physics and CeNS, Ludwig-Maximilians-Universität München, 80799, Munich, Germany

We report on the improvement of the device performance of polymer:fullerene bulk heterojunction solar cells by molecularly doping the active layer. 2,3,5,6-tetrafluoro-7,7,8,8-tetracyanoquinodimethane (F4-TCNQ) was used to p-dope the low bandgap polymer poly[2,6(4,4-bis-(2-ethylhexyl)-4H-cyclopenta[2,1-b:3,4-b0]-dithiophene)-alt-4,7-(2,1,3-benzothiadiazole)] (PCPDTBT) that was then blended with the soluble fullerene derivative [6,6]-phenyl-C61-butyric acid methyl ester (PCBM). Blends with different doping concentrations were investigated. We show how the short circuit current densities of the photovoltaic devices increase with the doping concentration as a result of an enhancement of the field effect mobilities.

HL 46: Organic Photovoltaics I

Time: Wednesday 10:15–13:30 Location: FOE Anorg

HL 46.1 Wed 10:15 FOE Anorg

Charge transport and electron trapping in a donor/acceptor-type copolymer — •Marcel Schubert[1], Eduard Preis[2], Ullrich Scherf[2], and Dieter Neher[1] — [1]Universität Potsdam, Institut für Physik und Astronomie, 14476 Potsdam — [2]Bergische Universität Wuppertal, Makromolekulare Chemie, 42119 Wuppertal

Low bandgap polymers are the driving force of the ongoing increase in efficiency of organic solar cells (OSC). Most of them are so called donor/acceptor-type copolymers. The polymer PFTBTT was one of the first of this material class, specially design for use in OSC [1]. It has been successfully incorporated as donor material in combination with soluble fullerenes or as acceptor in all-polymer solar cells.

Here, we present a detailed study of the electron transport properties of PFTBTT. By making use of an ultra thin charge generation layer, we were able to (1) selectively address the charge transport of electrons, (2) perform time-of-flight measurements on samples with less than 200 nm thickness and (3) to combine the time-of-flight and Photo-CELIV technique to investigate charge carrier dynamics. Our measurements proof that PFTBTT is an ambipolar material with a high electron bulk mobility. Furthermore, detailed investigations of the charge carrier dynamics with time-delayed extraction fields revealed a power law-type relaxation of the free electron mobility over two orders in time. These results help to quantify relaxation phenomena reported recently for PFTBTT containing all-polymer solar cells [2].

[1] M. Svensson et al., Adv. Mater. 15, 988 (2003).
[2] C. R. McNeill et al., J. Appl. Phys. 106, 024507 (2009).

HL 46.2 Wed 10:30 FOE Anorg

Investigation of Charge Transfer States in MDMO-PPV:PCBM Solar Cells — •Julia Kern[1], Sebastian Schwab[1], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Faculty of Physics and Astronomy, Julius-Maximilians-University of Würzburg, Am Hubland, D- 97074 Würzburg — [2]Center for Applied Energy Research (ZAE Bayern e. V.), Am Hubland, D-97074 Würzburg

In recent years, so called charge transfer states (CTS), i.e. interfacial states generated at the donor-acceptor heterojunction in organic so-

lar cells, have attracted a considerable amount of attention and their role in the processes of charge carrier dissociation and recombination has been discussed controversially. In this context, we investigated the photo- (PL) and electroluminescence (EL) originating from blends of MDMO-PPV and various fullerene derivatives. Upon blending donor and acceptor, a peak emerges at the lower energetic side of the pure material excitonic transitions which can be attributed to a CTS. Interestingly, a distinct red shift of this CTS emission is observed between the obtained EL and PL spectra. Furthermore, we studied the influence of temperature and voltage variations on the intensity and spectral shape of the CTS emission.

HL 46.3 Wed 10:45 FOE Anorg

Structure-Property-Relations in PPE-PPV based Polymer Solar Cells — •Christian Kästner[1], Burhan Muhsin[1], Adam Getachew[2], Christoph Ulbricht[2], Özlem Usluer[2], Daniel Ayuk Mbi Egbe[2], and Harald Hoppe[1] — [1]Institute of Physics, Ilmenau University of Technology, Ilmenau, Germany — [2]Linz Institute for Organic Solar Cells, Johannes Kepler University Linz, Austria

Abstract: Photophysical and photovoltaic properties of a series of anthracene-containing and ethylene-3,4-dioxythiophene (EDOT)-containing poly(p-phenylene-ethynylene)-alt-poly(p-phenylene-vinylene)s (PPE-PPV) copolymers with general constitutional units (Ph-C-tC-Anthr-C-tC-Ph-CH-dCH-Ph-CH-dCH-) n and (Ph-C-tC-EDOT-C-tC-Ph-CH-dCH-Ph-CH-dCH-) n have been studied. Mixed linear and branched alkoxy side chains were grafted to the backbone in order to tune the π-π-stacking ability of the materials, which significantly affects their photovoltaic response when used as donor components in a bulk heterojunction construct together with PCBM as acceptor.

HL 46.4 Wed 11:00 FOE Anorg

Morphological aspects of the exciton transport in molecular thin films — •A.K. Topczak[1], T. Roller[2], and J. Pflaum[1,3] — [1]Inst. Exp. Phys. VI, Würzburg University, 97074 Würzburg — [2]3rd Phys. Inst., Stuttgart University, 70550 Stuttgart — [3]ZAE Bayern, 97074 Würzburg

The exciton diffusion length is a key criteria to optimized design of organic thin film photonic devices. This optimisation requires fundamental understanding and control of the excitonic transport. It has been proposed that exciton transport should depend on the extension of crystalline domains [1]. Therefore we performed photoluminescence-quenching measurements to compare the exciton diffusion length (EDL) of the three archetypical semiconductors Diindenoperylene (DIP), Sexithiophene (α-6T) and tris-8-hydroxyquinolate-aluminum (Alq$_3$) and to link this quantity to the polycrystalline structure. A correlation between the exciton transport and the crystalline morphology is demonstrated. Long-range ordered thin films of DIP and α-6T show a high EDL. For these films the necessity of taking interference effects into account for a precise modeling became evident. In comparison, amorphous films of Alq$_3$ showed an EDL which is significantly smaller. We will elucidate the microscopic transport mechanisms and their respective energies by means of temperature dependent measurements. From our results, conclusions on the cell design of planar heterojunction thin film cells can be drawn. Financial support by the DFG (project PF385/4) is gratefully acknowledged. [1] D. Kurrle, J. Pflaum, Appl. Phys. Lett.92 (2008) 133306

HL 46.5 Wed 11:15 FOE Anorg

Electronic Trap States in Methanofullerenes and their Influence on Organic Solar Cells — •Julia Schafferhans[1], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Physical Institute, Julius-Maximilians University of Würzburg, Am Hubland, D-97074 Würzburg — [2]Bavarian Center for Applied Energy Research (ZAE Bayern e.V.), Am Hubland, D-97074 Würzburg, Germany

Methanofullerenes are the most commonly used electron acceptors in organic bulk heterojunction solar cells, due to their advantages that they can be easily processed from solution, possess a high electron affinity and form segregated phases in blends with common donor polymers.

Although trap states can have a significant impact on the performance of organic solar cells, as they can act as recombination centers, lower the mobility and disturb the internal field distribution, the traps in methanofullerenes have not been matter of research so far.

We investigated the trap states of three commonly used fullerene derivatives, namely $PC_{61}BM$, $PC_{71}BM$ and $bisPC_{61}BM$, by thermally stimulated current measurements. Each of the studied methanofullerenes exhibit a broad trap distribution, whereby the $PC_{71}BM$ and $bisPC_{61}BM$ reveal significantly deeper traps compared to $PC_{61}BM$. These findings will be discussed with respect to the solar cell performance.

HL 46.6 Wed 11:30 FOE Anorg

Luminescence imaging of polymer solar cells: visualization of progressing degradation — Marco Seeland, •Roland Rösch, and Harald Hoppe — Institute of Physics, Ilmenau University of Technology, Ilmenau, Germany

We apply luminescence imaging as tool for the non-destructive visualization of degradation processes within bulk heterojunction polymer solar cells. The imaging technique is based on luminescence detection with a highly sensitive silicon-ccd camera and is able to visualize the with time advancing degradation patterns of polymer solar cells. The devices investigated have been aged under defined conditions and were characterized periodically with current-voltage-sweeps. This allows determining the time evolution of the photovoltaic parameters and - in combination with the luminescence images - understanding differences in the observed degradation behaviour. The versatile usability of the method is demonstrated in a correlation between local reduction of lateral luminescence and a fast decrease of the short-circuit-current due to the loss of active area. Differences in the degradation of photovoltaic parameters under varied aging conditions are discussed.

15 min. break

HL 46.7 Wed 12:00 FOE Anorg

Quantitative Description of Electroluminescence Images of Polymer Solar Cells — •Marco Seeland, Roland Rösch, and Harald Hoppe — Institute of Physics, Ilmenau University of Technology, Ilmenau, Germany

We present a quantitative description of electroluminescence images obtained on organic solar cells, which is based on a device modeling employing a network of interconnected microdiodes. The equivalent circuit network model takes interface and bulk resistances as well as the sheet resistance of the transparent electrode into account. The application of this model allows direct calculation of the lateral current and voltage distribution as well as determination of internal resistances and the sheet resistance of the higher resistive electrode. Furthermore, we have extended the microdiode-model to also describe and predict current voltage characteristics for devices under illumation. Finally the local nature of this description enables important conclusions concerning the geometry dependent performance of thin film solar cells.

HL 46.8 Wed 12:15 FOE Anorg

Investigation of Field-dependent Charge Carrier Generation and Recombination in Polymer Based Solar Cells by Transient Extraction Currents — •Juliane Kniepert, James Blakesley, and Dieter Neher — University of Potsdam, Germany

There is an ongoing discussion as to whether photoinduced charge transfer in P3HT:PCBM solar cells leads to fully separated electrons and holes, independent of an electric field, or Coulombically bound interfacial charge pairs. While recent studies by R.A. Marsh et al. with transient absorption spectroscopy gave clear evidence for the formation and field-induced dissociation of bound polaron pairs, measurements by I.A. Howard et al. were in favour of hot exciton dissociation. Here, we present the results of bias-dependent Time Delayed Collection Field (TDCF) measurements to access directly the density of free charge carriers in P3HT:PCBM blends coated from dichlorobenzene. Solvent annealing was applied to yield a phase-separated morphology and the corresponding solar cells exhibit high values for the external quantum efficiency and fill factor. Our setup allowed us to follow the generation and recombination of photogenerated charges with a so far unattained time resolution of 40 ns. Our experiments show that the number of collected carriers is independent of the applied bias during pulsed illumination implying that extractable carriers in P3HT:PCBM blends are not generated by the field-assisted separation of bound polaron pairs. In addition, our experiments support the view that bimolecular recombination of free carriers is strongly suppressed in phase-separated P3HT:PBCM blends.

HL 46.9 Wed 12:30 FOE Anorg

Influence of phase separation on the recombination dynamics of trapped charges in disordered organic semiconductors — •Julien Gorenflot[1], Matthias Gunz[1], Andreas Kämpgen[1],

Jens Lohrmann[1], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius-Maximilians University, D-97074 Würzburg — [2]Bavarian Center for Applied Energy Research (ZAE Bayern), D-97074 Würzburg

Using a combination of steady-state and transient photoinduced absorption, we explore the recombination of polarons in pristine poly(3-hexylthiophene) (P3HT) as well as in its blend with [6,6]-phenyl-C61 butyric acid methyl ester(PCBM). Interestingly those two systems behave very differently with a recombination order of two for pure P3HT which contrasts with the much higher apparent order in the blend. We explain those results in terms of trap induced delay in the blend where energetically trapped polarons can be unavailable for recombination due to phase separation. We determine the activation energy of the bimolecular recombination in pure P3HT. Our results show that the polaron recombination is caused in both neat polymer and blend by intermolecular rather than intramolecular charge transport.

HL 46.10 Wed 12:45 FOE Anorg

Determination of the built-in voltage of BHJ solar cells by temperature dependent photocurrent measurements — •Markus Mingebach[1], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Physical Institute, Julius-Maximilians-University of Würzburg, Am Hubland, D-97074 Würzburg — [2]Bavarian Center of Applied Energy Research (ZAE Bayern e. V.), Am Hubland, D-97074 Würzburg

Despite all progresses in the performance of organic BHJ solar cells (up to 8% power conversion efficiency) some very important properties such as the voltage dependent photocurrent or the built-in potential are not fully understood yet. We investigate poly(3-hexyl thiophene) (P3HT) : [6,6]-phenyl-C_{61} butyric acid methyl ester (PCBM) solar cells by means of temperature dependent pulsed photocurrent measurements and impedance spectroscopy. We find a point of optimal symmetry (POS) that represents the case of quasi flat bands (QFB) in the bulk of the cell, which is lower than the built-in voltage. [1] This difference is due to band bending at the contacts, which is reduced at lower temperatures. Therefore we can identify the built-in voltage by measuring the POS (confirmed by temperature dependent current voltage measurements). This leads to the conclusion that the potential determined by Mott-Schottky analysis is not the built-in potential.
[1] M. Limpinsel, A. Wagenpfahl, M. Mingebach, C. Deibel and V. Dyakonov, Phys. Rev. B 81, 085203 (2010).

HL 46.11 Wed 13:00 FOE Anorg

Charge Transport and Recombination Dynamics in Oxygen Exposed P3HT:PCBM Bulk Heterojunction Solar Cells — •Alexander Foertig[1], Andreas Baumann[1], Julia Schafferhans[1], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Physical Institute, Julius-Maximilians-University of Würzburg, Am Hubland, D-97074 Würzburg — [2]Bavarian Centre for Applied Energy Research (ZAE Bayern e.V.), Am Hubland, D-97074 Würzburg, Germany

The effect of synthetic air exposure on the charge transport and recombination dynamics in poly(3-hexyl thiophene)(P3HT):[6,6]-phenyl-C_{61} butyric acid methyl ester (PCBM) bulk heterojunction solar cells was studied using the complementary measurement techniques of (photogenerated) charge carrier extraction by linearly increasing voltage (photo-CELIV) and transient photovoltage (TPV) and transient photocurrent (TPC). An additional extraction peak appeared in the photo-CELIV transient at larger extraction fields, which is assigned to a field dependent release of previously trapped charge carriers. The complementary techniques consistently revealed an increased charge carrier density and reduced recombination with exposure time to oxygen which we attribute to delayed release from oxygen induced traps and therefore reduced recombination.

HL 46.12 Wed 13:15 FOE Anorg

Charge transport measurements by transient techniques and their detailed evaluation — •Jens Lorrmann[1], David Vocke[1], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Physical Institute, Julius-Maximilian-University of Würzburg — [2]Bavarian Center for Applied Energy Research e.V. (ZAE Bayern e.V.), Würzburg

The charge carrier transport in pristine poly(3-hexyl thiophene-2,5-diyl) (P3HT) of different regioregularities and in blends with [6,6]-phenyl-C_{61} butyric acid methyl ester (PCBM) was investigated by time-of-flight measurements (TOF). We investigate the field and temperature dependence of hole and electron mobilities down to temperatures of 130 K in order to understand the effects of the transport on the solar cell efficiency. The results from the TOF measurements are compared with the outcome of complementary methods like charge extraction by linearly increasing voltage (CELIV) and field effect transistor measurements. We calculate the disorder parameters from the temperature and field dependencies of the charge mobility using a Gaussian disorder transport formalism. Furthermore, we present the detail evaluation of TOF current transients with an improved method by Scott et al. [1], which provides explicit distributions of the transit times and the mobilities instead of discrete values.

[1] J.C. Scott, L.T. Pautmeier and L.B. Schein, *Mean mobilities of charge carriers in disordered media*, Phys. Rev. B 46:8603, 1992

HL 47: GaN on Si

Time: Wednesday 10:15–11:30 Location: POT 51

HL 47.1 Wed 10:15 POT 51

Kathodolumineszenzuntersuchungen an GaN auf Si(211)- und Si(311)-Substraten — •Mathias Müller, Anja Dempewolf, Frank Bertram, Thomas Hempel, Jürgen Christen, Roghaiyeh Ravash, Armin Dadgar und Alois Krost — Institut für Experimentelle Physik, Otto-von-Guericke-Universität Magdeburg, Deutschland

Mittels spektral aufgelöster Kathodolumineszenzmikroskopie (KL) wurden die Lumineszenzeigenschaften von GaN-Schichten auf Si(211) und Si(311)-Substraten bei Heliumtemperatur untersucht. Nicht-c-Achsen orientiertes GaN Wachstum ermöglicht eine Reduktion der Polarisationsfelder und somit des quantum confined Stark effect (QCSE), welcher die Effizienz von optoelektronischen Bauelementen herabsetzt. Hierzu wurden systematisch geeignete hoch indizierte Si(h11)-Substrate benutzt, auf denen mittels MOVPE jeweils eine AlN-Keimschicht sowie eine AlGaN-Pufferschicht gewachsen wurde, gefolgt von zwei dicken GaN-Schichten, welche durch eine AlN-Zwischenschicht unterbrochen sind. Ortsintegrale Spektren zeigen bei tiefen Temperaturen drei dominante Lumineszenzkanäle: das gebundene Exziton (D^0,X), Donator-Akzeptor-Paarbande DAP sowie Basalflächenstapelfehlerlumineszenz BSF. Auf Si(211) ist die Stapelfehlerlumineszenz im Vergleich zum GaN auf Si(311) stark reduziert. An der Bruchkante zeigt sich mit zunehmender Schichtdicke die Entwicklung der dominanten Lumineszenzkanäle der Proben, welche auf Si(311) eine starke Inhomogenität im Vergleich zu Si(211) aufweist.

HL 47.2 Wed 10:30 POT 51

Semi-polar GaN heteroepitaxy an high index Si-surfaces — •Roghaiyeh Ravash, Jürgen Bläsing, Thomas Hempel, Armin Dadgar, Jürgen Christen, and Alois Krost — Otto-von-Guericke-University Magdeburg, FNW/IEP/AHE, Postfach 4120, 39016 Magdeburg, Germany

Due to the lack of GaN homosubstrates, the growth of GaN-based devices is usually performed on heterosubstrates as sapphire or SiC. These substrates are either insulating or expensive, and both unavailable in large diameters. Meanwhile, silicon can meet the requirements for a low price and thermally well conducting substrate and also enabling the integration of optoelectronic devices with Si-based electronics. Up to now, the good matching of hexagonal GaN with the threefold symmetry of Si(111) greatly promotes the c-axis orientated growth of GaN on this surface plane. A large spontaneous and piezoelectric polarization oriented along the c-axis exists in such hexagonal structure leading to low efficiencies for thick quantum wells. The attention to the growth of non-polar or semi-polar GaN based epitaxial structures has been increased recently because of reducing the effect of the polarization fields in these growth directions. Therefore we studied semi-polar GaN epilayers grown by metalorganic vapor phase epitaxy on silicon substrates with different orientations from Si(211) to Si(711). We observed that AlN seeding layer growth time play a significant role

in obtaining the different GaN texture.

HL 47.3 Wed 10:45 POT 51

Spatially resolved cathodoluminescence spectroscopy of InGaN/GaN heterostructures on m-plane GaN grown on patterned Si (112) substrates — •Christopher Karbaum[1], Frank Bertram[1], Sebastian Metzner[1], Jürgen Christen[1], Xianfeng Ni[2], Natalia Izyumskaya[2], Vitaliy Avrutin[2], Ümit Özgür[2], and Hadis Morkoç[2] — [1]Institute of Experimental Physics, Otto-von-Guericke-University Magdeburg, Germany — [2]Depart. of Electrical and Computer Engineering, VCU, Richmond, USA

The optical properties of GaN/InGaN heterostructures grown by MOVPE on pre-patterned Si substrate have been studied using cathodoluminescence (CL) at low temperatures (T=5.4 K). A stripe mask pattern was produced on the Si (112) substrate using photolithography and ICP-RIE. Anisotropic wet etching resulted in (-1-11) Si sidewalls and (112) Si terraces connected by (111) Si facets. After the growth of an AlN layer the (111) and (112) Si facets were masked with SiO_2. The lateral and vertical epitaxial growth of GaN was initiated at the (-1-11) Si sidewalls resulting in a partially coalesced m-plane surface. Finally, an InGaN layer capped with p-GaN was deposited. The GaN (D^0,X) emission observed from the +c-wing is red-shifted possibly due to tensile strain and the incorporation of impurities. Homogeneous and intense CL from InGaN is emitted from nearly the entire m-plane surface at about 3.2 eV with a FWHM of 98 meV. Just above the -c-wing the CL intensity from InGaN is reduced due to the presence of stacking faults and defects. The influence of BSFs on lifetimes of (D^0,X) and InGaN emissions will be discussed.

HL 47.4 Wed 11:00 POT 51

Monitoring the influence of interlayer thickness and Si doping on the stress behaviour of GaN grown on Si(111) — •S. Fritze[1], J. Bläsing[1], P. Drechsel[2], A. Dadgar[1], and A. Krost[1] — [1]Institute of Experimental Physics, Otto-von-Guericke-University Magdeburg, Universitätsplatz 2, 39106 Magdeburg — [2]OSRAM Opto Semiconductors, Leibnizstraße 4, 93055 Regensburg

GaN growth on Si substrates is a cost-effective alternative to replace conventional substrates like sapphire and SiC. Especially the large diameter availability of Si substrates up to 300 mm can increase chip yield and reduce production costs. To accomplish thick, crack free GaN layers of high crystalline quality an exact control of tensile thermal stress between GaN and Si and the reduction of high dislocation densities are essential. By inserting thin AlN interlayers during growth compressive stress is induced in the subsequent GaN layer and compensates part of the tensile stress. Here the influence of interlayer thickness and Si doping on wafer bow, crystal quality and vertical strain profile of MOVPE grown GaN structures on Si(111) has been studied. In symmetric and grazing incidence high resolution X-ray diffraction measurements we observe higher compressive stress in the GaN toplayer with increasing interlayer thickness. Additional X-ray transmission scattering measurements also show the stress state of the underlying GaN layers. Optical bow measurements demonstrate an increasing convex curvature with increasing interlayer thickness. With a Si doping level between $1 \cdot 10^{18} cm^{-3}$ and $4 \cdot 10^{18} cm^{-3}$ a wafer bow as low as 2.9 μm can be achieved using an optimized interlayer thickness.

HL 47.5 Wed 11:15 POT 51

Investigations of pn-junctions based on AlGaN / AlN structures for LEDs on Si(111) — •Antje Rohrbeck, Hartmut Witte, Phannee Saengkaew, Thomas Fey, Armin Dadgar, Jürgen Christen, and Alois Krost — nstitute of Experimental Physics, Otto-von-Guericke- University Magdeburg, Magdeburg, Germany

AlGaN/AlN - ultraviolet LEDs grown on Si(111) substrates are of high interest for many applications and have the advantages to easily be integrated within the silicon electronic. However, the large misfit between the AlGaN layers and the Si substrate introduces many defects in the layers. The most important part of the AlGaN/AlN-LED structure is the p- AlGaN / n-AlGaN junction involving the AlGaN/GaN multi-quantum well. We have investigated these pn-junctions within the LED structure grown by MOVPE in detail and n-type AlGaN layers as well as p-type AlGaN/p-type GaN multilayer which were grown separately. All AlGaN layers have an Al content of 10 % and the Si(111) substrates were highly n-type doped. For these investigations Hall-effect measurements, CV- and IV-characteristics, impedance spectroscopy, surface scanning potential and scanning capacitance microscopy were used. The p-type doping of the AlGaN/GaN multilayer structure shows a Mg-accumulation at the AlGaN/GaN interfaces. Furthermore, there are negative differential capacitances and currents within the CV- and IV-characteristics whose origins will be discussed considering the impact of surface defects or the AlGaN/GaN interfaces. Additionally, electroluminescence spectra of the whole LED structure give further indications that defects are located within or close to the pn-junctions.

HL 48: ZnO: Devices

Time: Wednesday 10:15–13:30 Location: POT 151

HL 48.1 Wed 10:15 POT 151

Optimization of optical and electrical properties of room temperature deposited ZnO:X (X = Al, Ga, In) TCO electrodes — •Tobias Diez, Alexander Lajn, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Fakultät für Physik und Geowissenschaften, Institut für Experimentelle Physik II, Linnéstr. 5, 04103 Leipzig

Transparent conductive oxides (TCOs) are commercially exploited as electrodes in transparent electronics (e.g., transparent displays) and optoelectronic device applications (e.g., thin-film solar cells). Indium-tin-oxide (ITO) has the biggest market share, however, the increasing usage of TCOs in connection with the high indium price demands to establish alternatives. Doped ZnO is such a promising and cheap alternative to ITO. We deposited smooth, amorphous ZnO thin films on quartz glass and sapphire substrates at room temperature using pulsed laser deposition (PLD). To optimize the optical and electrical properties we measured transmittance and conductivity as a function of the oxygen pressure applied during PLD. Additionally, we investigated the influence of different group III dopants (Al, Ga, In) and their doping concentration on these thin film properties. For Al-doped ZnO the highest figure of merit ($T^{10}/R_s = 1.9 \cdot 10^{-3}\,\Omega^{-1}$) was found at an oxygen pressure of 0.002 mbar and a doping concentration of 3 %. Furthermore, we analyzed the impact of this optimized growth condition on the device performance of transparent metal-semiconductor field-effect transistors (MESFET) using highly conductive ZnO as source and drain electrodes.

HL 48.2 Wed 10:30 POT 151

Dynamic Properties of (Mg,Zn)O-based MESFETs — •Fabian J. Klüpfel, Alexander Lajn, Heiko Frenzel, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Fakultät für Physik und Geowissenschaften, Abteilung Halbleiterphysik, Linnéstr. 5, 04103 Leipzig

Transparent electronics is an emerging technological field, in which oxide based transistors play a key role. Various materials have been used to fabricate transparent transistors, including ZnO, (In,Ga,Zn)O, SnO_2 and related compounds [1-4]. Besides the steady-state electrical characterization, dynamic properties of such devices have been studied using ring oscillators. However, this rather complex test structures are less suitable to investigate and identify the physical effects, which limit the working range in the frequency domain. We present dynamic measurements on single (Mg,Zn)O-based MESFETs with the gate materials Ag_xO, PtO_y and Au. A strong dependence of the dynamic properties on the gate material was observed. The usage of Ag_xO results in delayed response of the source-drain current even for frequencies below 1 kHz. For PtO_y and Au absence of such an effect was verified up to 1 Mhz. We attribute this difference to the diffusion of Ag into the channel material during device fabrication.

[1] K. Nomura et al. Science, 300, 1269 (2003)
[2] E. Fortunato, Thin Solid Films, 487, 205 (2005)
[3] Y. Ogo, Appl. Phys. Lett., 93, 032113 (2008)
[4] H. Frenzel et al., Adv. Mat., 10.1002/adma.201001375 (2010)

HL 48.3 Wed 10:45 POT 151

Carrier transport in nanocrystalline field-effect transistors: Impact of interface roughness and geometrical carrier trap —

•Koshi Okamura and Horst Hahn — Institute of Nanotechnology, Karlsruhe Institute of Technology (KIT), 76021 Karlsruhe, Germany

Nanocrystalline field-effect transistors (FETs) inherently have a certain level of roughness at the semiconductor-dielectric interface, which originates from the size of building blocks, i.e., nanocrystals ranging from a few to a few tens of nanometers. This interface roughness is expected to act like carrier traps, significantly preventing induced carriers from being transported along the channel in nanocrystalline FETs. In this study, a simple numerical calculation is performed for nanoparticulate zinc oxide (ZnO) FETs on the basis of Shockley's gradual channel approximation with the induced carriers classified into two components: (1) fixed carriers located within a threshold depth d_{th} from the interface and (2) mobile carriers located away from d_{th}. This calculation clearly indicates that the mobile carrier concentration is strongly dependent on the level of interface roughness; and the field-effect mobility is directly reflected by the mobile carrier concentration, significantly decreasing by a factor of 3.9x10^{-1}, 7.4x10^{-2}, 3.0x10^{-2}, 3.9x10^{-3}, and 7.3x10^{-4} for d_{th} of 1, 5, 10, 30, and 40 nm, respectively. These findings reveal that an interface roughness as small as a few nanometers results in a decrease in field-effect mobility as large as an order of magnitude, which is in qualitative agreement with experimental results.

HL 48.4 Wed 11:00 POT 151

Covalent functionalization of ZnO nanowires — •Andreia da Rosa, Ney Moreira, and Thomas Frauenheim — BCCMS, University of Bremen, Am Fallturm 1, 28359, Bremen, Germany

Understanding the interaction of organic species with inorganic nanostructures constitutes a step forward in the development of semiconductor based biosensors. In this work we have used density functional theory to investigate ZnO-(1010) nanowire surfaces modified with substituted methane molecules (Me-X, with X= OH, NH2, SH, COOH, and CN). We have found three relevant mechanisms for surface stabilization: passivation of surface oxygen lone-pairs via dissociative chemisorption processes, electrostatic adsorbate-interations involving Zn surface sites and hydrogen bonding interactions involving oxygen surface sites. Covalent adsorbate-substrate interactions were found to play only a marginal role on the surface stabilization. Contradicting the usual chemical intuition, we have found no significant evidence for the formation of classical Lewis acid-base adducts on Zn surface sites. Finally we suggest that the functionalization with Me-COOH is also expected to be stable under ordinary laboratory conditions or in aqueous media.

HL 48.5 Wed 11:15 POT 151

Excitonic Transport in a ZnMgO/ZnO Quantumwell — •Martin Noltemeyer[1], Thomas Hempel[1], Jürgen Christen[1], Matthias Brandt[2], Michael Lorenz[2], Marius Grundmann[2], Andrey Polyakov[3], and Mikhail Stepovich[3] — [1]Institute of Experimental Physics, Otto-von-Guericke-Universität Magdeburg — [2]Institut fuer Experimentelle Physik II, Universität Leipzig — [3]Tsiolkovsky Kaluga State University, Russia

Using highly spectrally and ps-time resolved cathodoluminescence (CL) the excitonic transport in a c-oriented PLD grown ZnMgO/ZnO quantumwell (QW) of about $b = 4nm$ thickness is indirectly measured as a function of temperature (T=5K-180K). In a first step, the initial exciton lifetime τ of the QW ($E_{QW}(5K) = 3.22eV$) is assigned by time resolved CL on the uncovered sample area. It decreases over one order of magnitude from $\tau(5K) = 3.75ns$ to $\tau(180K) = 0.38ns$. In a second step, the sample is excited by the pulsed e-beam in the center of a circular aperture ($d = 1.45\mu m$) in a completely light absorbing Ti-mask (thickness: 160nm). The analytic solution of the two-dimensional diffusion equation for this geometry is fitted to the initial decay of the CL with the given parameters $\tau(T)$ and $d(T)$. This directly gives the diffusion constant $D(T)$ which increases from $D(5K) = 0.25\,cm^2/s$ to $D(180K) = 1.4\,cm^2/s$. Using the Einstein-Relation, one can define an excitonic mobility that has a plateau around $\mu = 600\,cm^2/Vs$ at low T (5K-12K) with a decay at higher temperature following $\mu \propto T^{-\frac{2}{3}}$ which is close to scattering with Fröhlich-Interaction ($\mu \propto T^{-\frac{1}{2}}$).

HL 48.6 Wed 11:30 POT 151

First principles calculation of Auger recombination rates in ZnMgO — •Markus Heinemann and Christian Heiliger — I. Physikalisches Institut, Justus Liebig University Giessen, D-35392 Giessen, Germany

The variation of the band gap in $Zn_{1-x}Mg_xO$ with the Mg concentration x may open a channel for non-radiative recombination mechanisms. We use density functional theory to investigate the possibility of band-to-band Auger transitions in wurtzite $Zn_{1-x}Mg_xO$ alloys for $0 \leq x \leq 1$. Auger recombination rates for different Mg concentrations are computed by two different ways: (1) by interpolating the band structure and transition matrix elements from *ab initio* calculations of bulk ZnO, $Zn_{0.5}Mg_{0.5}O$, and MgO primitive cells, and (2) by using a supercell approach. We find that inter-band Auger recombination becomes possible at Mg concentrations $\gtrsim 50$ % where ZnMgO has not been reported to exist in a stable wurtzite phase.

15 min. break

HL 48.7 Wed 12:00 POT 151

Light emitting diodes based on ZnO — •Julian Benz, Christian Reindl, Stefan Lautenschläger, Sebastian Eisermann, Torsten Henning, Peter J. Klar, and Bruno K. Meyer — I. Physikalisches Institut, Justus-Liebig-Universität, Heinrich-Buff-Ring 16, 35392 Giessen

The oxide semiconductor zinc oxide (ZnO) is due to its wide band-gap potentially of interest for applications in blue and UV optoelectronic devices. The availability of crystalline ZnO substrates of different orientations offers new possibilities in this respect. However, before optoelectronic devices fully based on ZnO can be realized, one has to overcome the problem of p-type doping. A possible way to circumvent this problem is the use of p-GaN/n-ZnO heterostructures. In the last few years considerable progress has been made in the development of p-type ZnO. Doping with nitrogen is used in Giessen. We report on current-voltage characteristics and electroluminescence measurements of GaN/ZnO heterostructures and ZnO/ZnO:N homojunctions.

HL 48.8 Wed 12:15 POT 151

Optical spin orientation by linearly polarized light in ZnO — •Vera Klinke[1], Christoph Schwark[1], Christian Weier[1], Gernot Güntherodt[1], Matthias Althammer[2], Sebastian T.B. Goennenwein[2], Matthias Opel[2], Rudolf Gross[2], and Bernd Beschoten[1] — [1]Physikalisches Institut II A, RWTH Aachen University, Aachen, Germany — [2]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany

Optical absorption of circularly polarized light is well known to yield spin-polarized electrons. Recently, some of us have demonstrated that electron spin polarization can even be generated with high efficiency by absorption of linearly polarized light in InGaAs for laser energies near its fundamental band gap [1]. This method allows to selectively excite in-plane or out-of-plane spins. The excitation mechanism, however, has not been fully understood. We extend our studies to unintentionally doped ZnO samples. For laser excitation energies far below the band gap, we can resonantly spin-polarize donor bound excitons with linearly polarized light excitation. Surprisingly, the observed Faraday rotation for linearly polarized excitation can even be 10 times larger than for circularly polarized excitation.

This work has been supported by DFG through SPP 1285.

[1] K. Schmalbuch *et al., arXiv:1008.0157, Phys. Rev. Lett. (in press)*

HL 48.9 Wed 12:30 POT 151

Piezoelectric properties of ZnO and (Zn,Mg)O- microstructures — •Christina A. Fobbe[1], Irina Laubenstein[1], Marcel Ruth[1], Manuel H. W. Bader[1], Alexander M. Bernhart[2], Mark R. Kaspers[2], Christian A. Bobisch[2], Rolf Moeller[2], and Cedrik Meier[1] — [1]University of Paderborn, Experimental Physics & CeOPP, Warburger Str. 100, 33098 Paderborn — [2]University of Duisburg-Essen, Faculty of Physics, Lotharstr. 1, 47057 Duisburg

Zinc oxide (ZnO) is a highly attractive material for piezoelectric applications. The usage of ZnO crystals in applications such as sensors and actuators has already been demonstrated. *Ab-initio* calculations have shown that the piezoelectric constant for magnesium oxide (MgO) exceeds the value for bulk ZnO [1].

We present investigations of the piezoelectric properties of $Zn_{1-x}Mg_xO$-microstructures with different Mg concentrations in comparison to binary ZnO-microstructures. For these experiments ZnO based microstructure devices have been fabricated on hydrothermally grown ZnO samples as well as on (Zn,Mg)O-epilayers grown by plasma-assisted molecular beam epitaxy (MBE).

The piezoelectric properties of the devices were investigated by applying an external electric field using a UHV-four-probe scanning tunneling microscope (STM). This way, we were able to reproduce the

literature value of bulk ZnO and report on the results obtained for (Zn,Mg)O samples.

[1] G. Chambaud et al., Chem. Phys. 352, 147 (2008)

HL 48.10 Wed 12:45 POT 151

Synthesis and characterization of micro scaled free standing c-oriented piezoelectric ZnO needles — •Sören Kaps, Arnim Schuchardt, Yogendra Kumar Mishra, and Rainer Adelung — Functional Nanomaterials, Institute for Materials Science, University of Kiel, Kaiserstraße 2, 24143 Kiel

The combination of a piezoelectric and a magnetostrictive material on a microscopic scale allows the creation of magnetoelectric (ME) composites with a very high ME effect. For magnetic field sensors a freestanding ME composite has the advantage that no clamping of the composite is necessary and therefore no hindering of the deformation can occur. Since the preferred growth direction of ZnO is the c-axis which is also piezoelectric active and hence it becomes a potential candidate for building freestanding ME composites. The controlled growth and the piezoelectric properties of ME composites are highly important to realize ME composites by coating the ZnO with a magnetostrictive material. In the present work free standing ZnO needles with variable dimensions, have been synthesized by conventional vapor liquid solid (VLS) and a newly introduced flame transport synthesis (FTS) approach. The effect of different ZnO structures on piezoelectric properties will be discussed. Further the piezoelectric properties will be related to the electronic properties and it will be shown how reliable conductivity measurements can give a hint on the quality of the obtained structures.

HL 48.11 Wed 13:00 POT 151

Electrical properties of 1D to 3D ZnO nanostructures synthesized by flame transport synthesis approach — •Arnim Schuchardt, Sören Kaps, Yogendra Kumar Mishra, Ingo Paulowicz, and Rainer Adelung — Functional Nanomaterials, Institute for Material Science, Faculty of Engineering, Christian-Albrechts-University, Kaiserstraße 2, 24143 Kiel Germany

Due to the piezoelectricity and the strong tendency to grow self organised in one or two dimensional structures with high aspect ratios, ZnO has obtained huge interest for the application in nanogenerators. With a simple flame transport method self organised ZnO-structures with dimensions ranging from nm up to mm were synthesised. In first experiments to investigate the piezoelectric properties of ZnO rods, these rods where deformed periodically by a PZT piezo actuator including a simultaneous measurement of the voltage. The electrical properties of ZnO structures synthesised by the flame transport method and the influence of the metallic contacts will be shown and discussed. The occurrence of Schottky contacts in between the ZnO structures and the metallic contacts will be elaborated in more detail. With respect to the generator applications, the change of the electrical conductivity under normal and bended state for a ZnO rod was performed and preliminary results will be discussed. Apart from ZnO rods, electrical properties of 3-dimensional complex flexible network of ZnO nanostructures will also be discussed.

HL 48.12 Wed 13:15 POT 151

Trap-related behavior of charge carrier transport in transparent conductive oxides — •Marlis Ortel and Veit Wagner — School of Engineering and Science, Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

Recently significant progress was made in the field of wet-chemically processed metal oxide semiconductors. Even though these materials are amorphous they show high mobility values of up to 100 cm2/Vs. Furthermore metal oxide semiconductors are transparent due to their large band gap. The combination of both properties makes these materials important for applications such as transparent electronics.

However TCO-based devices often show hysteresis and stress-related threshold voltage shift, which is not acceptable in many applications. In this work the charge carrier transport in TCO-based transistors is analyzed. The semiconductor is wet-chemically deposited from a precursor solution and thermally converted into ZnO. The hysteresis and bias stress in these layers are attributed to trapping of charges. The observed threshold voltage shifts are strongly affected by charge carrier density, electric field strength, temperatures and ambient gases. To gain detailed information about the local threshold voltage shift within the channel is obtained via 4-probe setup. This setup includes two electrodes in the conducting channel which enable the determination of the potential in the channel while stressing the device and thus yield valuable information if charge density or electric field strength is more important. The analysis yields, among others, especially a strong influence of the electric field strength on the observed bias stress.

HL 49: Photonic Crystals and Metamaterials

Time: Wednesday 10:15–12:15 Location: POT 251

HL 49.1 Wed 10:15 POT 251

Optical Gain in Rolled-up Semiconductor/Metal Metamaterials — Stephan Schwaiger, Markus Broell, Ricardo Costa, Matthias Klingbeil, Aune Koitmae, Wolfgang Hansen, Detlef Heitmann, and •Stefan Mendach — Institute for Applied Physics, University of Hamburg, Jungiusstrasse 11, 20355 Hamburg, Germany

Stimulated emission from optically active gain material is one of the most promising ways to solve the problem of losses in metamaterials [1, 2]. Here, we present gain measurements on rolled-up semiconductor/metal hybrid metamaterials [3] containing InGaAs quantum wells. We find a characteristic increase and decrease of the transmission through the metamaterial when optically pumping the quantum well. We observe positive gain of up to 15% at the high energy tails of the photoluminescence peaks of the quantum well and negative gain of similar magnitude at the low energy tails. This behaviour can be well reproduced with transfer matrix calculations which model each peak in the quantum well photoluminescence by a Lorentz oscillator.

[1] Y. Sivan, S. Xiao, U. K. Chettiar, A.V. Kildishev, and V. M. Shalaev, Opt. Exp. 26, 24060 (2009). [2] S. Xiao, V. P. Drachev, A.V. Kildishev, X. Ni, U. K. Chettiar, H.-K. Yuan, and V.M. Shalaev, Nature 466, 735 (2010). [3] S. Schwaiger, M. Bröll, A. Krohn, A. Stemmann, C. Heyn, Y. Stark, D. Stickler, D. Heitmann, and S. Mendach, Physical Review Letters 102, 163903 (2009)

HL 49.2 Wed 10:30 POT 251

Calculation of Transmission through rolled-up three dimensional Metamaterials — •Andreas Rottler, Stephan Schwaiger, Aune Koitmäe, Matthias Klingbeil, Markus Bröll, Detlef Heitmann, and Stefan Mendach — Institute of Applied Physics, University of Hamburg, Germany

Metamaterials are artificial structures where permittivity and permeability can be designed on demand and may exhibit values which are not observed in nature. In this talk, we present finite-difference time-domain simulation results on a metamaterial which consists of curved alternating layers of metal/semiconductor films. Such structures can be prepared from self-rolling strained metal/semiconductor layers and exhibit an anisotropic permittivity with tunable plasma frequency allowing for hyperlensing in the visible [1]. We performed simulations where we varied the parameters of the structure in order to optimize the transmission through the curved metamaterial.

We gratefully acknowledge support by the DFG via the Graduiertenkolleg 1286.

[1] S. Schwaiger et al., Phys. Rev. Lett. 102, 163903 (2009)

HL 49.3 Wed 10:45 POT 251

Auxiliary basis functions for the Wannier function based 2D TE photonic crystal circuit design — •Patrick Mack, Christian Wolff, and Kurt Busch — Institut für Theoretische Festkörperphysik (TFP) and DFG-Center for Functional Nanostructures (CFN), Karlsruhe Institute of Technology (KIT), 76128 Karlsruhe, Germany

Photonic crystals are periodic dielectric heterostructures exhibiting a band structure for light. Adjusting fabricational parameters offers the possibility to open complete, photonic band gaps prohibiting light propagation regardless of direction. Purposely designed defect structures introduce localized light modes in these forbidden frequency ranges, creating resonator modes, waveguides and functional elements for photonic devices, whose design optimization has to be carried out

numerically.

The Wannier function (WF) approach yields a tight-binding like numerical method which expands these localized states in a set of localized basis functions and proved to be particularly efficient for E-polarized (TM) light in the combination with an S-matrix approach. In the H-polarized (TE) case, however, slow convergence limited the applicability of this Ansatz. We propose to use additional auxiliary basis functions, that improve convergence and are capable of modeling 2D TE large scale photonic circuitry (typically air holes in silicon) involving non-etched holes and tunable linear anisotropic media, such as liquid crystals and magneto-optic materials.

HL 49.4 Wed 11:00 POT 251

Coupling model for the derivation of optical resonances in stacked nanogratings — •Thomas Weiss[1,2], Nikolay A. Gippius[2,3], Sergei G. Tikhodeev[3], Gérard Granet[2], Liwei Fu[1], Richard Taubert[1], and Harald Giessen[1] — [1]4th Physics Institute and Research Center Scope, University of Stuttgart, Stuttgart, Germany — [2]LASEMA, University Blaise Pascal, Aubière, France — [3]A. M. Prokhorov General Physics Institute, Russian Academy of Sciences, Moscow, Russia

Nanogratings have become one of the most important structures in modern nanooptics over the last few years. They can be used in different fields such as photonic crystals and metamaterials. However, the experimental fabrication as well as the corresponding numerical calculation is usually very time-consuming. Hence, simple models are required for a qualitative derivation of the optical behavior of such structures. Here, we present a method to approximate the optical resonances of stacked nanogratings using the Fourier modal method and optical scattering matrix theory. The resulting equations form a low-dimensional linear eigenvalue problem that can easily be solved for varying grating distances, including near field effects as well as multiple scattering in the far field regime with strong coupling to Fabry-Perot resonances. The method is not only accurate and fast; it provides also additional physical insight, as the individual components of the coupling mechanism can be studied independently. Furthermore, the model involves no fitting parameters. All quantities can be derived ab initio by the scattering matrix formalism.

HL 49.5 Wed 11:15 POT 251

3D photonic crystal integrated in a mircomorph thin film silicon tandem cell — •Johannes Üpping[1], Thomas Beckers[2], Reinhard Carius[2], Uwe Rau[2], Stephan Fahr[3], Carsten Rockstuhl[3], Falk Lederer[3], Matthias Kroll[4], Thomas Pertsch[4], Lorenz Steidl[5], Rudolf Zentel[5], and Ralf B. Wehrspohn[1] — [1]Institute of Physics, mikroMD, University of Halle Wittenberg — [2]Institute of Energy Research, IEF-5 Photovoltaics, Forschungszentrum Jülich GmbH — [3]Institute of Condensed Matter Theory and Sold State Optics, Friedrich-Schiller-Universität Jena — [4]Institute of Applied Physics, Friedrich-Schiller-Universität Jena — [5]Institute of Organic Chemistry, Johannes Gutenberg-Universität Mainz

A 3D photonic intermediate reflector for textured micromorph silicon tandem solar cells has been investigated. In thin-film silicon tandem solar cells consisting of amorphous and microcrystalline silicon with two junctions of a-Si/μc-Si, efficiency enhancements can be achieved by increasing the current density in the a-Si top cell. It is one goal to provide an optimized current matching at high current densities. For an ideal photon-management between top and bottom cell, a spectrally selective intermediate reflective layer (IRL) is necessary. We we present the first fully integrated 3D photonic thin-film IRL device incorporated in a state-of-the-art textured tandem solar cell. The design, the preparation and numerical calculations of a 3D self organized inverted opal photonic crystal structure in a textured micromorph tandem solar cell are presented.

HL 49.6 Wed 11:30 POT 251

Angle-resolved fluorescence spectroscopy in photonic crystals — •Rebecca Wagner, Lars Heerklotz, and Frank Cichos — Molecular Nanophotonics, University of Leipzig, Germany

Photonic Crystals (PCs) are materials with periodically varying dielectric constant. Multiple scattering of light on this spatially modulated refractive index leads to the formation of a photonic band structure including photonic band gaps. The optical density of states is redistributed as compared to a homogeneous material and is described by the fractional local density of states (FLDoS). This leads to a modified propagation of light in the material.

The spectral and angular position of the band gaps can, for example, be probed by reflection spectroscopy. Since reflections can occur on different lattice plane families, the detection angle has to be varied for every angle of incidence, making this method very time consuming. Further, an average of the reflectivity over differently oriented crystal domains is taken.

We develop a method to overcome these problems using fluorescence spectroscopy of single internal emitters. By applying a special technique we are able to measure angle resolved fluorescence spectra for many emission angles at the same time. Comparison of these spectra to spectra of emitters outside the PC gives the FLDoS, which also contains information about the symmetry of the emitter's local environment. By varying emitters and lattice constants of the PC, different regions of the band structure can be probed.

HL 49.7 Wed 11:45 POT 251

The Concepts of Self-assembled 3D Photonic Crystals for High Temperature IR reflective coatings — •Hooi Sing Lee[1], Alexander Petrov[1], Manfred Eich[1], Roman Kubrin[2], Gerold Scheider[2], Julien Bachmann[3], and Kornelius Nielsch[3] — [1]Institut für Optische und Elektronische Materialien, TUHH, Hamburg, Deutschaland — [2]Institut für keramische Hochleistungswerkstoffe , TUHH, Hamburg, Deutschaland — [3]nstitut für Angewandte Physik, Uni Hamburg, Hamburg, Deutschaland

The study is undertaken to develope a self-assembled 3D microporous structure which is based solely on low thermal conductivity ceramic materials and is capable of reflecting IR radiation at any incident angle over a wide spectral range.The practical applications which will benefite most from this study are ceramic thermal barrier coatings (TBC) and selective filters for thermophotovoltaics (TPV). Finite Integration Technique (FIT) simulations have shown that yttria stabilized zirconia (YSZ) inverse opal with the pore size of $>$ 500nm possesses stopgap in the IR regime and can be tailored to reflect target range of wavelength by changing the lattice constants. The width of the stopgap can be effectively enlarged by stacking several inverse opal with different pore sizes in the subsequent layers and it was shown in simulation and experiment. It was estimated that 9 stacks of such structures can achieved 91% of total hemispherical reflectance in the wavelegth range of 1-6 *m, where the major blackbody radiant power at 1500 K tends to be concentrated. The optical properties of direct opal and inverse opal were measured and compared with the simulations.

HL 49.8 Wed 12:00 POT 251

Bio-inspired multifunctional photonic systems — •Mathias Kolle[1], Peter Vukusic[2], and Joanna Aizenberg[1] — [1]School of Engineering and Applied Sciences, Harvard University, 9 Oxford St, Cambridge, MA-02138, US — [2]School of Physics, Stocker Road, Exeter, EX4 4QL

Biomimetic and bio-inspired attempts to produce novel photonic structures have attracted increasing research interest in recent years. Nature offers an enormous amount of multifunctional micro- and nanostructures that provide outstanding, distinctive, dynamic and tailored coloration and high reflectivity. Various intriguing photonic structures have been identified on the wing scales of beetles, butterflies, the feathers of birds or in marine animals. Nature offers a huge reservoir of blueprints for novel artificial optical materials and photonic structures. We present the development of bio-inspired, dynamic, micro-optical elements that are comparable to some of natures efficient optical systems. Artificially controlled self-assembly combined with established nanofabrication techniques can be used for the development of new optically-adaptive devices. Novel optical elements have to address the aspect of tunability and multifunctionality to be versatile for a wide range of applications. Furthermore, we propose a technique to create fully organic adaptive optical systems based on elastic multilayer micro-rolls.

HL 50: SKM Symposium: Topological Insulators (SYTI)

Time: Wednesday 10:30–13:00 Location: TRE Ma

Invited Talk HL 50.1 Wed 10:30 TRE Ma
Topological insulators and topological superconductors — •Shoucheng Zhang — Stanford

Recently, a new class of topological states has been theoretically predicted and experimentally observed. The topological insulators have an insulating gap in the bulk, but have topologically protected edge or surface states due to the time reversal symmetry. Similarly, topological superconductors or superfluids have novel edge or surface states consisting of Majorana fermions. In this talk, I shall review the recent theoretical and experimental progress in the field, and focus on a number of outstanding issues, including the quantized anomalous Hall effect, quantized magneto-electric effect, the topological Mott insulators and the search for topological superconductors.

Invited Talk HL 50.2 Wed 11:00 TRE Ma
Dirac Fermions in HgTe Quantum Wells — •Laurens Molenkamp — Physikalisches Institut(EP3) der Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

HgTe quantum wells have a linear band dispersion at low energies and thus mimic the Dirac Hamiltonian. Changing the well width tunes the band gap (i.e., the Dirac mass) from positive, through zero, to negative. Wells with a negative Dirac mass are 2-dimensional topological insulators and exhibit the quantum spin Hall effect, where a pair of spin polarized helical edge channels develops when the bulk of the material is insulating. Our transport data provide very direct evidence for the existence of this third quantum Hall effect. Wells with a thickness of 6.3 nm are zero gap Dirac systems, similar to graphene. However, zero gap HgTe wells possess only a single Dirac valley, which avoids inter-valley scattering. This makes them especially suitable to study quantum interference effects under a Dirac Hamiltonian.

Invited Talk HL 50.3 Wed 11:30 TRE Ma
Interaction, disorder, and quantum criticality in Z_2 topological insulators — •Alexander Mirlin — Karlsruhe Institute of Technology, Germany

We study disorder and interaction effects in topological insulators with strong spin-orbit coupling. We find that the interplay of nontrivial topology, quantum interference, and Coulomb repulsion induces a novel critical state on the surface of a three-dimensional topological insulator. Remarkably, this interaction-induced criticality, characterized by a universal value of conductivity, emerges without any adjustable parameters. Further, we predict a direct quantum-spin-Hall transition in two dimensions that occurs via a similar critical state.

[1] P.M. Ostrovsky, I.V. Gornyi, A.D. Mirlin, Interaction-induced criticality in Z_2 topological insulators, Phys. Rev. Lett. 105, 036803 (2010)

[2] A. D. Mirlin, F. Evers, I. V. Gornyi, P. M. Ostrovsky, Anderson Transitions: Criticality, Symmetries, and Topologies, in "50 Years of Anderson Localization", ed. by E. Abrahams (World Scientific, 2010); reprinted in Int J Mod Phys B 24, 1577 (2010).

Invited Talk HL 50.4 Wed 12:00 TRE Ma
Disorder and Interactions in Topological Insulators — •Allan H. MacDonald — University of Texas, Austin TX, USA

Three-dimensional topological insulators have protected surface states that are described by massless Dirac equations. I will discuss some properties of these two-dimensional Dirac systems, emphasizing the importance of disorder and interactions. The magneto-optical properties of topological insulator thin films depend intricately on a competition between disorder and time-reversal symmetry breaking by either external magnetic fields or exchange coupling to external magnetic fields. Broken symmetry states, including notably nteraction-driven spontaneous phase coherence between top and bottom surfaces are likely to occur in the absence of a magnetic field. In addition a wide variety of unusual broken symmetry states are likely to be discovered in the presence of external magnetic fields as sample qualities improve.

Invited Talk HL 50.5 Wed 12:30 TRE Ma
Tunable multifunctional topological insulators in ternary Heusler and related compounds — •Claudia Felser[1], Stanislav Chadov[1], Lukas Müchler[1], Jürgen Kübler[2], Shou Cheng Zhang[3], Xiaoliang Qi[3], and Hai-Jun Zhang[3] — [1]University Mainz — [2]TU Darmstadt — [3]Stanford University

Recently the quantum spin Hall effect was theoretically predicted and experimentally realized in quantum wells based on the binary semiconductor HgTe. The quantum spin Hall state and topological insulators are new states of quantum matter interesting for both fundamental condensed-matter physics and material science. Many Heusler compounds with C1b structure are ternary semiconductors that are structurally and electronically related to the binary semiconductors. The diversity of Heusler materials opens wide possibilities for tuning the bandgap and setting the desired band inversion by choosing compounds with appropriate hybridization strength (by the lattice parameter) and magnitude of spinorbit coupling (by the atomic charge). Based on first-principle calculations we demonstrate that around 50 Heusler compounds show band inversion similar to that of HgTe. The topological state in these zero-gap semiconductors can be created by applying strain or by designing an appropriate quantumwell structure, similar to the case of HgTe. Many of these ternary zero-gap semiconductors (LnAuPb, LnPdBi, LnPtSb and LnPtBi) contain the rare-earth element Ln, which can realize additional properties ranging from superconductivity (for example LaPtBi) to magnetism (for example GdPtBi) and heavy fermion behaviour (for example YbPtBi).

HL 51: Joint Focussed Session: Theory and Computation of Electronic Structure: New Frontiers III

Time: Wednesday 11:15–13:00 Location: TRE Phy

HL 51.1 Wed 11:15 TRE Phy
Dynamical magnetic excitations of nanostructures from first-principles — •Samir Lounis[1,2], Antonio Costa[3], Roberto Muniz[3], and Douglas Mills[1] — [1]Department of Physics and Astronomy, University of California Irvine, California, 92697 USA — [2]Institut für Festkörperforschung and Institut for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — [3]Instituto d Fisica, Universidade Federal Fluminense, 24210-340 Niteroi, Rio de Janeiro, Brazil

Within the framework of time-dependent density functional theory combined with the Korringa-Kohn-Rostoker Green function formalism, we present a real space methodology to investigate dynamical magnetic excitations from first-principles [1]. We set forth a scheme which enables one to deduce the correct effective Coulomb potential needed to preserve the spin-invariance signature in the dynamical susceptibilities, i.e. the Goldstone mode. We use our approach to explore the spin dynamics of 3d adatoms and different dimers deposited on a Cu(001) surface[1] and a Cu(111) surface [2] with emphasis on their decay to particle-hole pairs.

Research supported by the U. S. Depart. of Energy through grant No. DE-FG03-84ER-45083. S. L. thanks the A.v. Humboldt Foundation for a Feodor Lynen Fellowship. R.B.M. acknowledges support from CNPq and FAPERJ, Brazil.

[1] Lounis *et al.* Phys. Rev. Lett. **105**, 187205 (2010); Lounis *et al.* arXiv:1010.1293. [2] Khajetoorians et al. arXiv:1010.1284v2.

HL 51.2 Wed 11:30 TRE Phy
Magnetic order of $LaVO_3/SrVO_3$ superlattices — •Cosima Schuster[1], Ulrike Lüders[2], Udo Schwingenschlögl[3], and Raymond Fresard[2] — [1]Institut für Physik, Universität Augsburg, D-86135 Augsburg — [2]Laboratoire CRISMAT, UMR CNRS-ENSICAEN(ISMRA) 6508, FR3095 Caen — [3]KAUST, PCSE Division, P.O. Box 55455, Jeddah 21534, Saudi Arabia

While stable ferromagnetic ground states are predicted based on model

calculations their experimental realizations are scarce. Experimental data obtained on $LaVO_3[m]/SrVO_3[1]$ superlattices show that these systems remain magnetic above room temperature for particular values of m, in contrast to the solid solutions with the same composition. To clarify the magnetic and orbital order in these heterostructures, we perform electronic structure calculations based on density functional theory. First, we discuss the magnetic and orbital order of strained $LaVO_3$, for the c/a ratio of the heterostructure, where two types of ordering are nearly degenerate. While both g-type and c-type antiferromagnetic ordering within the $LaVO_3$ favour a non-magnetic interface in case of odd m and a ferromagnetic interface in case of even m, the orbital ordering perpendicular to the interface is different in both cases. A detailed discussion of the particular combinations of the magnetic and orbital order at the interface is given.

HL 51.3 Wed 11:45 TRE Phy

First-principles quantum-mechanical methods for full prediction of NMR parameters in fluorides — •Aymeric Sadoc[1], Florent Boucher[1], Mamata Biswal[2], Monique Body[2], and Christophe Legein[2] — [1]Institut des matériaux Jean Rouxel (IMN) - Université de Nantes, CNRS, 2 rue de la houssinière, BP 32229, 44322 Nantes, France — [2]Institut de Recherche en Ingénierie Moléculaire et Matériaux Fonctionnels (IRIM2F) - Université du Maine, CNRS, Avenue Olivier Messiaen, 72085 Le Mans, France

^{19}F magic angle spinning (MAS) NMR is a powerful structural tool for complex fluoride crystalline materials having multiple crystallographic sites since ^{19}F (I=1/2) isotropic chemical shift (δ_{iso}) is very sensitive to the environment of the fluorine atom. However, in many cases, several fluorine sites have the same multiplicity preventing an unambiguous experimental assignment. Simulation of the response to an external magnetic field is then necessary to complete the analysis. The relation of the measured δ_{iso} values with the calculated isotropic chemical shieldings (σ_{iso}) is needed to interpret of NMR spectra.

^{19}F σ_{iso} values were calculated for alkali, alkaline earth and rare earth of column IIIB fluoride compounds using the GIPAW method implemented in the CASTEP software. Using DFT-PBE, we have established a linear relation between ^{19}F calculated σ_{iso} and experimental δ_{iso} values which enables full prediction of ^{19}F NMR spectra. In the case of complex NMR spectra, this calibration curve is successfully applied for the attribution from first-principles quantum-mechanical of ^{19}F chemical shifts.

HL 51.4 Wed 12:00 TRE Phy

***Ab-initio* study of MnO and NiO in various crystal structures – The failure of (semi)local density functionals** — •Andreas Schrön, Claudia Rödl, and Friedhelm Bechstedt — IFTO, FSU Jena, Max-Wien-Platz 1, 07743 Jena, Germany

Transition-metal oxides (TMOs) are of great interest for applications in e.g. dilute magnetic semiconductors (DMSs) which are supposed to allow for transparent ferromagnets with high critical temperatures. One of the most promising host materials is ZnO which crystallizes in the wurtzite structure. Although TMOs have been investigated a long time experimentally, their theoretical description is still unsatisfying.

The semilocal generalized-gradient approximation (GGA) to density functional theory (DFT) works well for many materials. Here we demonstrate that this approach predicts the wrong ground-state crystal structure for MnO, since it does not account sufficiently for the electron correlation effects in materials with strongly localized electrons. It is usually assumed, that approaches including an additional on-site Coulomb interaction U (GGA+U) or non-local exchange contributions like the hybrid functional HSE03 cure this failure.

The relative energetic ordering of the rock-salt, zinc-blende, and wurtzite crystal structures are investigated for various magnetic orderings. It is shown that neither GGA nor the HSE03 hybrid functional yields the experimentally observed ground-state structure. However, agreement with experiment is obtained if the GGA+U functional with $U > 4$ eV is applied. For NiO, on the other hand, all three functionals yield rock-salt as the equilibrium crystal structure.

HL 51.5 Wed 12:15 TRE Phy

Laser-induced ultrafast demagnetization: First-principles analysis of Elliott-Yafet processes — •Karel Carva[1,2] and Peter M. Oppeneer[2] — [1]Department of Condensed Matter Physics, Charles University, Ke Karlovu 5, CZ-12116 Prague 2, Czech Republic — [2]Department of Physics and Materials Science, Uppsala University, Box 530, SE-75121 Uppsala, Sweden

The laser-induced ultrafast demagnetization phenomenon has attracted a lot of attention since the first successful experiment on the fs timescale in 1996. However even now it is still far from being understood on the microscopic level. A number of possible microscopic mechanisms have been proposed.

Here we concentrate on Elliott-Yafet spin relaxation due to to electron-phonon scattering in Ni. The spin-flip probability associated with electron-phonon scattering in Ni has been estimated - employing the ab initio band structure - to be larger than expected. We calculate the spin-flip Eliashberg function based on ab initio electron-phonon coupling matrix elements to obtain the spin-flip probability with much higher accuracy. We extend this method to the regime of non-equilibrium electron distributions relevant for ultrafast processes. We find significant differences between the efficiency of this spin relaxation mechanism for highly non-equilibrium electron distributions pumped by the laser and thermalized ones (not in equilibrium with lattice).

HL 51.6 Wed 12:30 TRE Phy

Momentum Distribution and Renormalization Factor in Sodium and the Electron Gas — •Valerio Olevano — Institut Neel, CNRS & UJF, Grenoble, France

The homogeneous electron gas or jellium is one of the most fundamental models, canonical workbench to test different many-body theoretical approaches. Although really simple, still is very close to real solids, especially alkali metals, and sodium is one of its nature's closest realization. Here we present theoretical and also experimental results on the momentum distribution and the quasiparticle renormalization factor in sodium. From an x-ray Compton-profile measurement of the valence-electron momentum density, we derive its discontinuity at the Fermi wavevector. This yields for the first time an accurate measure of the renormalization factor, one of the most important quantities in many-body theory, that we compare with GW and quantum Monte Carlo calculations performed both on crystalline sodium and on the homogeneous electron gas. Our calculated results are in good agreement with the experiment.

References: S. Huotari, J. A. Soininen, T. Pylkkänen, K. Hämäläinen, A. Issolah, A. Titov, J. McMinis, J. Kim, K. Esler, D. M. Ceperley, M. Holzmann, and V. Olevano, Phys. Rev. Lett. 105, 086403 (2010).

HL 51.7 Wed 12:45 TRE Phy

Construction of low energy Hamiltonians using maximally localized Wannier functions — •Roman Kovacik and Claude Ederer — School of Physics, Trinity College Dublin, Ireland

The theoretical description of correlated electron systems, such as e.g. transition metal oxides, is often based on effective tight-binding (TB) models. A systematic way to obtain realistic TB model parameters from first principles calculations is the construction of maximally localized Wannier functions (MLWFs) [1]. The corresponding TB representation is given by the real space Hamiltonian matrix elements in the MLWF basis. We address two important issues: i) how many orbitals to include in the basis set for the TB model representation, and ii) what is the most appropriate reference point to connect the model and Kohn-Sham band structures (i.e. should the Kohn-Sham band structure be considered as "non-interacting" or as mean-field approximation to the interacting case). We use $LaMnO_3$, a prototype material for correlation-driven phenomena, as an example for the construction of model Hamiltonians. In particular, we compare a TB description based only on effective Mn e_g bands with a description that explicitly includes also the O p bands, and we analyze the effects of the Hubbard U and the Jahn-Teller distortion on the corresponding TB parameterizations. In addition, we discuss the suitability of different types of Wannier functions for the calculation of TB parameters.

[1] I. Souza, N. Marzari, and D. Vanderbilt, PRB 65, 035109 (2001).

HL 52: Nonpolar and Semipolar Nitrides

Time: Wednesday 11:45–13:15 Location: POT 51

HL 52.1 Wed 11:45 POT 51

Influence of Si-doping on heteroepitaxially grown a-plane GaN — •Matthias Wieneke, Barbara Bastek, Martin Noltemeyer, Thomas Hempel, Antje Rohrbeck, Harmut Witte, Peter Veit, Jürgen Bläsing, Armin Dadgar, Jürgen Christen, and Alois Krost — Otto-von-Guericke-Universität Magdeburg, FNW/IEP, Universitätsplatz 2, 39106 Magdeburg

Si-doped a-plane GaN samples with nominal doping levels up to 10^{20} cm^{-3} were grown on r-plane sapphire by metal organic vapor phase epitaxy. Silane flow rates higher than 59 nmol/min lead to three dimensional grown crystallites as revealed by scanning electron microscopy. High resolution X-ray diffraction, photoluminescence and cathodoluminescence suggest considerably reduced defect densities in the large micrometer-sized GaN crystallites. Especially, transmission electron microscopy images verify a very low density of basal plane stacking faults less than 10^4 cm^{-1} [1] in these crystallites consisting of heteroepitaxially grown a-plane GaN. In our presentation the influence of the Si doping on the basal plane stacking faults will be discussed. [1] Wieneke et al., Phys. Status Solidi B, 2010, 10.1002/pssb.201046372

HL 52.2 Wed 12:00 POT 51

Single phase semipolar ($11\bar{2}2$) GaN on ($10\bar{1}0$) sapphire — •S. Ploch[1], J. B. Park[2], J. Stellmach[1], T. Schwaner[1], M. Frentrup[1], T. Wernicke[1], T. Niermann[2], M. Pristovsek[1], M. Lehmann[2], and M. Kneissl[1] — [1]Institute of Solid States Physics, — [2]Institute of Optics and Atomic Physics, TU Berlin, Hardenbergstr. 36, 10623 Berlin

InGaN quantum well based light emitters grown on (0001) GaN suffer from poor quantum efficiencies with increasing indium mole fraction due to strong polarization fields along the polar crystal orientation. This effect can be greatly reduced by growing on semi- and non-polar GaN orientations. Semipolar ($11\bar{2}2$) GaN layers were deposited by metalorganic vapour phase epitaxy on ($10\bar{1}0$) sapphire. After sapphire substrate nitridation at 1000°C, a GaN nucleation layer was deposited at high temperature, followed by the deposition of 1.5 nm thick GaN buffer layers. The samples show predominantly ($11\bar{2}2$) orientation with a small fraction of ($10\bar{1}3$) oriented domains. With increasing nitridation layer thickness the ($10\bar{1}3$) phase is suppressed leading to a very smooth surface morphology (rms roughness $<$ 4nm). PL measurements show dominant basel plane stacking fault (BSF) I_1 luminescence without any other defects. Transmission electron microscopy measurements reveal a high BSF density. The FWHM of the X-ray diffraction rocking curve measurements of the ($11\bar{2}2$) reflection decreases to 1193 arcsec and 739 arcsec along [$1\bar{1}00$] and [$11\bar{2}3$] respectively with increasing nucleation temperature. Using high temperature nucleation smooth and homogeneous ($11\bar{2}2$) phase GaN layers have been obtained.

HL 52.3 Wed 12:15 POT 51

Polarisation of the spontaneous emission from nonpolar and semipolar InGaN quantum wells — •Lukas Schade[1,2], Ulrich Schwarz[1,2], Simon Ploch[3], Tim Wernicke[3], Arne Knauer[4], Veit Hoffmann[4], Markus Weyers[4], and Michael Kneissl[3,4] — [1]Department of Microsystems Engineering, University of Freiburg (IMTEK) — [2]Fraunhofer Institute for Applied Solid State Physics (IAF) — [3]Institute of Solid State Physics, Technical University Berlin — [4]Ferdinand-Braun-Institute, (FBH)

Spontaneously emitted light stemming from semipolar and nonpolar InGaN quantum wells is polarized. This property is a consequence of the broken in-plane symmetry of non c-plane wurtzite quantum wells. We studied the polarized photoluminescence of semipolar and nonpolar InGaN/InGaN multi quantum wells grown on low defect density GaN substrates with a setup for confocal microscopy. For excitation of charge carriers we use a 375 nm diode laser. The photoluminescence is collected with an objective of small NA, to avoid polarisation scrambling, and analyzed with a broadband polarizer and a spectrometer. The experimental results are compared to k·p band structure calculations for semipolar and nonpolar InGaN quantum wells. These simulations provide the polarisation degree of the confined states of the valence band and their energetic splitting. Next, from the thermal occupation the polarized spectra are calculated. The comparison with experimental results allows the determination of the valence subband splitting. Our experiments show a splitting of the two topmost valence subbands in nonpolar direction which is larger than predicted.

HL 52.4 Wed 12:30 POT 51

Spatially and spectrally resolved photoluminescence of InGaN MQWs grown on highly Si doped a-plane GaN buffer — •Martin Thunert, Matthias Wieneke, Anja Dempewolf, Frank Bertram, Armin Dadgar, Alois Krost, and Jürgen Christen — Institute of Experimental Physics, Otto-von-Guericke-University Magdeburg, Germany

A set of InGaN multi quantum well (MQW) samples grown by MOVPE on highly Si doped a-plane GaN on r-plane sapphire templates has been investigated using spatially resolved photoluminescence spectroscopy (μ-PL). The Si doping level of nominal about 10^{20} cm^{-3} leads to three dimensionally grown crystallites mostly terminated by m-facets. The MQW thickness has been systematically varied from nominally 2.1 to 4.2 nm, as well as the InGaN growth temperature, which was varied from 760 °C to 700 °C. The growth of a-plane GaN based devices leads to a non-polar growth direction avoiding the polarization field affected Quantum-Confined-Stark-Effect. Spatially resolved PL studies show for all samples low near band edge (NBE) GaN emission intensity over the whole area under investigation accompanied by highly intense InGaN MQW emission for single crystallites. The MQW luminescence shows a systematic blueshift with increasing InGaN growth temperature due to lower In incorporation as well as a systematic redshift with increasing MQW thickness. Excitation power dependent spectra at 4 K as well as temperature dependent PL spectra will be presented.

HL 52.5 Wed 12:45 POT 51

Highly spatially and spectrally resolved cathodoluminescence microscopy of planar semipolar InGaN/GaN MQWs grown on pre-patterned sapphire substrate — •Silvio Neugebauer[1], Sebastian Metzner[1], Frank Bertram[1], Thomas Hempel[1], Jürgen Christen[1], Stephan Schwaiger[2], and Ferdinand Scholz[2] — [1]Institute of Experimental Physics, Otto-von-Guericke-University Magdeburg, Germany — [2]Institute of Optoelectronics, Ulm University, Germany

The optical properties of a 5-fold InGaN multiple quantum well (MQW) grown on planar semipolar ($11\bar{2}2$) GaN directly grown on prepatterned r-sapphire substrate by MOVPE have been investigated using highly spatially and spectrally resolved cathodoluminescence (CL) microscopy. The sapphire was masked and structured via RIE generating grooves with c-plane-like sidewalls. Here the growth of GaN is initiated and single stripes are formed along the sapphire a-direction. The integral spectrum of the GaN substructure exhibits a dominant (D^0,X) emission at 357,4 nm and a weak luminescence at about 361,7 nm related to basal plane stacking faults (BSFs). The BSF-CL was exclusively observed at the -c-wing of the stripes. Dark stripes in CL intensity image running from the c-plane-like sidewalls to the surface indicate bundles of dislocations acting as nonradiative recombination centers. In complete contrast, the area of the +c-wing exhibits a homogeneous CL distribution without any BSF contribution. The luminescence of the InGaN MQW shows three different emission wavelengths at 425 nm, 445 nm and 470 nm according to surface morphology.

HL 52.6 Wed 13:00 POT 51

Indium incorporation in GaInN quantum wells on various surface orientations — •Holger Jönen[1], Uwe Rossow[1], Heiko Bremers[1], Stephan Schwaiger[2], Ferdinand Scholz[2], Sebastian Metzner[3], Frank Bertram[3], Jürgen Christen[3], and Andreas Hangleiter[1] — [1]Institut für Angewandte Physik, TU Braunschweig — [2]Institut für Optoelektronik, Universität Ulm — [3]Institut für Experimentelle Physik, Otto-von-Guericke-Universität Magdeburg

While GaN based blue-violet lasers are commercially available, several problems occur on the way towards the green spectral region. Among others the high indium contents needed for green emission result in high piezoelectric fields which dramatically reduce the oscillator strength. One promising approach to reduce the influence of polarization fields is to grow on non- or semipolar surfaces of the wurtzite structure. In this contribution we compare the In incorporation in GaInN multiple quantum wells on various surface orientations. Our samples were grown by MOVPE on bulk GaN substrates, (HVPE) GaN templates or foreign substrates. The In content in the QWs was determined by high res-

olution X-ray diffraction and photoluminescence. Applying the same growth conditions we find similar growth rates and In contents for the nonpolar layers compared to conventional c-plane structures. Preliminary experiments indicate that the In incorporation on the semipolar $(11\bar{2}2)$-plane is significantly larger which is assigned to a reduction of the strain-induced repulsive interaction between incorporated In atoms on the surface[1].

[1] J. Northrup, Appl. Phys. Letters **95**, 133107 (2009).

HL 53: Optical Properties I

Time: Wednesday 12:30–13:30 Location: POT 251

HL 53.1 Wed 12:30 POT 251

Microscopic theory of phonons in the semiconductor microcavity luminescence — •Christoph N. Böttge, Thomas Feldtmann, Mackillo Kira, and Stephan W. Koch — Department of Physics and Material Sciences Center, Philipps-University, Renthof 5, D-35032 Marburg, Germany

The strong interaction between electrons and longitudinal optical (LO) phonons in ZnO gives rise to pronounced phonon sidebands in the photoluminescence (PL) spectrum as strikingly shown in recent experiments and theoretical investigations. To develop a consistent microscopic theory of the sideband emission, we have generalized the semiconductor luminescence equations (SLE) by including phonon-assisted processes. This approach allows us to compute both spontaneous and stimulated emission at the excitonic resonance and its first phonon sideband. In addition, we have developed an analytic model to describe phonon-assisted luminescence in a cavity.

Because phonon-assisted emission and absorption take place on different sides of the excitonic resonance, we found that no normal-mode splitting occurs for the phonon sideband. This is in pronounced contrast to the usual case where the cavity mode coincides with the zero phonon line leading to strong qualitative changes in the spectra due to the normal-mode coupling. Our numerical and analytical results confirm that the sideband intensity is strongly enhanced when the reflectivity of the mirrors reaches a critical value. We show that also ZnO-based systems can reach normal-mode coupling for the zero-phonon line and strongly enhanced emission for the first phonon sideband.

HL 53.2 Wed 12:45 POT 251

Many-body effects in phonon-sideband luminescence — •Alexej Chernikov[1], Verena Bornwasser[1], Christoph N. Böttge[1], Thomas Feldtmann[1], Sangam Chatterjee[1], Martin Koch[1], Mackillo Kira[1], Stephan W. Koch[1], Thomas Wassner[2], Stefan Lautenschlaeger[2], Bruno K. Meyer[2], and Martin Eickhoff[2] — [1]Faculty of Physics and Material Sciences Center, Philipps-Universität Marburg, Renthof 5, D-35032 Marburg, Germany — [2]I. Physikalisches Institut,Justus-Liebig-Universität Giessen,Heinrich-Buff-Ring 16, D-35392 Giessen, Germany.

The photoluminescence spectra of high-quality intrinsic semiconductors with a direct bandgap are usually dominated by the excitonic resonance. The spectra may also feature one or more additional lines, commonly referred to as phonon sidebands (PSBs), traced back to the phonon-assisted recombination. In theory, PSB luminescence is traditionally treated using a perturbative approach with excitons coupled directly to LO-phonons via polar Froehlich interaction. However, the many-body properties of the interacting carrier system yield a more complex picture. Already the luminescence at the main excitonic resonance does not necessarily require excitonic population. In addition, the Froehlich coupling is expected to be suppressed in case of the exciton-phonon interaction. Here, we study the time-resolved PSB emission of direct polar semiconductors and apply a microscopic many-body approach to analyze the experimental observations. Our results show that excitonic population is not required for the observation of PSBs.

HL 53.3 Wed 13:00 POT 251

THz studies of strong-coupling microcavity systems — •Andrea C Klettke[1], Johannes T Steiner[1], Mackillo Kira[1], Stephan W Koch[1], and Yun-Shik Lee[2] — [1]Department of Physics and Material Sciences Center, Philipps-University Marburg, Renthof 5, D-35032 Marburg, Germany — [2]Department of Physics, Oregon State University, Corvallis, Oregon 97331, USA

We study semiconductor quantum wells inside a cavity assuming the simultaneous presence of optical and terahertz radiation. Light-matter coupling of semiconductor quantum wells inside Bragg-mirror microcavities leads in the linear regime to a polaritonic mixing of the excitonic quantum well resonance and the cavity mode. The resulting normal mode splitting into low (LEP) and high energy peak (HEP) provides a basis for the conversion of $1s \rightarrow 2p$ population via strong THz radiation.

We present a microscopic theory allowing us to quantitatively evaluate the combined influence of the optical and THz field and their interaction with the microcavity exciton resonance. We use the parameters appropriate to study the response of a system investigated experimentally in the group at Oregon State University. The major observation is that we can selectively switch off either the low or the high energy peak. Non-linear contributions will be discussed as well as multi-photon absorption and higher harmonics.

HL 53.4 Wed 13:15 POT 251

Quantum-optical correlations in dissipative quantum-dot systems — •Martin Mootz, Mackillo Kira, and Stephan W. Koch — Department of Physics and Material Sciences Center, Philipps-University Marburg, Renthof 5, D-35032 Marburg

Quantum-optical spectroscopy is based on a concept where the system interactions are controlled and characterized through the quantum fluctuations of the light. We apply this scheme to semiconductor systems which exhibit a complicated many-body problem dominated by the Coulomb interaction among electrons and holes and by coupling with the semiconductor environment. To gain insights on the quantum-optical spectroscopy, we model quantum-dot systems via the Jaynes-Cummings model coupled to a reservoir. We characterize the quantum features of the light source and the resonance fluorescence via the cluster-expansion transformation that yields a one-to-one mapping between correlated clusters and the traditional phase-space distributions. We investigate the transition from strong-to-weak coupling, which is typically considered to be the border between quantum-optical and classical studies. We show that quantum-optical spectroscopy can detect nonclassical features even in the weak-coupling regime where dephasing completely removes direct quantum-optical signatures such as revivals and quantum-Rabi flopping.

HL 54: Joint Session: Organic Semiconductors IV: Excitations and Charges

Time: Wednesday 14:00–17:00 Location: ZEU 222

Topical Talk HL 54.1 Wed 14:00 ZEU 222

Control of Charge Carrier Dynamics in Disordered Conjugated Polymers — •Dirk Hertel — Physical Chemistry, University of Cologne, Luxemburgerstr. 116, 50939 Cologne, Germany,

We developed a new method to probe charge carrier mobility on ultrafast time scale [1]. It is based on electric field induced second harmonic generation. The method is applied to prototypical amorphous conjugated polymers of the polyphenylene- and polyfluorene-type. Typically the carrier mobility in these organic polymers decreases with time in a power law fashion from about 1 cm^2Vs^{-1} at 1 ps to its stationary value of about 10^{-6} cm^2Vs^{-1} in hundreds of ns.

The dynamics of the mobility is discussed. It will be shown, that in nanoscale devices the macroscopic mobility is not adequate to describe charge transport. We study the influence of disorder, morphology and temperature on ultrafast transport. At early times the transport is dominated by tunneling [2] and disorder plays already an essential role. Comparison of transient photocurrents with Monte-Carlo simu-

lation reveals that on-chain transport has to be invoked to rationalize our results [3]. The hopping rates for intrachain transport are much larger compared with interchain transport. The results give access to essential transport properties for the development of advanced theoretical models and may help to design improved solar cells.

[1] A. Devižis, et al. *Phys. Rev. Lett.* **103**, (2009) 027404.
[2] A. Devižis, et al. *Phys. Rev. B* **82**, (2010) 155204.
[3] A. Devizis, et al. *Chem. Phys. Lett.* **498**, (2010) 302.

HL 54.2 Wed 14:30 ZEU 222

Light-Emitting Organic Memory — •Peter O. Körner, R. Clayton Shallcross, Vincent Aubert, Eduard Maibach, Philipp Zacharias, and Klaus Meerholz — Department of Chemistry, University of Cologne

We report on light-emitting organic memory (LE-OMEM) devices composed of multiple solution-processed layers. The active layer of our LE-OMEM devices is comprised of crosslinkable dithienylethene photochromes (XDTE) that can be optically switched between two energetically distinct and thermally stable isomers. Exploiting the difference in the HOMO and LUMO levels of these two isomers we use such a layer as an electrical switch within our OLED layer stack. We demonstrate that the ON/OFF ratio in current (OOR_j) as well as in electroluminescence (OOR_L) of such devices is exponentially dependent on the difference in the largest charge injection barrier between the ON and OFF state of the device. Optimized devices displayed impressive fatigue resistance and afforded values for OOR_j and OOR_L of greater than 10^3. We focus on a variety of crosslinkable DTE molecules of varying structure and functionality with an emphasis on OOR, device stability over multiple read/write/erase cycles (fatigue resistance) and switching rates. Current induced switching allows for electrical writing and reading of grey level information in these XDTE devices. We studied this electrical switching behavior to gain further insight into the distinct switching mechanisms within the XDTE layer. These fundamental studies are a first step towards a completely electrically driven LE-OMEM.

HL 54.3 Wed 14:45 ZEU 222

Determination of the effective radiative quantum efficiency of light-emitting guest-host systems — •Tobias Schmidt[1], Daniel-Steffen Setz[2], Benjamin Lebsanft[1], Thomas Wehlus[1], Jörg Frischeisen[1], Benjamin Krummacher[2], Michael Flämmich[3], Norbert Danz[3], and Wolfgang Brütting[1] — [1]Experimentalphysik IV, Universität Augsburg — [2]OSRAM Opto Semiconductors, Regensburg — [3]Fraunhofer-Institut für angewandte Optik und Feinmechanik (IOF), Jena

The efficiency of organic light-emitting diodes (OLEDs) is still limited as only a small part of the applied electrical power is converted into light and finally extracted from the device to air. Especially the radiative quantum efficiency (RQE) of the used guest-host system is often declared to be unity in phosphorescent emitter/matrix combinations. Due to interference effects, the radiative lifetime of the emitter and thus the effective RQE of the light-emitting guest-host system is influenced by coupling to different modes of the cavity formed by the metallic mirror and the partially reflecting ITO/glass interface. The effective RQE can be determined by measuring the external quantum efficiency of the electrically driven OLED or the photoluminescence lifetime of the emitter inside the OLED at different emitter positions in the cavity. We have investigated the RQE of the commonly used emitter $Ir(ppy)_3$ in neat films with PMMA and CBP as matrices, yielding values of about 70 %, and compare it to OLEDs, where significantly lower values of only 40 % are obtained.

HL 54.4 Wed 15:00 ZEU 222

Exciton quenching in light emitting organic field-effect transistors studied by localized Spectroscopy — •Wouter Koopman, Stefano Toffanin, and Michele Muccini — ISMN-CNR, Via P. Gobetti 101, 40129 Bologna, Italy

The recent development of organic light-emitting transistors (OLETs) promises a new generation of light-emitting organic devices surpassing the efficiency of organic LEDs. The transistor structure prevents non-radiative processes connected to charge-carrier injection as for the ideal OLET the full recombination takes place inside the channel.

In this work we present an investigation of the influence of field-induced quenching on the luminescence intensity in OLETs based on *N,N' ditridecyl-perylene-3,4,9,10-tetracarboxylic diimide* (PTCDI-C13H27) as a model compound. We have used localized photoluminescence and lifetime spectroscopy to study the quenching processes at the electrodes and in the channel region in working devices. Our measurements show a reduction of luminescence intensity up to 20% by applying a forward gate voltage, with a gate field in the order of $1\times10^8 Vm^{-1}$. Upon application of a reverse bias a counter-intuitive enhancement of the PL spectrum was found. Excluding polaron-injection by a dielectric barrier, we can identify field induced effects to be responsible for the observed effects.

These results clarify the role of external electric field induced exciton-quenching on the luminescence efficiency of OLETs and establish a bases for the understanding of the limiting processes in more complex devices.

HL 54.5 Wed 15:15 ZEU 222

Triplet Excimer Emission in a Series of CBP-Derivatives — •Sebastian Hoffmann[1], Pamela Schrögel[2], Rodrigo Albuquerque[1], Michael Rothmann[2], Peter Strohriegl[2], and Anna Köhler[1] — [1]Department of Physics, University of Bayreuth, 95440 Bayreuth — [2]Macromolecular Chemistry I, Department of Chemistry, University of Bayreuth, Bayreuth 95440, Germany

Carbazole-based materials such as 4,4*-bis(N-carbazolyl)-2,2*-biphenyl (CBP) and its derivatives are frequently used as matrix materials for phosphorescent emitters in organic light emitting diodes. An essential requirement for such matrix materials is a high energy of their first triplet excited state. Here we present a detailed spectroscopic investigation supported by DFT calculations on two series of CBP derivatives, where CH3 and CF3 substituents introduce strong torsion into the molecular structure. The resulting poor coupling between the two halves of the molecules leads to an electronic structure similar to that of N-phenyl-3,6-dimethyl-carbazole, with high triplet state energy of 2.95 eV. However, we also observe a triplet excimer emission centred at about 2.5-2.6 eV in all compounds. We associate this triplet excimer with a sandwich geometry of neighboring carbazole moieties. For compounds with more polar CF3 substituents, the lifetime of the intermolecular triplet excited state extends into the millisecond range for neat films at room temperature. We attribute this to an increased charge-transfer character of the intermolecular excited state for the more polar substituents. [1] S.T. Hoffmann et al, J. Phys.Chem. B, in press.

15 min. break

HL 54.6 Wed 15:45 ZEU 222

The effect of energetic disorder on the spectral diffusion of singlet and triplet states in phenylene-type polymers — •Anna Köhler[1], Sebastian T Hoffmann[1], Heinz Bässler[1], Jan-Moritz Koenen[2], and Ullrich Scherf[2] — [1]Experimental physics II, Universität Bayreuth — [2]Macromolecular Chemistry, Bergische Universität Wuppertal

We have employed quasicontinuous temperature dependent fluorescence and phosphorescence spectroscopy to monitor the spectral diffusion of singlet and triplet excitons in a series of pi-conjugated polymers.(1) The experimental results are complemented by Monte-Carlo simulations. We investigated (i) how spectral diffusion is controlled by the degree of energetic disorder present in the amorphous film and (ii) how this process depends on the range of the electronic coupling by comparing singlet exciton diffusion via long-range Förster transfer against triplet exciton diffusion by short-range Dexter transfer. For singlets, we find that the fluorescence spectra bear out a bathochromic shift upon cooling the sample down to a critical temperature below which the shift saturates. This bathochromic shift is a signature of spectral relaxation. In contrast we observe a hypsochromic shift of the phosphorescence spectra below a characteristic temperature for triplets in systems with at least moderate energetic disorder. We show that Random-walk theory applied to excitation transport within a Gaussian density-of-states distribution is both necessary and sufficient to rationalize the experimental results in a quantitative fashion. (1) S.T. Hoffmann et al. PRB 81, 115103 (2010)

HL 54.7 Wed 16:00 ZEU 222

Surface Doping of Conjugated-polymer/Insulating-polymer Composite Film for Field-effect-transistor — •Guanghao Lu[1,2], Patrick Pingel[2], Ingo Salzmann[1], Norbert Koch[1], and Dieter Neher[2] — [1]Institut für Physik, Humboldt-Universität zu Berlin, Berlin, Germany — [2]Institut für Physik und Astronomie, Universität Potsdam, Potsdam, Germany

In organic field-effect-transistors, optimized devices are usually

achieved at inert environment together with passivated dielectric surface, in order to prevent the possible doping by oxygen or polar groups at dielectric surface. However, in this work, we find that the field-effect properties of poly(3-hexylthiophene)/polystyrene (P3HT/PS) composite can be greatly improved upon surface doping. Upon exposure to air and using oxidablely active dielectric surface, we doped the top surface and bottom surface of P3HT/PS film for top-contact and bottom-contact devices, respectively. The field-effect mobility of these films with only 2-5 wt% P3HT can be enhanced by more than 3 orders, reaching 0.05-0.2 cm2V-1s-1. This phenomenon is strongly contrary to the case of pure P3HT film. We proposed that, for pure P3HT, doping inevitably induces negatively charged sites or charge-transfer complexes, which act as new traps or undesired low energy sites. However, for conjugated-polymer incorporated within insulating-polymer matrix, the interaction between hole and surrounding negative sites is weaker because of the spatial occupation of a-PS among P3HT domains, which largely optimizes the positive aspect of doping and meanwhile restrained its negative role.

HL 54.8 Wed 16:15 ZEU 222

Investigation of single grains in nanoscale P3HT OFETs — •Dileep Dhakal, Steve Pittner, Torsten Balster, and Veit Wagner — School of Engineering and Science, Jacobs University Bremen, Campus Ring 1, 28759 Bremen

Regio-regular poly(3-hexylthiophene) (P3HT) has a chain length in the range of several nm up to more than 100 nm, depending on the molecular weight. In addition, the lateral correlation length of 50 nm thick spin-coated P3HT-layers was found to be 150 nm [1] corresponding to the range of structural order within the film. Therefore, the reduction of the channel length L in organic field effect transistors towards the sub-100 nm range will open up the possibility for channels formed by single grains or individual P3HT chains. For this investigation transistor templates on oxidized silicon substrates are prepared by 2 approaches i) by electron beam lithography (EBL) and ii) by metal deposition under defined tilt angle at a preexisting contact edge. The resulting channel length between the source and drain electrode is in the range from 1 μm to 100 nm for EBL and reaches even lower channel sizes using the second approach. At L = 1 μm a mobility of 10^{-2} cm^2/Vs is typically extracted from transfer curve measurements. Without optimization of the gold/P3HT-interface we find a decrease of mobility by more than one order of magnitude for 100 nm devices, which is attributed to an increased influence of the contact resistance. The ratio can be clearly improved by optimizing the interface. [1] B. Gburek and V. Wagner, Org. Electronics 11 (2010) 814.

HL 54.9 Wed 16:30 ZEU 222

The impact of polar bonds on electron transport through self-assembled monolayers — •David A. Egger[1], Ferdinand Rissner[1], Egbert Zojer[1], and Georg Heimel[2] — [1]Institute of Solid State Physics, Graz University of Technology, Austria — [2]Institut für Physik, Humboldt-Universität zu Berlin, Germany

Density functional theory based surface- and transport-calculations are performed to elucidate the role of intra-molecular polar bonds built into self-assembled monolayers (SAMs) sandwiched between two metal electrodes. Conjugated (oligo)phenylene-ethynylenethiols (also known as 'Tour wires') on gold are chosen due to their frequent appearance in past experimental and theoretical studies. Here, we substitute carbon by nitrogen atoms in a systematic way to realize two different molecules with zero dipole moment and virtually identical frontier molecular orbital energies. Despite this similarity in the electronic structure of the isolated species, the charge-transport characteristics of the corresponding SAMs are vastly different. We give a sound explanation for our observations based on an intuitive electrostatic rationale and conclude that the actual orientation of polar bonds in monolayers of preferentially oriented molecules crucially impacts characteristic parameters of molecular electronic devices, such as conductance gap or threshold voltage.

HL 54.10 Wed 16:45 ZEU 222

Photoinduced magnetoresistance in organic field-effect transistors — •Thomas Reichert and Tobat P. I. Saragi — Department of Mathematics and Science and Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, Heinrich-Plett-Strasse 40, D 34132 Kassel, Germany

We report on negative magnetoresistance (MR) in low external magnetic fields in organic field-effect transistors. This effect can only be observed if the device is irradiated. MR strongly depends on gate voltage but is independent of drain voltage. Furthermore, the MR increases as the intensity of irradiation increases and the relationship of both parameters is not linear. The dependency of MR on magnetic field is not linear either, but it follows Non-Lorentian function. The triplet exciton-charge reaction model is a possible explanation for negative MR in irradiated organic field-effect transistors.

HL 55: Photovoltaics: mainly Technology and Photon Management

Time: Wednesday 14:30–17:45 Location: FOE Anorg

HL 55.1 Wed 14:30 FOE Anorg

Spectral down-conversion in Sm-doped borate glasses for photovoltaic applications — •Marcel Dyrba[1], Katharina Baumgartner[2], Reinhard Carius[2], Paul-Tiberiu Miclea[3,4], and Stefan Schweizer[1,3] — [1]Centre for Innovation Competence SiLi-nano®, Martin Luther University of Halle-Wittenberg, Karl-Freiherr-von-Fritsch-Str. 3, 06120 Halle (Saale) — [2]Institut für Energieforschung 5 (Photovoltaics), Forschungszentrum Jülich GmbH, 52425 Jülich — [3]Fraunhofer Center for Silicon Photovoltaics, Walter-Hülse-Str. 1, 06120 Halle (Saale) — [4]Institute of Physics, Martin Luther University of Halle-Wittenberg, Heinrich-Damerow-Str. 4, 06120 Halle (Saale)

A class of Sm-doped borate glasses has been developed for photovoltaic applications. The fluorescent glass is placed on top of a solar cell and, in the case of Sm^{3+} doping, converts the incident violet/blue part of the solar spectrum to visible red light which is efficiently converted to a photocurrent and enhances the solar cell efficiency. Borate glasses are good candidates as a matrix material since they offer a high optical transparency and they are robust and inexpensive. The chemical base composition of borates glasses consists of the network former boron oxide and metal oxides as network modifiers. The system can easily be doped with Sm^{3+} ions. However, the spectroscopic properties of Sm^{3+}, in particular the fluorescence efficiency, are significantly influenced by the electron negativity of the network modifier. The external quantum efficiency (EQE) and spectral response of amorphous thin film silicon solar cells covered with fluorescent borate glasses have been evaluated.

HL 55.2 Wed 14:45 FOE Anorg

Spectral and angle dependent emission of solar fluorescence collectors — •Hendrik Sträter, Sebastian Knabe, and Gottfried H. Bauer — Institute of Physics, Carl von Ossietzky University Oldenburg, D-26111 Oldenburg

Fluorescence collectors (FCs) provide the option for concentration and simultaneous spectral selection of solar photons of direct or diffuse light. The energetic and commercial benefit of these systems depend on the yield of the conversion of solar photons into luminescence photons and on the efficiency of their respective conductance to the edges of the FC where they are coupled into appropriate solar cells. For the characterization of the performance of FCs and the identification of losses, we have performed angle and spectrally resolved measurements of fluorescence photons from FC with two different types of optical designs, a PMMA substrate with homogeneous depth dependent dye concentration and a novel type of FC, which consist of a transparent substrate with a thin overlayer containing the absorbing and emitting dye. We have recorded the edge fluorescence when illuminating the entire FC surface laterally homogeneously, as well as for slit-like excitation on the front surface with variation of the distance of the illuminated slit from the edge. We compare the experimental fluorescence results with a 2-dimensional ray-tracing approach and verify the spectral and angle dependent edge emission. Moreover we illuminate the FC with long wavelength photons which are not absorbed and conclude, again from angle dependent and spectrally resolved edge emission, on scattering losses at surfaces and in the bulk.

HL 55.3 Wed 15:00 FOE Anorg

Light scattering by rough surfaces for increase of absorption

of low band gap light in solar cells — •Konstantin Kloppstech, Sebastian Knabe, and Gottfried H. Bauer — Institute of Physics, Carl von Ossietzky University Oldenburg, Germany

Scattering of low band gap light for the increase of the absorption of low band gap photons is commonly formulated in phenomenological magnitudes such as haze factors resulting from experiments at particular scattering media. We have formulated analytically and described by numerical simulations the scattering of light by the interaction of photons with rough surfaces based on wave numbers of photons k_λ and wave numbers of the topological surface contour k_s that has been derived in 2 dimensions via AFM analyses of the contour function $h(x, y)$ of the scattering medium, e.g. a glassy diffusor. We have distinguished two regimes: **i)** $k_\lambda < k_s$ in which we apply a ray tracing approach with respect to *Snellius' Law* for photon propagation at phase border between different media, and **ii)** $k_\lambda \propto k_s$, where the propagation of photons after scattering has been formulated on *Huygens' Principle* with generation of spherical waves at the respective position $h(x, y)$. The experimental scattering of photons with different wavelengths - recorded with a standard type goniometer - are compared with the simulation of numerically generated far field results in dependence of distance r from the scattering medium and scattering angle β. In particular for the wave optical approach we find a "scattering function" that contains the contour function $h(x, y)$ however that substiantially departs from its puristic *Fourier Transform*.

HL 55.4 Wed 15:15 FOE Anorg

Silver nanoparticles for enhanced light absorption in thin film amorphous silicon solar cells — •Florian Lükermann[1], Frank Hamelmann[2], Helmut Stiebig[2], and Ulrich Heinzmann[1] — [1]Molecular and Surface Physics, Bielefeld University, 33615 Bielefeld, Germany — [2]Malibu GmbH & Co. KG, 33609 Bielefeld, Germany

Illuminating metal nanoparticles (NPs) with electromagnetic radiation leads to collective dipolar oscillations of the conduction electrons. Depending on the size, shape and surrounding material strong wavelength dependent resonances in the absorption and scattering spectra are the consequence. This so called localized surface plasmon (LSP) resonances go along with an enhanced electromagnetic field inside and in the close proximity of the NPs.

We fabricated silver NPs by thermal evaporation respectively sputtering of silver to gain thin metallic films in the range of a few nm. These films are subsequently annealed at temperatures in the order of 150 °C which leads to the formation of nanosized silver islands from a few nm to approximately 50 nm average diameter, depending on the film thickness. The nanoparticle films are incorporated in direct contact to the active layer of photosensitive amorphous silicon (a-Si) devices to investigate the influence of the enhanced electromagnetic field on the generation of photoexcited charge carriers.

External quantum efficiency measurements demonstrate an enhanced photocurrent in the near infrared region where a-Si in general shows no absorption. MIE simulations indicate that this effect can be associated to the LSP resonances of the incorporated NPs.

HL 55.5 Wed 15:30 FOE Anorg

Conformal Al doped ZnO on rough silicon surfaces — •Martin Otto[1], Matthias Kroll[2], Thomas Käsebier[2], Roland Salzer[3], Paul T. Miclea[1], and Ralf B. Wehrspohn[1,3] — [1]Martin-Luther-University Halle-Wittenberg, μMD Group - Institute of Physics, Heinrich Damerow Str. 4, 06120 Halle, Germany — [2]Friedrich-Schiller-University Jena, Institute for Applied Physics, Max-Wien-Platz 1, 07743 Jena, Germany — [3]Fraunhofer Institute for Mechanics of Materials Halle IWM, Walter-Hülse-Str.1, 06120 Halle, Germany

The feasibility of perfectly conformal deposition of transparent but highly conductive ZnO thin films on rough silicon surfaces for photovoltaic applications has been investigated. Aluminum doped zinc oxide (AZO) deposited via thermal ALD was used as a conformal cover layer for plasma etched black silicon. The coated structures achieve reflectances as low as 2.5% throughout the whole visible spectrum whereas the films exhibit resistivities of only $1.1 \cdot 10^{-3}\Omega$cm. An absorption enhancement of nearly a factor of 10 at a wavelength of 1150 nm compared to a simulated perfect ARC was observed.

HL 55.6 Wed 15:45 FOE Anorg

Comparative characterisation of sputtered ZnO:Al TCO-layers on float glass produced by large ceramic and metallic targets — •Sebastian Wohner[1], Hartmut Witte[1], Fahri Uslu[2], Jörg Günther[2], Jürgen Bläsing[1], Martin Bähr[2], and Alois Krost[1] — [1]Institut für Experimentelle Physik, Otto-von-Guericke-Universität Magdeburg — [2]Euroglas GmbH, Haldensleben

One of the main parts of photovoltaic cells is the conductive and transparent front contact which is often realized by wide bandgap ZnO. D.C magnetron sputtering with ceramic $ZnO{:}Al_2O_3$ targets is one of the commonly used processes to produce ZnO-layers on float glass. Disadvantages are the fixed stoichiometric proportions and the high temperatures.
Alternatively, Al-doped ZnO-layers were deposited by reactive d.c. magnetron sputtering from a large, planar Zn(Al) under oxygen ambience. Hereby the operating point has to be within the unstable transition region of the power - oxygen pressure characteristic.
For comparison ZnO layers were produced by reactive and by ceramic magnetron d.c. sputtering using large targets. The ZnO layers were characterized and compared by resistivity, Hall-effect as well as by optical transmission- and reflection measurements to get the electron concentration using the Drude-model. The surface and the crystal structure were analysed by AFM and Bragg-Brentano X-ray diffraction, respectively. The results show the potential for the production of qualitatively good ZnO-layers as TCO by reactive d.c. magnetron sputtering on large cathodes using adapted process controlling.

15 min. break

HL 55.7 Wed 16:15 FOE Anorg

Time Resolved Measurement of Interface and Bulk Recombination of Solar Cell Materials — •Anja Dobrich, Nadine Szabó, Klaus Schwarzburg, and Thomas Hannappel — Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

Today's state-of-the-art multi-junction solar cells are based on III-V semiconductor compounds grown by MOVPE. The current record multi junction solar cell grown on germanium, having Ge, Ga(In)As and GaInP subcells, have reached a record efficiency of 41.6%. This could be improved further if the low bandgap Ge subcell would be replaced by a more efficient double junction solar cell. For this purpose the low bandgap absorbers InGaAs and InGaAsP grown lattice-matched on InP(100) are suitable. Due to the enhanced bandgap composition a better yield of the solar spectrum is feasible.

Here, we study how the preparation routine of the critical InGaAs to InP interface effects the spatial homogeneity. As a probe for bulk and interface defects time resolved photoluminescence (TRPL) was used. For the lifetime measurements we have grown double hetero (DH) test structures. Due to the arsenic carry over in the InP layer, the InGaAs/InP interface is well-known to be critical with respect to the quality of the interface. The interfaces were prepared via different preparation routes starting with either III- or V-rich InGaAs surface terminations. In order to evaluate the interface formation we analysed the surface reconstruction in situ with reflection difference (RD) spectroscopy and via a contamination-free transfer to UHV with LEED.

HL 55.8 Wed 16:30 FOE Anorg

Nanowire based heterojunction Semiconductor-Insulator-Semiconductor solar cells — •Björn Hoffmann[1], Vladimir Sivakov[1], Florian Talkenberg[1], Gerald Brönstrup[1], and Silke Christiansen[1,2] — [1]Institut für Photonische Technologien, Jena — [2]Max-Planck-Institut für die Physik des Lichts, Erlangen

Semiconductor-Insulator-Semiconductor (SIS) solar cells based on wet-chemically etched silicon nanowires are promising candidates for 3rd generation photovoltaics due to very good electro-optical properties and low production costs. Atomic layer deposition (ALD) is used to form a homogeneous layer of Al_2O_3 as a tunnel barrier around the nanowires followed by a thick layer of Al doped ZnO as transparent front contact. Electron beam induced current (EBIC) is used to visualize the areas of effective charge carrier separation which happens in the bulk wafer as well as in the nanowires. The cells reach short-circuit current densities of $J_{SC} = 33\,mA/cm^2$, open-circuit voltage of $V_{OC} = 470\,mV$ and power conversion efficiencies of up to $\eta = 8,6\%$.

HL 55.9 Wed 16:45 FOE Anorg

From Point to the Line: The Incubation Effect during Laser Scribing of Silicon Thin-Film Photovoltaic Modules — •Michael Richter[1], Christof Schultz[1], Frank Fink[1], Volker Quaschning[1], Bert Stegemann[1], Hans-Ulrich Pahl[2], Heinrich Endert[2], and Bernd Stannowski[3] — [1]Hochschule für Technik und Wirtschaft Berlin, Wilhelminenhofstr. 75a, 12459 Berlin, Germany — [2]Newport Spectra-Physics GmbH, Ruhlsdorfer Strasse 95, 14532

Stahnsdorf, Germany — [3]PVcomB - Kompetenzzentrum Dünnschicht- und Nanotechnologie für Photovoltaik Berlin, Schwarzschildstr. 3, 12489 Berlin, Germany

Serial interconnection of thin film solar cells by laser ablation requires precise and layer-selective scribing of narrow grooves. We have determined the ablation energy fluence thresholds by variation of spot overlap and laser fluence for different photovoltaic materials used for silicon based thin-film solar cells and derived the respective incubation coefficients as a function of the laser pulse duration. The results provide a detailed description of the incubation behavior and allow an accurate prediction of the specific laser scribing results. Moreover, we found good agreement between experiment and theoretical estimations.

HL 55.10 Wed 17:00 FOE Anorg

Numerical simulations for the effiency improvement of hybrid dye-microcrystalline silicon pin-solar cells — •Sven Burdorf, Gottfried Heinrich Bauer, and Rudolf Brüggemann — Institut für Physik, Carl von Ossietzky Universität Oldenburg, Germany

Hybrid solar cells consisting of dye sensitizers incorporated in the i-layer of microcrystalline silicon pin solar cell have been proposed and even recently processed [1,2]. The dye sensitizer molecules are embedded in the matrix and enhance the overall absorption of the dye-matrix system due to their high absorption coefficient in the spectral range interesting for photovoltaic applications. However, the charge transport properties of dyes are quite poor. Microcrystalline silicon on the other hand has acceptable charge transport properties, while the absorption, given a layer thickness in the micron range, is relatively poor. This contribution investigates the effiency improvement of hybrid dye-microcrystalline solar cells compared to pure microcrystalline solar cells by simulation. The results indicate that, under optimal conditions, the effiency can be improved by more than 20 % compared to a pure microcrystalline silicon cell. The thickness reduction for the hybrid system can be as large as 50 % for the same effiency. [1] T. Mayer, U. Weiler, C. Kelting, D. Schlettwein, S. Makarov, D. Wöhrle, O. Abdallah, M. Kunst and W. Jaegermann 2007 Solar Energy Materials and Solar Cells 91 1873-1886. [2] T. Mayer, U. Weiler, E. Mankel, W. Jaegermann, C. Kelting, D. Schlettwein, N. Baziakina and D. Wöhrle 2008 Renewable Energy 33 262-266.

HL 55.11 Wed 17:15 FOE Anorg

Picosecond Excited State Spectroscopy of Organic Bulk Heterojunctions — •Björn Gieseking[1], Berthold Jäck[1], Carsten Deibel[1], and Vladimir Dyakonov[1,2] — [1]11Experimental Physics VI, Faculty of Physics and Astronomy, Julius- Maximilians-University Würzburg, D-97074 Würzburg — [2]2Bavarian Centre for Applied Energy Research (ZAE Bayern), D-97074 Würzburg

Bulk heterojunction solar cells comprised of conjugated polymers and fullerene derivatives approach efficiencies of 8 % making this composite system a promising candidate for the application in organic photovoltaics. Different approaches for improving the device performance aim at the physical properties of the material system itself, but a further optimization requires a deeper insight into the elementary processes following the photoexcitation of these blends.

Here we present recent time-resolved spectroscopic studies on the conjugated Polymer P3HT blended with different fullerene derivatives employing femtosecond transient absorption (TA) and photoluminescence (PL) spectroscopy. For both methods we use an Ti:sapphire-based femtosecond laser system together with two optical parametric amplifiers and a streak camera providing a time resolution in the sub picosecond (TA) and picosecond (PL) regime, respectively. Applying these techniques we studied the recombination dynamics of singlet excitons and polarons after photoexcitation. We will discuss our results in terms of performance optimisation of organic solar cells.

HL 55.12 Wed 17:30 FOE Anorg

Defect and charge transfer studies on hybrid solar cells with silicon nanocrystals — •Sabrina Niesar[1], Daniel Herrmann[2], Wolfgang Fabian[1], Nadine Erhard[1], Andre Stegner[1], Rui Pereira[3], Hartmut Wiggers[4], Martin Brandt[1], Eberhard Riedle[2], and Martin Stutzmann[1] — [1]Walter Schottky Institut, Technische Universität München, 85748 Garching — [2]Ludwig-Maximilians-Universität München, 80538 München — [3]University of Aveiro, 3810-193 Aveiro, Portugal — [4]Institut für Verbrennung und Gasdynamik, Universität Duisburg-Essen, 47057 Duisburg

Hybrid inorganic nanoparticle-polymer solar cells are a promising alternative to purely organic devices due to the broad spectral range of absorption of the inorganic material. In this work, a combination of P3HT and silicon nanocrystals (Si-ncs), which are synthesized in a microwave plasma reactor, is studied. In particular, we focus on methods to decrease the concentration of silicon dangling bond defects which negatively affect the electronic properties of the hybrid solar cells. HF etching in combination with vacuum annealing at 200°C leads to the lowest defect densities. Conductivity measurements in vacuum show that the defect reduction results in improved electrical properties of Si-nc thin films. Electron paramagnetic resonance and Fourier transform infrared spectroscopy are used to study the stability of the different post-growth treatments. The charge transfer across the organic-inorganic interface is investigated via broadband-femtosecond optical pump-probe spectroscopy. We find that the addition of the Si-ncs leads to an increase of the charge separation as compared to pure P3HT.

HL 56: Invited Talk: Holger Eisele

Time: Wednesday 14:30–15:00 Location: POT 51

Invited Talk HL 56.1 Wed 14:30 POT 51

Cross-sectional Scanning Tunneling Microscopy on Semiconductor Nanostructures — •Holger Eisele — Institut für Festkörperphysik, Technische Universität Berlin, 10623 Berlin

The growth of semiconductor nanostructures is crucially determined by kinetic, thermodynamic, and quantum mechanic effects. In order to obtain optimized opto-electronic properties a detailed understanding of atomistic processes during growth is necessary. Here, cross-sectional scanning tunneling microscopy provides a unique access to the spatial structure of semiconductor nanostructures embedded in devices.

The principle of application of cross-sectional scanning tunneling microscopy on different semiconductor nanostructures will be presented in this contribution. In particular, it will be shown how to determine the main spatial parameters as they are the size, the shape and the stoichiometric arrangement of the constituent materials.

Among the wide variety of semiconductor nanostructure systems, this contribution will concentrate on examples. For InAs/GaAs a material reorganization during the capping is observed, which determines mostly the quantum dot structure [1]. In the InAs/InGaAsP/InP system the influence of the quaternary separation layers on the quantum dash stacking and the strain field is demonstrated [2]. During submonolayer InAs/GaAs growth quantum dot like structures form [3].

[1] H. Eisele, A. Lenz, R. Heitz, et al., J. Appl. Phys. 104, 124301 (2008). [2] A. Lenz, F. Genz, H. Eisele, et al., Appl. Phys. Lett. 95, 203105 (2009). [3] A. Lenz, H. Eisele, J. Becker, et al., Appl. Phys. Express 3, 105602 (2010).

HL 57: ZnO: Optical Properties

Time: Wednesday 14:30–15:30 Location: POT 151

HL 57.1 Wed 14:30 POT 151

Localization of light in ZnO nano-needle arrays — •David Leipold, Christoph Minz, and Erich Runge — Technische Universität Ilmenau, 98693 Ilmenau, Germany

Localization of electromagnetic waves due to multiple scattering is an astonishing phenomenon. The strong electromagnetic fields concentrated to small spatial dimensions allow for novel ultrafast, non-linear, nano-optical experiments and applications. Recent experiments provide strong evidence for the existence of highly localized photon modes in a system of homogeneous, randomly distributed, vertically aligned ZnO nano-needles: Hot spots with hugely enhanced intensity were observed in the spatial distribution of the second harmonic generation (SHG) signal. We present results of full 3D solutions of Maxwell's equations for a model system. Several aspects of these results are quantitatively compared to experimental data.

We thank Manfred Maschek, Slawa Schmidt, Martin Silies, and Christoph Lienau from the Carl von Ossietzky Universität Oldenburg as well as Takashi Yatsui, Kokoro Kitamura and Motoichi Ohtsu from the University of Tokyo, who did the experiments which inspired this theoretical work.

HL 57.2 Wed 14:45 POT 151

Time-resolved photoluminescence spectroscopy of ZnO / (ZnMg)O heterostructures — •Verena Bornwasser[1], Alexej Chernikov[1], Martin Koch[1], Sangam Chatterjee[1], Stephan W. Koch[1], Bernhard Laumer[2], and Martin Eickhoff[3] — [1]Department of Physics and Material Sciences Center, Philipps-Universität Marburg, Renthof 5, D 35032 Marburg — [2]Walter Schottky Institut, Technische Universität München, Am Coulombwall 4, D 85748 Garching — [3]Physikalisches Institut, Justus-Liebig-Universität Giessen, Heinrich-Buff-Ring 16, D 35392 Giessen

ZnO-based materials are promising for the realization of optoelectronic devices operating in the UV. ZnO has a band gap energy of about 3.4eV, a large exciton binding energy of 60meV and a high material quality due to recently improved growth methods. Hence, a detailed understanding of the optical properties and carrier dynamics in this system is crucial to further optimize growth procedures and device performance. Here we present time-resolved photoluminescence measurements of the hetero- and homoepitaxially grown ZnO quantum wells and (ZnMg)O barrier layers. Our results show a strong correlation between the substrate and the material quality for the quantum well system. In the case of the (ZnMg)O barriers, post-growth annealing significantly improves the material quality. In addition a structural phase separation is observed as the annealing temperature exceeds 950°C.

HL 57.3 Wed 15:00 POT 151

Low-temperature dielectric tensor of MgZnO thin films and ZnO single crystals — •David Schumacher, Rüdiger Schmidt-Grund, Helena Hilmer, Chirs Sturm, Holger Hochmuth, Michael Lorenz, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Linnestr. 5, Leipzig, Germany

We determined the temperature evolution of the spin-orbit interaction and crystal field splitting energies in a-plane $Mg_xZn_{1-x}O$ ($x < 0.1$) thin films and m-plane ZnO single crystals. In so doing we obtained hints on the ZnO valence band (VB) ordering, which is still under debate.

The temperature dependent dielectric tensor has been obtained by means of spectroscopic ellipsometry in the near band-gap spectral range (1 - 4.5) eV and temperatures (10 - 470) K. We derived the near bandgap band-to-band transition energies, amplitudes and broadening parameters. In order to get insight in the VB ordering of wurtzite ZnO our model dielectric function were constrained to satisfy the quasi cubic model, which gives expressions for the energy differences of the split-off bands due to spin-orbit interaction and crystal field splitting. We discuss the evolution of these quasi-cubic parameters, Δ_{so} and Δ_{cf}, as a function of temperature and Mg-content under the assumption of positive as well as negative spin-orbit-coupling.

We would like to stress that during the analysis our model had to be expanded by an additional ZnO surface-near-region layer in order to describe the data adequately. We ascribe this finding to the influence of electronic surface states and to mechanical damages of the surface.

HL 57.4 Wed 15:15 POT 151

Emission Properties of ZnMgO/ZnO Quantum Wells — •Pascal Becker[1], Bernhard Laumer[1,2], Fabian Schuster[2], Martin Eickhoff[1], and Detlev M. Hofmann[1] — [1]I. Physikalisches Institut, Justus-Liebig-Universität Giessen, Heinrich-Buff-Ring 16, D-35392 Giessen — [2]Walter Schottky Institut, Technische Universität München, Am Coulombwall 3, D-85748 Garching

ZnO quantum wells embedded in $Zn_{(1-x)}Mg_xO$ barriers are possible candidates for the realization of light emitters in the blue and near UV spectral range and exhibit interesting optical properties due to the presence of spontaneous and piezoelectric polarisation fields, which give rise to the quantum confined Stark effect. Here, we investigated MBE-grown ZnO quantum wells with different thickness and barrier composition x by luminescence and magneto-optical spectroscopy. The properties of wide quantum wells (> 5nm) are in good agreement to published data. However, for narrow quantum wells we observe an opposite sign of the magnetic circular polarisation of the emission (MCPE) and an inverted slope of the magnetic field dependence. We will discuss this effect in terms of changes in the valence band ordering.

HL 58: Invited Talk: Martin Geller

Time: Wednesday 14:30–15:00 Location: POT 251

Invited Talk HL 58.1 Wed 14:30 POT 251

Transport spectroscopy on non-equilibrium spin and charge states in self-organized quantum dots — •Martin Geller — Faculty of Physics and CeNIDE, University of Duisburg-Essen, Germany.

Self-organized quantum dots (QDs) are perfectly suited for fundamental studies on many-particle interactions in artificial semiconductor atoms. However, detailed investigations on the pure excited (non-equilibrium) many-particle states in self-organized QDs are still missing. Non-equilibrium charge/spin states were always studied in optical experiments, where electron-hole interactions are in addition present.

An all-electrical spectroscopy technique on an ensemble of self-organized InAs QDs is presented in this talk. It allows to prepare and detect the pure non-equilibrium many-particle electron states with their spin-singlet, -doublet and -triplet configurations, using a time-resolved measurement detection scheme via a two-dimensional electron gas. The energy spectrum of the first three "QD elements", the QD-Hydrogen, -Helium and -Lithium, are shown and compared with a theory based on a numerical solution of a many-particle Hamiltonian of a two-dimensional parabolic potential. This all-electrical measurement scheme also enables to address the two-electron excited state of the QD Helium configuration and measure the spin-relaxation time of this "qubit" without an applied magnetic field up to 50 K. This constitutes an important step towards electrical quantum operations in self-organized QDs for temperatures well above 4 K.

HL 59: SKM Symposium: Semiconductor Nanophotonics - Quantum Optics and Devices (SYNP)

Time: Wednesday 14:30–17:15 Location: TRE Ma

Invited Talk HL 59.1 Wed 14:30 TRE Ma

Quantum Optics on Photonic Chips — •Dirk Englund[1], Brendan Shields[2], Hongkun Park[2], Mikhail Lukin[2], Kelley Rivoire[3], Jelena Vuckovic[3], and Fariba Hatami[4] — [1]Columbia University — [2]Harvard University — [3]Stanford University — [4]Humboldt University

Nanoscale optical structures present a path towards controlling the interaction of photons with single emitters in solids, such as semiconductor quantum dots or color centers. I will describe how this controlled light matter interaction may enable the construction of basic components for quantum information science. I will discuss recent work on cavity-enhanced generation of single photons; nonlinear optical interactions at the single photon level; and some recent work towards cavity-enhanced optical interactions with long-lived spin states in the diamond nitrogen vacancy center.

Invited Talk HL 59.2 Wed 15:00 TRE Ma

Two-photon Interference from Separate Quantum Dots — Edward Flagg, Andreas Muller, Sergey Polyakov, Alexander Ling, Alan Migdall, and •Glenn S. Solomon — Joint Quantum Institute, NIST & University of Maryland, Gaithersburg, MD USA

Semiconductor quantum dots (QDs) are attractive sources of single photons. When single photons emitted by two separate QDs are indistinguishable they will interfere when brought together at a beam splitter in a Hong-Ou-Mandel (HOM)-type experiment. This two-photon interference is needed in many proposed schemes for quantum computation and quantum networking involving quantum repeaters. However, while photons emitted by a single QD in a microcavity have been shown to be highly indistinguishable, mutually indistinguishable photons from separate QDs have only recently been produced [1].

Here we discuss results from an HOM experiment in which interference of photons from two QDs located in different samples is observed and is below the classical limit. We use strain-induced InAs QDs excited by a common pulsed laser. One QD is embedded in a planar optical microcavity of fixed resonant frequency, the other QD resides in a fiber-semiconductor tunable cavity. Despite having non-identical emission properties, the photons emitted from the QDs interfere in the HOM experiment. We obtain a probability of coalescence of the two photons of 18 %, which is increased to 47 % when post-selection within a small detection time window is applied. Dephasing processes limiting the coalescence, and extension to other quantum interfaces will be discussed. [1] E. B. Flagg, et al., Phys. Rev. Lett. 104, 137401 (2010).

Invited Talk HL 59.3 Wed 15:30 TRE Ma

Coherent optoelectronic control of a single exciton qubit — •Artur Zrenner[1], Steffen Michaelis de Vasconcellos[1], Simon Gordon[1], Dirk Mantei[1], Wadim Quiring[1], Mohannad Al-Hmoud[1], Torsten Meier[1], Max Bichler[2], Andreas D. Wieck[3], and Dirk Reuter[3] — [1]Universität Paderborn, D-33095 Paderborn — [2]Walter Schottky Institut, Technische Universität München, D-85748 Garching — [3]Ruhr-Universität Bochum, D-44780 Bochum

Due to their excellent coupling to light, excitons in semiconductor quantum dots are in particular interesting for the implementation of coherent optoelectronic devices. In our present contribution we present results on the coherent manipulation of an exciton by fast electric signals. The new scheme employs fixed optical clocking and a synchronous electric gate signal, which is designed to coherently control the phase of the exciton qubit. A first picosecond laser clock pulse turns thereby the qubit in a coherent superposition state. Afterwards, the phase of the qubit is manipulated by an electric signal, which is phase locked to the laser pulses. A second laser pulse and subsequent state projection by tunneling are used to analyze the quantum state after the coherent manipulation. Using this protocol, we are able to achieve a quantum phase shift of up to pi by varying the electric signal. To verify the experimental data we performed calculations based on the optical Bloch equations. Such voltage controlled qubit manipulations seem to be essential for new types of scalable optoelectronic quantum phase gates and novel applications in the field of coherent optoelectronics.

Coffee Break

Invited Talk HL 59.4 Wed 16:15 TRE Ma

Generation of non-classical states of light with site- and potential-controlled pyramidal quantum dots — •Eli Kapon — Ecole Polytechnique Fédérale de Lausanne Laboratory of Physics of Nanostructures 1018 Lausanne, Switzerland

Generation of non-classical states of light, such as single photons, bunched photons and entangled photos, using semiconductor quantum dots (QDs) has been of major interest both for fundamental studies as well as for applications in quantum information processing. Here we review recent progress of such light generation using (In)GaAs/(Al)GaAs pyramidal QDs grown on patterned (111)B GaAs substrates, for which the location on a substrate, the heterostructure potential, and the emission wavelength can be controlled to a large extent. The control over nucleation site and 3D heterostructure configuration permits the design of the QD states energies and barriers, as well as the polarization of the emitted photons. The site- and emission wavelength-control make possible the integration of the QDs with optical nano-cavities in a reproducible and scalable manner. The (111) substrate orientation yields QDs of higher (C3v) symmetry as compared with most conventional QD systems, which leads to virtually vanishing fine structure splitting and high yield of 2X-X entangled photons emission. Recent results on polarization-entangled photon emission [1] and first observation of phonon-assisted coupling of 3D-confined excitons with optical cavity modes [2] will be presented and discussed. [1] A. Mohan et al., Nature Photonics 4, 302 (2010). [2] M. Calic et al., submitted (2010).

Invited Talk HL 59.5 Wed 16:45 TRE Ma

Semiconductor Devices for Quantum Photonics — •Andrew Shields[1], Anthony Bennett[1], Mark Stevenson[1], Cameron Salter[1,2], Raj Patel[1,2], Ian Farrer[2], Christine Nicoll[2], and David Ritchie[2] — [1]Toshiba Research Europe Ltd, 208, Cambridge Science Park, Milton Rd, Cambridge CB40GZ. UK — [2]Cavendish Laboratory, University of Cambridge, Madingley Road, Cambridge CB30HE. UK

Often referred to as "artificial atoms", quantum dots possess discrete energy levels that make them viable hosts for electronic qubits or sources of photonic qubits. However, unlike atoms, no two quantum dots are alike, a complication for quantum information schemes requiring either indistinguishable electronic states in different quantum dots, or indistinguishable photons emitted from different quantum dots. We demonstrate here that the transition energy of a quantum dot can be continuously varied, over a range much larger than the linewidth, using an electric field applied in a diode structure. By tuning individual quantum dots to identical energies we demonstrate two-photon interference of photons emitted from truly remote, independent quantum dots, thereby overcoming a significant barrier to scalable quantum information processing. Quantum dots may be used not only to generate single photons, but also polarization entangled pairs. We demonstrate here an electrically-driven entangled light source, based upon the electroluminescence of a single quantum dot in a semiconductor light emitting diode (LED). The device can be operated with continuous or pulsed current injection, with an entanglement fidelity in the latter case of up to 0.83+/-0.03. We also observe a violation of Bell's inequality with the device emission.

HL 60: Quantum Dots: Transport

Time: Wednesday 15:00–16:15 Location: POT 251

HL 60.1 Wed 15:00 POT 251

Light sensing and room temperature memory application of a single-electron memory with positioned InAs quantum dots — •Sebastian Göpfert[1], Lukas Worschech[1], Stephan Lingemann[1], Christian Schneider[1], David Press[2], Sven Höfling[1], and Alfred Forchel[1] — [1]Technische Physik, Physikalisches Institut, Wilhelm Conrad Röntgen Research Center for Complex Material Systems, Universität Würzburg, Am Hubland, D-97074Würzburg, Germany — [2]Stanford University, Edward L Ginzton Lab, Stanford, CA 94305 USA

Electron-beam lithography and try etching techniques were applied for the fabrication of single-electron memories. The device is based on two site-controlled InAs quantum dots (QDs) embedded in a GaAs/AlGaAs quantum-wire transistor. A pattern of nanoholes on a modulation doped GaAs/AlGaAs heterostructure was used to serve as nucleation centers for the QDs. Large shifts of the transistor threshold occur by charging of the QDs with single electrons. At low bias voltages transport spectroscopy shows clear regimes of single-electron transport. Single-electron read and write functionalities up to room temperature were observed. Light with a wavelength in the telecommunication range can be used to control the memory function and to observe single electron charging events at room temperature.

S. Göpfert, L. Worschech, S. Lingemann, C. Schneider, D. Press, S. Höfling, and A. Forchel, Appl. Phys. Lett. accepted (2010)

HL 60.2 Wed 15:15 POT 251

All-electrical measurement of the relaxation time of a two-electron spin-triplet state in InAs quantum dots — Bastian Marquardt[1], •Martin Geller[1], Andreas Beckel[1], Benjamin Baxevanis[2], Daniela Pfannkuche[2], Andreas D. Wieck[3], Dirk Reuter[3], and Axel Lorke[1] — [1]Faculty of Physics and CeNIDE, University of Duisburg-Essen, Germany — [2]I. Institut für Theoretische Physik, University Hamburg, Hamburg, Germany — [3]Chair of Applied Solid State Physics, Ruhr University, Bochum, Germany

Many-particle spin states in self-assembled quantum dots (QDs) could serve as qubits in quantum information processing devices [1]. However, in optical experiments always the excitonic states are measured, hence, electrical preparation and detection of pure excited many-particle states without electron-hole interaction are still missing. We demonstrate an all-electrical spectroscopy technique on an ensemble of InAs QDs [2]. It allows us to prepare and detect the pure many-particle electron states with their spin-singlet and -triplet configurations, using a time-resolved measurement detection scheme via a 2DEG [3]. This all-electrical measurement scheme enables us to determine the electron spin-relaxation time without an applied magnetic field and without optical excitation to 5 ms at 4 K. The spin relaxation time is independent on the applied magnetic field (up to 2 T) and slightly decreases down to 3 ms at 50 K.

[1] T. D. Ladd et al., Nature 464, 45 (2010). [2] B. Marquardt et al., submitted (2010), Preprint: arXiv: 1007.0392v1. [3] B. Marquardt et al., Appl. Phys. Lett. 95, 22113, (2009).

HL 60.3 Wed 15:30 POT 251

Quantum dot memories based on antimony — •Tobias Nowozin, Annika Högner, Andreas Marent, Andrei Schliwa, and Dieter Bimberg — Institut für Festkörperphysik, Fakultät II, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin

A promising option to enhance the performance of today's Flash memories is to use quantum dots (QDs) as a storage unit for charge carriers. In contrast to the Si/SiO_2-based Flash, QDs based on III-V semiconductors could facilitate long storage times in combination with fast write speeds (<nanoseconds). Especially type-II QDs based on GaSb with their exclusive hole localization in combination with other materials such as GaP are promising for non-volatile performance (i.e. >10 years storage time at room temperature). We present results of 8-band-k·p calculations for GaSb QDs and investigate the dependence of the localization energy on the size, shape, and composition of the dots. Storage times in various Sb-based QD heterostructures are predicted.

HL 60.4 Wed 15:45 POT 251

Tunable g-factors in SiGe quantum dots — •Georgios Katsaros[1,2], Natalia Ares[1], Panayotis Spathis[1], Mathieu Stoffel[2], Frank Fournel[3], Massimo Mongillo[1], Vincent Bouchiat[4], Francois Lefloch[1], Armando Rastelli[2], Oliver G. Schmidt[2], and Silvano De Franceschi[1] — [1]CEA, INAC/SPSMS/LaTEQS, 17 Rue des Martyrs, 38054 Grenoble, France — [2]IFW-Dresden, Institute for Integrative Nanosciences, Helmholtzstrasse 20, 01069 Dresden, Germany — [3]CEA, LETI, MINATEC, F38054 Grenoble, France — [4]Institut Néel, CNRS and Université Joseph Fourier, BP 166, 38042 Grenoble cedex 9, France

A prominent branch of spintronics aims at exploiting the electronic spin degree of freedom either for encoding and manipulating quantum information or for switching the state of transistors in a more efficient way. While ground-breaking achievements could be made mainly on GaAs-based heterostructures, the importance of exploring alternative material systems with favourable properties such as long spin coherence is now widely recognized. Si and Ge are attractive materials because in these materials electronic spins can have a long coherence time due to the absence of hyperfine interaction (in isotopically purified crystals). Here we report for the first time the realisation of single-hole transistors based on individual self-assembled SiGe quantum dots [1]. Transport spectroscopy reveals largely anisotropic and electrically tunable hole g-factors, which make SiGe self-assembled QDs an interesting material system for performing all-electrical spin coherent manipulations. Ref. : [1] G. Katsaros et al., Nature Nanotechnology , 2010, 5, 458.

HL 60.5 Wed 16:00 POT 251

Transmission phases and conductance through quantum dots in Fano regime of transport — •Elena Roxana Racec — Technische Universität Cottbus, Fakultät 1, Postfach 101344, 03013 Cottbus, Germany — University of Bucharest, Faculty of Physics, PO Box MG-11, 077125 Bucharest Magurele, Romania

We analyze a quantum dot strongly coupled to the conducting leads via quantum point contacts - Fano regime of transport - and report a variety of resonant states that demonstrate the dominance of the interacting resonances in the scattering process in a low confining potential [1]. As effects of the interaction between resonances, the line shapes of the conductance peaks are described by Fano functions with complex asymmetry parameters and the phases of the transmission amplitudes do not increase monotonically by π through each conductance peak anymore. The phase lapses, typical for the universal behaviour, are obtained as a particular case for weak interacting resonances, while the strong interaction regime is associated with the mesoscopic phase evolution.

[1] E. R. Racec, U. Wulf, P. N. Racec, Phys. Rev. B 82, 085313 (2010) [16 pages]

HL 61: Joint Focussed Session: Theory and Computation of Electronic Structure: New Frontiers IV

Time: Wednesday 15:00–17:00 Location: TRE Phy

Topical Talk HL 61.1 Wed 15:00 TRE Phy

Progress in diffusion quantum Monte Carlo calculations — •Richard Needs — Cavendish Laboratory, J J Thomson Avenue, Cambridge CB3 0HE, UK

My group has developed the CASINO code [1] for performing variational and diffusion quantum Monte Carlo calculations. Fixed-node diffusion quantum Monte Carlo is the most accurate method known for calculating the energies of large many-particle quantum systems. The key ingredient is an accurate trial many-body wave function which controls the statistical efficiency and accuracy of the calculations. Accurate wave functions can be obtained by building correlation effects

on top of mean field descriptions such as density functional theory or Hartree-Fock theory. About 80% of the correlation energy can typically be included by multiplying the mean-field determinant by a Jastrow factor which is small when electrons are close together and tends to unity at large separations. Such wave functions provide an excellent description of electron correlation in closed shell molecules but are often not much better than density functionals for small open shell systems. The wave functions of open shell systems can, however, be greatly improved by introducing more determinants, pairing functions, and backflow transformations, and extremely good results can be obtained. The calculations are expensive but the polynomial scaling with system size allows calculations for 1000 or more particles. The discussion of the methodology will be illustrated by recent applications to atoms, molecules and extended systems.

[1] http://www.tcm.phy.cam.ac.uk/~mdt26/casino2.html

HL 61.2 Wed 15:30 TRE Phy

N^3 implementation for molecules and clusters of Hedin's GW scheme — •Dietrich Foerster[1], Peter Koval[2], and Daniel Sanchez-Portal[2] — [1]CPMOH, University of Bordeaux 1, Cours de la Liberation 351, Talence, France — [2]Centro de Fisica de Materiales, Paseo Manuel Lardizabal, 5, Donostia-San Sebastian, Spain

In the context of organic semiconductors it is useful to be able to predict key properties of their molecular constituents, such as their lumo and homo levels.

To make such predictions possible, we developed a new implementation of Hedin's GW approach for one-electron Green's function that scales like N^3 rather than N^4 with the number of atoms (see also the contribution by Peter Koval).

We achieved an N^3 scaling by using a local basis in the space of dominant orbital products.

This local basis has already been applied in a TDDFT code and it is also suitable in the Bethe Salpeter approach. To accelerate calculations in these frameworks for large molecules, we reanalyze the product basis and reduce its dimension.

HL 61.3 Wed 15:45 TRE Phy

Applications of a dominant product basis in many-body perturbation theory — •Peter Koval[1], Dietrich Foerster[2], and Daniel Sanchez-Portal[1] — [1]Centro de Fisica de Materiales, Paseo Manuel Lardizabal, 5, Donostia-San Sebastian, Spain — [2]CPMOH, Universite Bordeaux 1, Cours de la Liberation 351, Talence, France

The knowledge of excitation properties of molecules is crucial in developing organic semiconductor devices. Many-body perturbation theory is one of the most promising theories for characterization of excitations in electronic systems. In particular, Hedin's GW approximation for one-electron Green's function is capable of calculating lumo and homo of molecules with $O(N^3)$ computational complexity like TDDFT (see the contribution of Dietrich Foerster).

In this work, we implement the Hedin's G_0W_0 approximation on top of DFT calculations performed with SIESTA [1] code. We apply a dominant product technique [2] to span the space of orbital products and to reduce the dimensionality of dielectric matrix.

We discuss several results for ionization potentials and electron affinities of large molecules, revealing strengths and limitations of our implementation.

[1] J. M. Soler, E. Artacho, J. D. Gale, A. García, J. Junquera, P. Ordejón, D. Sánchez-Portal, J. Phys. **C 14**, 2745 (2002).

[2] P. Koval, D. Foerster, and O. Coulaud, J. Chem. Theory Comput. **6**, 2654 (2010); and references therein.

HL 61.4 Wed 16:00 TRE Phy

Using Finite Element method to tackle the Hartree-Fock equations — •Amélie Fau and Denis Aubry — MSSMat laboratory, Ecole Centrale Paris

It is well know that the Schrödinger equation cannot be solved exactly, except maybe for very simple cases, as it represents a many-body interaction problem. However, it is possible to derive approximations of the Schrödinger equation from variational principles. The Hartree-Fock equations are then generally solved thanks to a set of basis functions, e.g. Gaussians, Slater-type orbitals or plane waves.

To avoid to impose a general form to the approximate wave function, we use localized trial functions. We consider here the Finite Element Method as a new approach to solve these Hartree-Fock equations. We shall present the main properties of our computations with the different advantages and drawbacks involved by this strategy. We will present numerical results about different electronic systems: such as atoms or molecules (LiH, BeH2).

HL 61.5 Wed 16:15 TRE Phy

Finite-basis correction applied to the optimized effective potential within the FLAPW method — •Christoph Friedrich, Markus Betzinger, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The optimized-effective-potential (OEP) method is a special technique to construct local exchange-correlation (xc) potentials from general orbital-dependent xc energy functionals. Recently, we showed that particular care must be taken to construct local potentials within the all-electron full-potential augmented-plane-wave (FLAPW) approach. In fact, we found that the LAPW basis had to be converged to an accuracy that was far beyond that in calculations using conventional functionals, leading to a very high computational cost. This could be traced back to the convergence behavior of the density response function: only a highly converged basis lends the density enough flexibility to react adequately to changes of the potential. In this work we derive a numerical correction for the response function, which vanishes in the limit of an infinite, complete basis. It is constructed in the atomic spheres from the response of the basis functions themselves to changes of the potential. We show that such a finite-basis correction reduces the computational demand of OEP calculations considerably: the local potential converges at much smaller basis sets than before and its construction becomes numerically stable. We also discuss a similar correction scheme for *GW* calculations.

HL 61.6 Wed 16:30 TRE Phy

A conventional, massively parallel eigensolver for electronic structure theory[1] — •V. Blum[1], M. Scheffler[1], R. Johanni[2], H. Lederer[2], Th. Auckenthaler[3], Th. Huckle[3], H.-J. Bungartz[3], L. Krämer[4], P. Willems[4], B. Lang[4], and V. Havu[5] — [1]Fritz Haber Institute, Berlin — [2]RZ Garching — [3]TU München — [4]BU Wuppertal — [5]Aalto University, Helsinki

We demonstrate a robust large-scale, massively parallel conventional eigensolver for first-principles theory of molecules and materials. Despite much research into $O(N)$ methods, standard approaches (Kohn-Sham or Hartree-Fock theory and excited-state formalisms) must still rely on conventional but robust $O(N^3)$ solvers for many system classes, most notably metals. In particular, our eigensolver overcomes parallel scalability limitations where standard implementations of certain steps (reduction to tridiagonal form, solution of reduced tridiagonal eigenproblem) can be a serious bottleneck already for a few hundred CPUs. We demonstrate scalable implementations of these and all other steps of the full generalized eigenvalue problem. Our largest example is a production run with 1046 Pt (heavy-metal) atoms [1] with converged all-electron accuracy in the numeric atom-centered orbital code FHI-aims,[2] but the implementation is generic and should easily be portable to other codes. [1] P. Havu *et al.*, Phys. Rev. B **82**, 161418 (2010). [2] V. Blum *et al.*, Comp. Phys. Comm. **180**, 2175 (2009). [1] ELPA research consortium, funded by German Ministry of Research and Education (BMBF). http://elpa.rzg.mpg.de

HL 61.7 Wed 16:45 TRE Phy

Accurate and efficient density-functional calculations for the electronic entropy — •Rudolf Zeller — Institute for Advanced Simulation, Forschungszentrum Jülich, D-52425 Jülich

The calculation of the electronic entropy S(T) as function of temperature is a numerically demanding problem for metallic systems because S(T) depends logarithmically on the Fermi-Dirac distribution which varies rapidly near the Fermi level. Therefore, very accurate Brillouin zone samplings are usually needed.

I will present a technique based on complex energy contour integration and show how significant reduction of the number of sampling points can be achieved and how the problem of undetermined phases of complex valued logarithms can be avoided. The technique exploits the analytical properties of the Green function of the single-particle Kohn-Sham equation and has been implemented within the full-potential Korringa-Kohn-Rostoker method, where the use of Lloyd's formula guarantees fast convergence with respect to the angular momentum cutoff.

As a by-product I obtain a broadening scheme for total energy calculations with error elimination up to the sixth power of T. I will also explain particular advantages of Fermi-Dirac broadening (besides its direct physical significance) compared to other broadening schemes.

HL 62: Nitrides: Advanced Characterization Techniques

Time: Wednesday 15:15–16:45 Location: POT 51

HL 62.1 Wed 15:15 POT 51

Temperature dependent microscopic energy relaxation in semipolar InGaN SQW imaged by spatio-spectrally-time-resolved cathodoluminescence — •Sebastian Metzner[1], Frank Bertram[1], Jürgen Christen[1], Thomas Wunderer[2,3], Frank Lipski[2], Stephan Schwaiger[2], and Ferdinand Scholz[2] — [1]Inst. of Exp. Physics, OvG-University Magdeburg — [2]Inst. of Optoelectronics, Ulm University — [3]Palo Alto Res. Center Inc., USA

We present ps-time- and nm-spatially resolved cathodoluminescence (CL) spectroscopy at 4...300K of semipolar InGaN SQW on top of {11-22} GaN facets of 3D inverse pyramids, which were grown by MOVPE using hexagonal SiO_2 masks and selective area overgrowth. The microscopic local differences in strain, polarization fields, In-incorporation, and SQW-thickness result in an extremely complex interaction of relaxation, recombination in energy, space, and time via real space transport of the excited carriers. The CL mapping at 300K reveals a huge spectral shift of SQW emission from the center (380nm) to the ridge (535nm) of the inverse pyramids which is accompanied by a drastically increasing recombination time of 200ps (center) to >10ns (ridge) as observed in microscopic CL lifetime maps. To analyze the nanoscopic kinetic in detail, monochromatic spatio-time-resolved CL linescans and local time-delayed spectra have been recorded giving direct access to the microscopic transport mechanism of excited carriers. Using these techniques, we discuss the temperature dependence of energy relaxation via an efficient spatial transfer of carriers inside the SQW from high energy regions near the center towards the ridge.

HL 62.2 Wed 15:30 POT 51

Lateral transport in InGaN/GaN quantum wells: time-of-flight experiments — •Julia Danhof[1,2], Ulrich T. Schwarz[1,2], Yoichi Kawakami[3], and Akio Kaneta[3] — [1]Fraunhofer IAF, Tullastr. 72, 79108 Freiburg, Germany — [2]Institut für Mikrosystemtechnik, Georges-Köhler-Allee 106, 79110 Freiburg, Germany — [3]Kyoto University, Katsura Campus, Nishikyo-ku, Kyoto, 615-2312, Japan

The Indium Gallium Nitride material system is known to have very small lateral charge carrier diffusion constant. In case of quantum well structures this is most likely due to Indium fluctuations and defects. We present a method to directly observe travelling charge carriers in quantum wells by solely optical means. By combining a confocal setup with a pulsed laser, a streak camera and the possibility to perform so called pinhole scans we were able perform time-of flight experiments and observe lateral diffusion in a green emitting InGaN/GaN multiple quantum well. Our measurement results can be described quantitatively by continuity and rate equation. This quantitative description also provides us with a local charge carrier diffusion constant for this sample.

HL 62.3 Wed 15:45 POT 51

A (S)TEM and Atom Probe Tomography Study of InGaN — •Thorsten Mehrtens[1], Stephanie Bley[1], Marco Schowalter[1], Kathrin Sebald[1], Moritz Seyfried[1], Jürgen Gutowski[1], Stephan S.A. Gerstl[2], Pyuck-Pa Choi[2], Dierk Raabe[2], Adrian Avramescu[3], and Andreas Rosenauer[1] — [1]Institut für Festkörperphysik, Universität Bremen, Bremen — [2]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf — [3]OSRAM Opto Semiconductors GmbH, Regensburg

InGaN is a well suited material for opto-electronic devices such as LEDs and laser-diodes in spite of its high dislocation density. The reason for this is still under discussion, but small fluctuations of the indium concentration or layer thickness are assumed to be the origin. We have investigated an InGaN/GaN multi quantum well structure via quantitative high-angle annular dark field scanning transmission electron microscopy (HAADF-STEM) and atom probe tomography (APT). For the (S)TEM study the preparation process was optimized by low-energy milling in order to reduce amorphous surface layers. The indium concentration of the quantum wells were deduced by comparing HAADF-STEM images, where measured intensities strongly depend on the nuclear charges of the scattering atoms (Z-contrast), with multislice simulations. An indium concentration of around 16% was obtained. This value is in good agreement with the concentrations obtained with APT and energy-dispersive X-ray analysis (EDX).
Existence of short and long-range fluctuations in these layers will be discussed in comparison to μ-photoluminescence measurements.

HL 62.4 Wed 16:00 POT 51

Liquid He Temperature Cathodoluminescence Spectroscopy in a Scanning Transmission Electron Microscope — •Gordon Schmidt, Barbara Bastek, Peter Veit, Frank Bertram, and Jürgen Christen — Institute of Experimental Physics, Otto-von-Guericke-University Magdeburg, Germany

The technique of low temperature scanning transmission electron microscopy cathodoluminescence spectroscopy (STEM-CL) provides a unique and extremely powerful tool for the optical nanocharacterization of semiconductors and their heterostructures and interfaces. The combination of cathodoluminescence spectroscopy – in particular at liquid He temperatures – with the high spatial resolution of a scanning transmission electron microscope (STEM) allows a spatial excitation resolution below 5 nm.

Our CL-system is integrated in a field emission (S)TEM (FEI Tecnai F20) equipped with a liquid helium stage (T=10K / 300K) and a light collecting parabolic mirror. Optimizing the excitation conditions, such as TEM acceleration voltage, is necessary to minimize sample damage and prevent luminescence degeneration. Panchromatic as well as spectrally resolved CL imaging is used. In CL-imaging mode the CL-intensity is collected simultaneously to the STEM signal – typically the dark field image signal recorded by an HAADF detector at each pixel. This enables a direct microscopic correlation of structural defects, interfaces and their influence on the luminescence. We will present results of room temperature and liquid helium temperature STEM-CL studies of thin GaN, AlInN and GaN/InGaN heterostructures.

HL 62.5 Wed 16:15 POT 51

Time correlated single Photon Counting on GaN nanowires — •Aram Gorgis, Timur Flissikowski, Carsten Pfüller, Oliver Brandt, and Holger T. Grahn — Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5-7, 10117 Berlin

GaN nanowires (GaN NWs) received much interest in the last years because they can be grown in excellent quality on foreign substrates such as Si. We have investigated the photoluminescence (PL) of GaN NW ensembles as well as of single GaN NWs in the time domain. For the ensemble, we find the PL transients to be non-exponential even for low excitation densities. This observation agrees with the reports of several other groups.

The NWs constituting the ensemble experience a size distribution, hence the surface-to-volume-ratio can vary significantly from NW to NW. Surface recombination, being inversely proportional to the NW diameter, is thus expected to contribute more to the PL decay of thin NWs than for thick ones. Consequently, the PL decay from a single NW should be exponential, but the decay time may differ from NW to NW.

To obtain PL transients of single, freestanding NWs from the same sample with a high dynamic range, we utilize time-correlated single photon counting which allows even very weak signals to be detected with high signal-to-noise ratio. For all single NWs investigated, we indeed observe a single exponential decay.

HL 62.6 Wed 16:30 POT 51

Highly resolved optical spectroscopy on homoepitaxial AlN layers in magnetic fields — •Benjamin Neuschl[1], Martin Feneberg[1], Klaus Thonke[1], Ramon Collazo[2], and Zlatko Sitar[2] — [1]Institut für Quantenmaterie / Gruppe Halbleiterphysik, Universität Ulm, 89069 Ulm — [2]Department of Materials Science and Engineering, North Carolina State University, Raleigh, North Carolina, USA

We present optical emission spectroscopy studies on high quality c-plane AlN layers homoepitaxially grown by MOCVD on bulk AlN. The best full width at half maximum of an excitonic transition found by macroscopic photoluminescence is below 500 μeV exhibiting the unique sample quality. A detailed analysis of the excitonic bandgap region has been carried out by means of photoluminescence and cathodoluminescence. Temperature and polarization dependent measurements allowed an identification of the observed transitions and the according valence bands.We accomplished magneto photoluminescence measurements on our best sample and found multiple splittings allowing further insight into the nature of the observed transitions.

HL 63: II-VI-Compounds

Time: Wednesday 15:45–18:30 Location: POT 151

HL 63.1 Wed 15:45 POT 151

Band gap bowing of binary alloys: Experimental results compared to theoretical tight-binding supercell calculations for $Cd_xZn_{1-x}Se$ — •Daniel Mourad[1], Gerd Czycholl[1], Carsten Kruse[2], Sebastian Klembt[2], Reiner Retzlaff[2], Detlef Hommel[2], Mariuca Gartner[3], and Mihai Anastasescu[3] — [1]Institut für Theoretische Physik, Universität Bremen — [2]Institut für Festkörperphysik, Universität Bremen — [3]Institute für Physikalische Chemie "Ilie Murgulescu", Rumänische Akademie

Compound semiconductor alloys of the type $A_xB_{1-x}C$ find widespread applications as their electronic bulk band gap varies continuously with x, and therefore a tayloring of the energy gap is possible by variation of the concentration. We model the electronic properties of such semiconductor alloys by a multiband sp^3 tight-binding model on a finite ensemble of supercells and determine the band gap of the alloy. This treatment allows for an intrinsic reproduction of band bowing effects as a function of the concentration x and is exact in the alloy-induced disorder. In the present talk, we concentrate on bulk $Cd_xZn_{1-x}Se$ as a well-defined model system and give a careful analysis on the proper choice of the basis set and supercell size, as well as on the necessary number of realizations. The results are compared to experimental results obtained from ellipsometric measurements of $Cd_xZn_{1-x}Se$ layers prepared by molecular beam epitaxy (MBE) and photoluminescence (PL) measurements on $Cd_xZn_{1-x}Se$ nanowires reported in the literature.

HL 63.2 Wed 16:00 POT 151

Optical properties of photonic molecules on base of the II-VI material system — •Moritz Seyfried, Kathrin Sebald, Arne Gust, Carsten Kruse, Detlef Hommel, and Jürgen Gutowski — Institute of Solid State Physics, University of Bremen, P.O. Box 330 440, D-28334 Bremen, Germany

Photonic molecules (PMs), consisting of pillar microcavities (MCs) which are connected by a small bar, offer the possibility to couple spatially separated quantum dots (QDs) in the individual pillars via the moderation of the electromagnetic field. Therefore, PMs with pillar diameters of 2.78μm and different center-to-center (CC) distances of the individual pillars were prepared out of planar monolithic VCSEL structures by using focused-ion-beam etching. The structures were grown by molecular beam epitaxy containing either one CdSe/ZnSSe QD layer or, as a more homogeneous illumination source for the far field studies, three quantum well layers as active material. Quality factors of up to 6000 could be determined from the measured discrete mode spectra of the PMs. The photoluminescence spectra were studied in dependence on the excitation position on the PM as well as on the CC distance of the individual pillars. A reduction of the spectral separation of the fundamental mode and the first higher mode with increasing CC distance was found and attributed to the reduced mode coupling for PMs with a larger CC distance. Furthermore, the electromagnetic field distribution was studied by means of the far-field pattern and is discussed with respect to the different CC distances. For a better insight the experimental data are compared with simulations.

HL 63.3 Wed 16:15 POT 151

Long-lived electron spincoherence in ZnSe-based quantum wells — •Alexander Schwan[1], Evgeny A. Zhukov[2], Dmitri R. Yakovlev[1], and Manfred Bayer[1] — [1]Experimentelle Physik 2, TU Dortmund, 44221 Dortmund — [2]Faculty of Physics, M. V. Lomonosov Moscow State University, 119992 Moscow, Russia

Carrier spin coherence in low-dimensional structures is in focus of current interest due to spintronics applications. We have studied carrier spin coherence in ZnSe/(Zn,Be,Mg)Se quantum wells (QWs) characterized by a type-I band alignment and binary QW material. The spin dephasing time T_2^* of the electron spin coherence is experimentally determined by time-resolved Kerr rotation (TRKR) and resonant spin amplification (RSA) measurements in magnetic fields up to 4 Tesla. The Larmor precession of the electron spins in the ZnSe layers is clearly observed in both the TRKR and RSA signals. Times T_2^* up to 30 ns have been evaluated for localized resident electrons of a temperature of 2 K. The temperature dependence of the electron spin coherence is investigated up to 150 K. For higher temperatures exceeding 20 K, where the electrons are delocalized, the dominant spin dephasing mechanism is the D'yakonov-Perel mechanism.

HL 63.4 Wed 16:30 POT 151

Energy transfer dynamics of the Mn $3d^5$ luminescence in ZnS:Mn nanostructures — •Uwe Kaiser[1], Limei Chen[1], Wolfram Heimbrodt[1], Sebastian Geburt[2], and Carsten Ronning[2] — [1]Dept. Physics, Philipps-University Marburg, Germany — [2]Institute of Solid State Physics, Friedrich-Schiller University, Germany

The energy transfer characteristics of $Zn_{1-x}Mn_xS$ bulk material can be described by the well known Förster model. For wires and belts in the range of several nanometers, which where studied in this work, this transfer model has to be modified, becuase of the reduced dimensionality. To prove this modified Förster model $Zn_{1-x}Mn_xS$ samples were prepared, which permited access to the different parameters of the model. The temporal behavior of the internal $Mn^{2+}(3d^5)$ luminescence, which enables access to the energy transfer, was measuered over four orders of magnitude. Different concentrations of Manganese from $4 \cdot 10^{-6}$ % to 4 % were incorporated by ion implantation into ZnS structures of differnet morphologies. For wires as well as for belts an enhancement of the effective dimensionality with the increase of the manganese concentration could be shown. To examine the influence of nonradiative killer centers different attempts for the introduction of defects were studied. With 1) ion implantation of neon as well as 2) different temperature treatements the concentration of killercenters could be controlled. The aim of this work was to prove the validitiy of the modified Förster model for a variety of $Zn_{1-x}Mn_xS$ nanostructures by the transients of the Mn photoluminescence.

HL 63.5 Wed 16:45 POT 151

Einfluss von Metallfilmen auf die Diffusion von Ag in CdTe — •Johannes Lehnert[1], Jörg Kronenberg[1], Herbert Wolf[1], Thomas Wichert[1] und ISOLDE Collaboration[2] — [1]Technische Physik, Universität des Saarlandes, D-66123 Saarbrücken — [2]CERN, CH-1211 Geneva 23

Es ist bekannt, dass für Gruppe I Elemente in CdTe, wie z.B. Ag, unter geeigneten externen Bedingungen bei ca. 800 K peakförmige Konzentrationsprofile erzeugt werden können [1]. In diesem Beitrag wird gezeigt, dass mit Hilfe von aufgedampften Metallfilmen solche Profile bei signifikant niedrigeren Temperaturen von unter 600 K gebildet werden können. Im ersteren Fall war nach einseitiger Implantation von ^{111}Ag in Te-reiches, p-leitendes CdTe (Dicke ca. 800 μm) die Probe bei 800 K (60 min) unter Cd-Dampfdruck diffundiert worden. Das ^{111}Ag-Profil spiegelt bei diesem Prozess die sukzessive Umwandlung des Te-reichen, p-leitenden Material in Cd-reiches, n-leitendes Material wider. Im zweiten Fall wird nach der Implantation, aber vor der Diffusion, ein Metallfilm auf die Oberfläche aufgedampft. In Fall von aufgedampftem Au genügt dann bereits eine Diffusionstemperatur von 580 K (30 min), um das entsprechende Profil zu erzeugen. Der Einfluss unterschiedlicher Metallfilme auf diesen Prozess wird diskutiert werden. Aufgrund der in beiden Experimenten übereinstimmenden Form der Ag-Profile gehen wir davon aus, dass die aufgedampften Metallfilme Ursache für eine Quelle von eindiffundierenden Cd-Atomen sind.

Gefördert durch das BMBF, Projekt 05 KK7TS1

[1] H. Wolf et al., Phys. Rev. Lett. 94 (2005) 125901

15 min. break

HL 63.6 Wed 17:15 POT 151

Ion-beam-induced damage formation in CdTe at 15K — Carl Willem Rischau, •Claudia Sarah Schnohr, Elke Wendler, and Werner Wesch — Friedrich-Schiller-Universität Jena, Institut für Festkörperphysik, Max-Wien-Platz 1, 07743 Jena, Germany

Ion implantation studies on CdTe are of interest regarding a possible application of this technique in the fabrication of CdTe devices, but also with respect to the fundamental understanding of ion-beam-induced damage formation in II-VI compounds. Studies at room temperature exhibit some interesting features like defects extending much deeper into the crystal than the calculated range of the ions and a high resistance to amorphization even after prolonged irradiation with ion fluences as high as several 10^{16}ions/cm^2.

In order to study a possible thermal origin of these effects, we irradi-

ated CdTe single crystals with 270keV Ar and 730keV Sb ions at 15K and analyzed the damage formation in-situ using Rutherford backscattering spectrometry (RBS) in channeling direction. Defect profiles calculated from the RBS spectra using the computer code DICADA show a flat defect distribution which extends to a depth of up to five times the projected range of the ions despite the very low temperature. The post-range defects in CdTe thus do not seem to be of thermal origin, but are instead believed to result from migration driven by the electronic energy loss. Furthermore, CdTe is not rendered amorphous at 15K even after irradiation with several 10^{16}ions/cm^2, suggesting that the high resistance to amorphization of CdTe is caused by the high ionicity of the material rather than thermal effects.

HL 63.7 Wed 17:30 POT 151

Birefringent effect in a two dimensional electron gas — •Mathias J. Mühlbauer, Christoph Brüne, Timo Wagner, Hartmut Buhmann, and Laurens W. Molenkamp — Physikalisches Institut (EP3), Universität Würzburg, 97074 Würzburg, Germany

Rashba spin-orbit interaction is one of the most promising effects for the creation and manipulation of spin polarizations in low-dimensional electronic semiconductor systems without using external magnetic fields. In systems with strong spin orbit coupling (SOC) it should be possible to observe the electronic analogue of the birefringent effect for polarized light as proposed by M.Khodas et al. [1]. The polarization takes place at an interface between regions with different SOC. HgTe/HgCdTe quantum wells are the basis for our studies. In theses heterostructures, electron beam injection and detection can be realized by Quantum point contacts (QPC) while the SOC can be altered through gate electrodes. However, the realization of QPCs in HgTe/HgCdTe is not trivial due to the narrow band gap and the presence of the Quantum Spin Hall Effect [2]. Here, we demonstrate the possibility to fabricate QPCs using electron beam lithography and dry etching and to control its transmission with a top gate. We will present measurements of conductance and beam collimation. The conductance sequence shows steps of e^2/h suggesting that spin polarization is already taking part within the QPC. Additionaly we will show and discuss measurements on two coupled QPCs separated by a beamsplitter.

[1] M. Khodas et al.,PRL 92, 086602 (2004).
[2] M. König et al. Science, 318, 766, (2007).

HL 63.8 Wed 17:45 POT 151

optical properties of ZnO-nanowire/CdSe-colloidal-quantum-dot hybrid structures — •dongchao hou, jan-peter richters, apurba dev, and tobias voss — Semiconductor Optics, Institute of Solid State Physics, University of Bremen

One of the research interests in modern nanotechnology is the assembly and study of hybrid heterostructures composed of different materials that offer enhanced properties through the interactions between their different constituents. ZnO nanowires functionalized with colloidal semiconductor quantum dots (QDs) display tailored optical properties due to energy and electron transfer processes between these two components, and have a huge potential for applications in light-emitting and photovoltaic devices.

Using a facile method, we synthesized water-soluble CdSe QDs with cadmium acetate and sodium selenosulfate as Cd and Se precursors, respectively. 3-mercaptopropionic acid (MPA) was used to cap the QDs, acting as the stabilizer, making the QDs water soluble and preventing them from agglomeration. TEM measurements demonstrated a narrow size distribution of the as-prepared QDs with the average diameter around 3 nm, consistent with UV-Vis absorption measurements. The carboxylic groups at the outer surface of the MPA-capped CdSe QDs render a tight and uniform attachment onto the surface of ZnO nanowires with high coverage efficiency possible. We studied the optical properties of the hybrid structures by photoluminescence spectroscopy under different temperatures to analyze the energy and electron transfer dynamics between the nanowires and the QDs.

HL 63.9 Wed 18:00 POT 151

Infrared absorption study of hydrogen shallow donors in rutile TiO_2 — •Frank Herklotz, Eduard Lavrov, and Jörg Weber — Technische Universität Dresden, 01062, Dresden, Germany

An IR absorption study of hydrogen-related defects in rutile TiO_2 has been performed. The previously reported O–H vibrational mode at 3288 cm^{-1} [1] is found to consist of two components. The modes are assigned to an acceptor-hydrogen complex of an unidentified acceptor and a hydrogen located in the open c-channels [2,3]. The latter is split into two modes due to the neutral and positively charge states of the defect. Based on the temperature dependence of the stretch mode intensities we identify this defect as a shallow donor with an ionization energy of 10 meV. The effective mass of electrons in the conduction band of TiO_2 is found to be $17m_e$.

[1] B. Soffer, J. Chem. Phys. **35**, 940 (1961).
[2] M. Koudriachova, S. de Leeuw, and N. M. Harrison, Phys. Rev. B **70**, 165421 (2004).
[3] S. Klauer and M. Wöhlecke, Phys. Rev. B **49**, 158 (1994).

HL 63.10 Wed 18:15 POT 151

Investigation on multibarrier Schottky contacts — •Stefan Müller[1], Holger von Wenckstern[1], Otwin Breitenstein[2], Jörg Lenzner[1], and Marius Grundmann[1] — [1]Universität Leipzig, Semiconductor Physics Group, Institut für Experimentelle Physik II, Leipzig, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik Weinberg 2, D-06120 Halle, Germany

We present current-voltage(I-V)-characteristics of multi-barrier PdO_y/ZnO-Schottky contacts fabricated by reactive dc-sputtering. The ZnO nominally undoped thin films were grown by pulsed-laser deposition on a ZnO:Al buffer on a-Al_2O_3[1].

The I-V-characteristics were fitted by assuming a parallel connection of two or three individual diodes with different barrier heights(e.g. $\phi_{B1} = 0.872\,\text{eV}$, $\phi_{B2} = 0.66\,\text{eV}$, $\phi_{B3} = 0.547\,\text{eV}$ at room temperature), ideality factors ($n_1 = 2.1$, $n_2 = 2.4$, $n_3 = 1.8$) and areas(A_0, $0.03A_0$, $4 \cdot 10^{-4}A_0$)[2]. Using dark lock-in thermography low-barrier patches were visualized for small forward currents.

These regions were investigated with additional techniques, like electron beam induced current and scanning electron microscope revealing origins for the local decrease of barrier height.

[1] H. von Wenckstern, Appl. Phys. Lett. 88, 092102 (2006)
[2] D. Defives, IEEE Trans. Electron Devices 46, 449 (1999)

HL 64: Quantum Wires: Transport

Time: Wednesday 16:30–19:30 Location: POT 251

HL 64.1 Wed 16:30 POT 251

Electronic Transport Properties of Nb/InAs-Nanowire/Nb Josephson Junctions — Yusuf Günel[1], Igor Batov[2], •Hilde Hardtdegen[1], Kamil Sladek[1], Andreas Einden[1], Gregor Panaitov[3], Detlev Grützmacher[1], and Thomas Schäpers[1] — [1]Instut für Halbleiter Nanoelektronik, Peter Grünberg Institut - 9 und Jülich Aachen Research Alliance on Fundamentals of Future Information Technology (JARA-FIT) Forschungszentrum Jülich, 52525 Jülich — [2]Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka, Moscow district, Institutskaya 2, 142432 Russia — [3]Institut für Bioelektronik, Peter grünberg Institut - 8 and JARA-Fundamentals of Future Information Technology, Forschungszentrum Jülich, 52425 Jülich

We experimentally studied the electronic transport properties of Nb/InAs-Nanowire/Nb Josephson junctions. Highly doped InAs nanowires were used as a weak link between two superconducting electrodes, in order to form a Josephson junction (JJs). At temperatures below the critical temperature of Nb (Tc~7K) a clear supercurrent was observed in the current *voltage characteristics. In addition, we analyzed the temperature and magnetic field dependence of the Josephson supercurrent. A complete suppression of the supercurrent was observed at a temperature of around 7 K and a magnetic field of 0.5 T, respectively. In detailed magnetic field dependent measurements clear oscillations were observed in the differential resistance. Furthermore, at zero magnetic field the differential resistance revealed characteristic features of multiple Andreev reflections.

HL 64.2 Wed 16:45 POT 251

Mode-filtered electron injection into a waveguide interferometer — •S.S. Buchholz[1], S.F. Fischer[1], U. Kunze[1], D. Reuter[2], and A.D. Wieck[2] — [1]Werkstoffe und Nanoelektronik — [2]Angewandte Festkörperphysik, Ruhr-Universität Bochum

Injection of mode-filtered electrons into a phase-sensitive waveguide Aharonov-Bohm (AB) ring is studied for the lowest one-dimensional (1D) transport mode. An individually tuneable quantum point contact (QPC) couples coherently to 1D modes in the ring. Thus, we demonstrate single-mode transport in a multi-mode waveguide structure.

QPCs and electronic waveguides (EWGs) show the distinctive property of quantized transverse momentum resulting in conductance quantization, which makes them attractive as electronic beam splitters and sensitive single charge detectors. QPCs in the "0.7-anomaly" have been discussed as all-electrical spin polarizers. The degree of spin polarization can be probed in a quantum ring - quantum dot device.[1] However, in order to investigate QPCs as spin polarizers, firstly their application as mode-filters in the lowest subband calls for experimental realization.

Here, we study transport in an EWG interferometer[2] (etched from a GaAs/AlGaAs-heterostructure) in which a QPC is embedded in one of the waveguide leads. The QPC was tuned to the regime of the first and second subbands. By means of bend resistance and electron interference, we show that the selective coupling of 1D subbands in the EWGs to modes in the QPC leads to coherent mode-filtered transport.

[1] B. Hiltscher et al., Phys. Rev. B 82, 165452 (2010).
[2] S.S. Buchholz et al., Phys. Rev. B 82, 045432 (2010).

HL 64.3 Wed 17:00 POT 251

Quantum Faraday Effect and Gauge Invariance in Aharonov-Bohm loops — •Kicheon Kang — Department of Physics, Chonnam National University, Gwangju 500-757, Republic of Korea — Institute for Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany

We investigate an isolated Aharonov-Bohm (AB) loop composed of tunnel-coupled two quantum dots with a flux Φ penetrating the loop. Let us consider the following experiment of the state evolution with a flux switching: Initially, the loop is in the ground state at finite value of the flux Φ_i. Then, the flux is suddenly switched to another value Φ_f. Finally, the charge in one of the two dots ($n_j(t)$, $j = 1, 2$) is measured as a function of time.

We find that the flux $\Phi(t)$ does not uniquely determine the physics of this system, and Faraday induction should be taken into account. Indeed, the Faraday induction gives additional phase shift of the wave function. The Faraday-induced phase shift depends on the geometry of the system as well as the amount of the flux change. For identical tunnel couplings with circular symmetric flux, $n_i(t)$ shows a $2\Phi_0$ periodicity.

In addition, we show that the Faraday-induced phase shift is directly observable with an adiabatic change of the flux, for a nonstationary initial state. Interestingly, this *quantum Faraday effect* can be understood in terms of a nontopological geometric phase.

HL 64.4 Wed 17:15 POT 251

Single ion implantation in semiconductor nanowires — •Raphael Niepelt, Andreas Johannes, Martin Gnauck, Irma Slowik, Sebastian Geburt und Carsten Ronning — Institut für Festkörperphysik, Friedrich-Schiller-Universität, Max-Wien-Platz 1, 07743 Jena

Ion implantation is well established as a standard doping technique for semiconductor nanowires. The concentration of dopant atoms per area is typically determined by total beam current monitoring during the irradiation. However, at extremely low ion fluencies, it is not possible to distinguish the exact number of implanted ions in a nanometer sized structure, as the ions are distributed statistically over the irradiated area that is usually far wider than the nanostructure of interest. In our experiments we implanted electrically contacted semiconductor nanostructures that were connected to a preamplifier/amplifier setup. As with every impinging ion a certain amount of energy is deposited inside the material, one can detect signals directly induced by the ion implantation and the nanostructures themselves can act as a radiation sensor. This leads to a countable and very precisely adjustable ion dose during the implantation down to doping with single ions.

HL 64.5 Wed 17:30 POT 251

Persistent Ion Beam induced Conduction in Semiconductor Nanowires — •Andreas Johannes, Raphael Niepelt, Martin Gnauck, Irma Slowik, Andreas Thielmann, Sebastian Geburt, Ulrich Schröder, David Stoll, and Carsten Ronning — Institut für Festkörper Physik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743

The electrical conductance of single, semiconductor nanowires is investigated in-situ during ion beam exposure. A stark increase in conductance proportional to ion flux and ion energy is observed. The increase in conductance shows remarkable similarities to the persistent photoconduction effect (PPC), which is well known yet not comprehensively understood. Especially ZnO nanowires show a strong increase in conductance (photo and ion induced) that only decays over days. Experiments are performed to investigate the parallels between ion and photo induced conductivity and to examine the underlying mechanisms. The decay rate is very sensitive to the external environment so that surface effects are considered to cause the conduction enhancement.

HL 64.6 Wed 17:45 POT 251

Efficient simulation of cylindrical nanowire heterostructures by means of the R-matrix formalism — •Paul Nicolae Racec, Hans-Christoph Kaiser, and Klaus Gärtner — Weierstrass Institute, Mohrenstr. 39, 10117 Berlin, Germany

The Landauer-Bütiker formalism is a well established method for describing ballistic transport in semiconductor nanostructures in the framework of scattering theory. However, direct 2d and 3d simulations of complex heterostructures with this method require a considerable computational effort. The R-matrix formalism is a potent means to reduce the computational costs to the solution of an eigenproblem for the electronic Schrödinger operator in effective mass approximation on a bounded domain with mixed Dirichlet and Neumann boundary conditions. For complex heterostructures this eigenproblem has to be solved numerically and provides the real Wigner-Eisenbud eigenfunctions and -energies. Our numerical approach is based upon a Delaunay triangulation of the rotational symmetric device domain and a finite volume discretization. Thus we can describe any complex geometry and take into account the inhomogeneities and the anisotropy of material properties, like the effective mass. The Wigner-Eisenbud functions and energies are used further on to compute explicitly the energy dependent scattering matrix elements and wave functions which feed into the Landauer-Bütiker formalism. We present results (tunneling coefficients and resonant scattering states) for cylindrical nanowires with embedded substructures like double barriers, quantum dots or quantum rings.

15 min. break

HL 64.7 Wed 18:15 POT 251

Anomalous structures in the conductance of Si/SiGe quantum wires — •Joeren von Pock[1], Daniel Salloch[1], Gang Qiao[1], Ulrich Kunze[1], and Thomas Hackbarth[2] — [1]Lehrstuhl für Werkstoffe und Nanoelektronik, Ruhr-Universität Bochum, D-44780 Bochum — [2]DaimlerChrysler Forschungszentrum Ulm, D-89081 Ulm

We observe an anomaly in the differential conductance below the first plateau at $G_0 = 4e^2/h$ in Si/SiGe quantum wires (QWRs), in contrast to [1]. This anomaly is investigated in its magnetic ($B \leq 15$ T) and thermal behaviour (20 mK $\leq T \leq$ 4200 mK). The QWRs are fabricated from Si/SiGe heterostructures with an electron mobility of $\mu = 207{,}000$ (125,000) cm^2/Vs and a density of $n_{2D} = 8.4 \cdot 10^{11}$ ($2.3{\cdot}10^{11}$) cm^{-2} at 1.5 K. The QWRs are constricted by an etch transfer in a low damage CF_4/O_2-Plasma, which causes a strong 1D-confinement potential. The anomalous conductance plateau is located near 0.6 G_0 at $B =$ 0 T. As B increases parallel to the wire, the anomaly shifts down to 0.5 G_0, indicating Zeeman splitting. Our results are similar to the 0.7 anomaly in GaAs/AlGaAs quantum point contacts and QWRs [2]. Additional to the 0.7 anomaly a zero bias anomaly [3] is observed in transport spectroscopy at $T = 22$ mK. This anomaly is investigated as a function of magnetic field and temperature. At $B > 1.5$ T the anomaly splits into two peaks, and at $T > 100$ mK it does the same, which is untypical for GaAs/AlGaAs.

[1] S. Scappucci *et al.*, Phys. Rev. B **74**, 035321 (2006)
[2] K. J. Thomas *et al.*, Phys. Rev. Lett. **77**, 135 (1996)
[3] S. M. Cronenwett *et al.*, Phys. Rev. Lett. **88**, 226805 (2002)

HL 64.8 Wed 18:30 POT 251

Electronic transport in tapered triangular-shaped InN nanowires — •Christian Blömers[1], Jia Grace Lu[2], Christopher Witte[2], Hans Lüth[1], Detlev Grützmacher[1], and Thomas Schäpers[1] — [1]Institute of Bio- and Nanosystems (IBN-1) and JARA

- Fundamentals of Future Information Technology, Forschungszentrum Jülich GmbH, D-52425 Jülich, Germany — [2]Department of Physics and Astronomy, University of Southern California, Los Angeles, CA 90089-0484, USA

Among the group-III nitrides InN exhibits the lowest effective mass and the highest predicted electron mobility and peak drift velocity. Recently intense research has been carried out to elucidate the usability of InN nanowires for several applications, e.g. high density and low power consuming FET devices, high efficiency solar cells or high sensitivity detectors. We report on electrical measurements on triangular-shaped InN nanowires grown by chemical vapor deposition. The wires are tapered with triangle side lengths ranging from 300 nm down to 40 nm. We obtain an unexpected increase in resistivity with decreasing cross section area for wire segments with a side length smaller than $l_t = 80$ nm. Additionally, we analyzed the temperature dependence of the resistivity and found a transition from metal-like to semiconductor-like behavior at the same transition side length $l_t = 80$ nm. We explain our observations in terms of quantum confinement and donor deactivation.

HL 64.9 Wed 18:45 POT 251

Formation of p-Si/ZnO nanowire heterostrcutures for light emitting devices — •Yaser Haj Hmeidi, Rapheal Niepelt, Martin Gnauck, Frank Schmidl, and Carsten Ronning — Institut für Festkörperphysik, Universität Jena, Max-Wien-Platz 1, 07743 Jena

The development of scalable techniques for assembling nanowire devices needs practical circuits, which are highly parallel and reproducible overlarge areas. ZnO nanowires can be grown easily via vapor-liquid-solid (VLS) mechanism and are suitable for this application. Furthermore, they have an emission wavelength in the UV, but p-type doping is not possible so far. Therefore, light emitting devices must be based on heterostructures with other suitable p-type materials. In this presentation, we will demonstrate p-n heterojunctions between n-type ZnO nanowires and highly doped p-type Si substrates. We developed a simple and powerful approach on the basis of spin-on-glass SiO_2 [1]. This approach is intrinsically scalable since every step involved can be carried out in parallel over an entire wafer. The challenge in this particular geometry is the fabrication of top metallic contacts on top of the nanowires in a way that the contact dose not short with the substrate. The resulting devices exhibit rectifying properties and under certain conditions, also light emission.

HL 64.10 Wed 19:00 POT 251

Coupling molecular spin states by photon-assisted tunneling — •Lars Schreiber[1], Floris Braakman[1], Tristan Meunier[1], Victor Calado[1], Jeroen Danon[2], Jake Taylor[3], Werner Wegscheider[4], and Lieven Vandersypen[1] — [1]Kavli Institute of Nanoscience, TU Delft, The Netherlands — [2]Dahlem Center for Complex Quantum Systems, FU Berlin, Germany — [3]Joint Quantum Institute of Standards and Technology, University of Maryland, USA — [4]Solid State Physics Laboratory, ETH Zurich, Switzerland

Artificial molecules containing just one or two electrons provide a powerful platform for studies of orbital and spin quantum dynamics in nanoscale devices. A well-known example of these dynamics is tunneling of electrons between two coupled quantum dots triggered by microwave irradiation. So far, these tunneling processes have been treated as electric dipole-allowed spin-conserving events.

Here we report that microwaves can also excite tunneling transitions between states with different spin. In this work, we create an artificial hydrogen molecule by a gate-defined double quantum dot formed in a GaAs/(Al,Ga)As 2DEG. The dominant mechanism responsible for violation of spin conservation is the spin-orbit interaction. These transitions make it possible to perform detailed microwave spectroscopy of the molecular spin states and open up the possibility of realizing full quantum control of a two spin system via microwave excitation.

HL 64.11 Wed 19:15 POT 251

The 0.7-anomaly of quantum point contacts — towards understanding its microscopic origin — •David Borowsky[1], Enrico Schubert[1], Daniela Taubert[1], Werner Wegscheider[2], and Stefan Ludwig[1] — [1]Center for NanoScience and Fakultät für Physik, Universität München, Germany — [2]Solid State Physics Laboratory, ETH Zürich, Switzerland

The 0.7-anomaly of a quantum point contact (QPC) has been a subject of intense research since it was first studied in 1996 [1], but its microscopic origin is still controversially discussed. The temperature dependence of the conductance G at the 0.7-anomaly revealed a scaling behaviour reminiscent of the Kondo effect [2], which lead to an interpretation in terms of a quasi-bound state in the Kondo regime [3].

Motivated by many unanswered questions, we used highly tunable QPCs in the 2D electron system (2DES) of a GaAs/AlGaAs heterostructure to study the 0.7-anomaly. We measured G at the 0.7-anomaly as a function of the microscopic confinement potential and in-plane magnetic field. Our experiments show scaling behaviour as a function of magnetic field similar to the temperature dependence [2]. Our results favor a model predicting a magnetic susceptibility enhancement at the 1D-constriction which leads to phenomenologically similar behaviour as the Kondo effect of a quasi-bound state [4].

[1] Thomas et al, Phys. Rev. Lett., 1996, **77**, 135 - 138
[2] Cronenwett et al, Phys. Rev. Lett., 2002, **88**, 226805
[3] Meir et al, Phys. Rev. Lett., 2002, **89**, 196802
[4] Jan von Delft (private communication)

HL 65: Nitrides: AlGaN

Time: Wednesday 17:00–18:00 Location: POT 51

HL 65.1 Wed 17:00 POT 51

Si Doping Studies in AlGaN — •Kamran Forghani[1], Mohammadreza Gharavipour[1], Ferdinand Scholz[1], Benjamin Neuschl[2], Tobias Meisch[2], Ingo Tischer[2], Klaus Thonke[2], Oliver Klein[3], and Ute Kaiser[3] — [1]Institute of Optoelectronics, Ulm University, 89069 Ulm, Germany — [2]Institute of Quantum Matter, Ulm University, 89069 Ulm, Germany — [3]Transmission Electron Microscopy Group, Ulm University, 89069 Ulm, Germany

Realization of n-type conductivity in AlGaN is essential for the growth of deep-UV LED devices. For MOVPE grown layers, we have investigated the relation between Si concentration and carrier concentration at different Al contents up to about 45%. For higher Al contents, the samples suffer from micro cracks as the doping concentration increases. The cracks could be suppressed by growing the Si-doped AlGaN layers on short period super lattice buffer structures. In order to determine the dopant ionization energy, we have performed temperature-dependent Hall measurements on the samples with different Al content, Si concentration, and crystal quality. Moreover, we performed TEM, XRD, and AFM to quantify threading dislocations behavior, crystal quality and surface properties, respectively. The photoluminescence from GaN quantum wells grown on these doped layers was used as a monitor to evaluate their influence on future UV-LED device performance.

HL 65.2 Wed 17:15 POT 51

Growth and characterization of highly reflective AlInN/AlGaN Bragg reflectors — •Christoph Berger, Jürgen Bläsing, Armin Dadgar, Thomas Hempel, Jürgen Christen, and Alois Krost — Otto-von-Guericke-Universität Magdeburg, Deutschland

We report on the growth of distributed Bragg reflectors (DBRs) with up to 40 periods based on lattice matched $Al_{0.85}In_{0.15}N/Al_{0.2}Ga_{0.8}N$ layers. Using an $Al_{0.2}Ga_{0.8}N$ buffer, which is directly grown on the c-plane sapphire substrate, stress relief through crack formation or by relaxation processes can be prevented, which is confirmed by Nomarski microscopy and X-ray reciprocal space maps. The structures exhibit homogenous layer thicknesses and sharp interfaces, as revealed by FE-SEM images, in-situ reflectivity measurements and high resolution X-ray diffraction. These properties allow the growth of DBRs with reflectivities higher than 99 % at a wavelength of ≈360 nm. Such mirrors are very promising for the use in high Q-factor microcavities for the subsequent realization of GaN-based VCSELs or the observation of strong exciton-photon coupling.

HL 65.3 Wed 17:30 POT 51

Ultraviolet photoluminescence excitation spectroscopy of AlGaN and AlN — •Martin Feneberg[1,2], Benjamin Neuschl[2],

Tobias Meisch[2], Klaus Thonke[2], Robert Metzner[1], Bernd Garke[1], and Rüdiger Goldhahn[1] — [1]Abteilung Materialphysik, Otto-von-Guericke-Universität Magdeburg — [2]Institut für Quantenmaterie/ Gruppe Halbleiterphysik, Universität Ulm

We present first results of photoluminescence excitation spectroscopy on AlN thin films and high aluminum content AlGaN layers. These studies were performed at the DORIS III synchrotron, DESY, Hamburg. The origin of observed deep emission bands in AlN can be distinguished between substrate and epilayer. In high aluminum content AlGaN, position and shape of the ordinary absorption edge can be observed. These data are compared to the ordinary dielectric function obtained by spectroscopic ellipsometry and to low temperature photoluminescence spectra obtained by ArF excimer laser excitation ($\lambda = 193nm$). We discuss possible origins of so-called "near band-gap" luminescence in AlGaN. Furthermore, the experimental data allows insight into energy positions of semi-core level states in AlGaN, which opens a way to determine the Fermi level energy in these materials.

HL 65.4 Wed 17:45 POT 51

Factors affecting the excitation process of Europium(Eu^{+3}) ion in Europium-implanted AlGaN — •Jayanta Kumar Mishra[1], Torsten Langer[1], Uwe Rossow[1], Kirill Trunov[2], Andreas Wieck[2], and Andreas Hangleiter[1] — [1]Institut für Angewandte Physik, TU Braunschweig — [2]Angewandte Festkörperphysik,Ruhr-Universität Bochum, Germany

Rare earth ions implanted into GaN are promising for optoelectronic applications. They show luminescence in the visible range while the luminescence from this material system is sharper as well as independent of temperature due to intra 4f transition of rare earth ions. To improve the emission efficiency we implanted Europium in GaN codoped with Mg at dose range from $10^9 cm^{-2}$ to $10^{14} cm^{-2}$ with an energy of 100keV. The red emission from $^5D_0 \rightarrow ^7F_2$ of europium was remarkably enhanced by Mg codoping. When we tried Eu implanted AlGaN, Eu^{3+} shows more promising luminescence. The transition probability or the energy transfer efficiency enhances the Eu^{3+} luminescence in AlGaN. We show that Eu occupies a C_{3v} symmetry site in AlGaN but in case of Mg doped GaN, Eu occupies a different site. The energy transfer from the host to Eu ions depends on the position of Eu ions in the host lattice. We also investigated the role of carriers (electrons/holes) in the excitation process of Eu ion by doping AlGaN with different kind of carriers (p-type and n-type).

HL 66: Joint Session: Plasmonics and Nanophotonics

Time: Wednesday 17:15–19:15 Location: GER 38

HL 66.1 Wed 17:15 GER 38

Simulation of second harmonic generation from split ring resonators with the Discontinuous Galerkin Time Domain method — •Yevgen Grynko, Torsten Meier, and Jens Förstner — Universität Paderborn, Warburger Str. 100, 33098 Paderborn

We report our results of the application of the Discontinuous Galerkin Time Domain (DGTD) method [1] for the simulation of the linear and non-linear response of plasmonic nanostructures. We use DGTD as it has a number of attractive features including adaptive grid refinement and nonlinear stability. In this work, we consider an array of U-shaped split ring resonators. Metallic dispersion is described with a current density equation based on the representation of electron dynamics in terms of electron plasma. It includes linear Drude terms and nonlinear terms for the Lorentz force and convective acceleration of the electron flow. The nonlinear part of the equation causes the doubling of the transmitted frequency leading to the the SH peak in the spectrum. Switching between the terms shows that the "convective" term plays the main role in the observed phenomena. The strength of the the SH peak is comparable to the values reported previously in the experiments [2] and FDTD simulations [3].

[1] J. S. Hesthaven, T. Warburton, 2002, J. Comp. Phys., 181, 186-221. [2] M. W. Klein, et al., 2007, Opt. Express, 15, 5238. [3] Y. Zeng, et al., 2009, Phys. Rev. B 79, 235109-1 - 235109-9.

HL 66.2 Wed 17:30 GER 38

Analysis of optimization techniques for coherent optical control in nanostructures — •Tobias Fankhänel, Torsten Meier, and Jens Förstner — University of Paderborn, Department of Physics and CeOPP, Warburger Str. 100, D-33098 Paderborn, Germany

We compare the efficiency of optimization approaches for shaping coherent optical control in nanostructures. The optical response of various structures is calculated using the Finite-Difference Time-Domain (FDTD, [1]) method. Standard optimization algorithms (L-BFGS gradient method [2], genetic algorithm [3]) are used to maximize target function like the flux transmission or spatio-temporal response; the algorithms' convergence time and computational effort is analyzed.

[1] A. Taflove, S. C. Hagness. Computational electrodynamics: the finite-difference time-domain method, third edition (Artech House Inc., Norwood 2005)

[2] J. Nocedal. Updating Quasi-Newton Matrices with Limited Storage (1980), Mathematics of Computation 35, pp. 773-782.

[3] GALib, http://lancet.mit.edu/ga/

HL 66.3 Wed 17:45 GER 38

Two state lasing from a quantum dot laser — •Diana Khabipova, Kathy Lüdge, Niels Majer, and Eckehard Schöll — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

We investigate the emission properties of a quantum dot (QD) laser with two confined electron and two hole levels, respectively. Our microscopically based rate equation model for quantum dot lasers [1] is extended by including the first excited state of the QDs as a second lasing state besides the ground state. The model treats separately the dynamics of QD electrons and holes, photon densities of the ground and excited state lasing, respectively, and the electron and hole densities in the 2D wetting layer as carrier reservoir. The carrier-carrier scattering rates include the direct capture from the wetting layer into the ground and excited state as well as relaxation processes from excited to ground state. The influence of the energy differences between the excited state, ground state, and wetting layer on the turn-on dynamics is investigated. We analyse also the effect of the excited state upon the relaxation oscillations, their turn-on delay and damping rate. Furthermore we study the excited state dynamics under thermal heating conditions and for different device dimensions.

[1] K. Lüdge, R. Aust, G. Fiol, M. Stubenrauch, D. Arsenijevic, D. Bimberg, and E. Schöll, IEEE J.Quantum Electron. 46, 12, 1755 (2010).

HL 66.4 Wed 18:00 GER 38

Analytical approach to modulation properties of quantum dot lasers — •Kathy Lüdge[1], Evgeny Viktorov[2], Thomas Erneux[2], and Eckehard Schöll[1] — [1]Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Universite Libre de Bruxelles, Optique Nonlineaire Theorique, Campus Plaine, C.P. 231, 1050 Bruxelles, Belgium

We analyze a microscopically based rate equation model for quantum dot lasers. The model separately treats the dynamics of electrons and holes, and the carrier-carrier scattering rates depend nonlinearly on the wetting layer carrier densities [1]. Our objective is to determine analytical expressions for the relaxation oscillation frequency and damping rate. To this end, we consider the Class B limit of the five rate equations and apply asymptotic techniques. We consider two cases corresponding to either equivalent or drastically different decay rates for the electrons and holes. We show how they contribute to increase the relaxation oscillation damping rate compared to the damping rate of the conventional laser and that there exist optimal conditions on the control parameters in order to observe maximum damping.

[1] K. Lüdge, E. Schöll, IEEE J.Quantum Electron. 45, 1396 (2009).

HL 66.5 Wed 18:15 GER 38

Periodic Nanostructures: Spatial dispersion mimics chirality — •Bruno Gompf[1], Julia Braun[1], Thomas Weiss[1], Harald Giessen[1], Martin Dressel[1], and Uwe Hübner[2] — [1]Physikalisches Institut and Research Center SCOPE, Universität Stuttgart — [2]Institut für Photonische Technologien, Jena

The underlying idea of metamaterials is that it should be possible to construct artificial materials with completely new effective dielectric properties from nanometer-sized photonic atoms. One of these new fascinating properties is, for example, the recently achieved optical activity in photonic metamaterials. In our work we demonstrate that even a simple isotropic metal-dielectric nanostructure, i.e., a subwavelength hole array on a square lattice in a semitransparent Au film, rotates the polarization state at oblique incidence, but this behaviour cannot be explained by effective optical parameters. The structure was characterized by Mueller matrix spectroscopic ellipsometry at various angles of incidence and azimuthal orientations in the energy range of 0.73 to 4.6 eV. For the additional theoretical simulations, we employed a Fourier modal approach. To visualize the theoretical and experimental results, we plot the matrix elements in polar coordinates. Already from a brief look at the off-diagonal elements, it becomes obvious that the hole array mixes different incoming polarization states upon reflection in a complex way, which can not be explained by purely dielectric optical constants. It can be shown that for our square array even a bi-anisotropic model must fail. Rather spatial dispersion has to be taken into account.

HL 66.6 Wed 18:30 GER 38

New transparent conductive metal based on polymer composite — •Mehdi Keshavarz Hedayati[1], Mohammad Jamali[1], Thomas Strunkus[2], Vladimir Zaporochentko[2], Franz Faupel[2], and Mady Elbahri[1,3] — [1]Nanochemistry and Nanoengineering, Institute for Materials Science, Faculty of engineering, Christian-Albrechts-University of Kiel — [2]Multicomponent Materials, Institute for Materials Science, Faculty of engineering, Christian-Albrechts-University of Kiel — [3]Helmholtz-Zentrum Geesthacht GmbH, Institute of Polymer Research, Nanochemistry and Nanoengineering

Currently great efforts are made to develop new kind of transparent conductors (TCs) to replace ITO. In this regard different materials and composites have been proposed and studied including conductive polymers, carbon nanotubes (CNTs), metal grids, and random networks of metallic nanowires. But so far none of them could be used as a replacing material, since either they are either fragile and brittle or their electrical conductivity is below the typical ITO. Thin metallic films due to their high electrical conductivity could be one of the best replacing materials for ITO, however their poor transparency makes their application as TCs limited. Here we design and fabricate a new polymeric composite coating which enhances the transparency of the thin metal film up to 100% relative to the initial value while having a high electrical conductivity of typical metals. Therefore our proposed device has a great potential to be used as new transparent conductor.

HL 66.7 Wed 18:45 GER 38

A self-assembly route to mesoporous Bragg reflectors — •Stefan Guldin[1], Matthias Kolle[1], Morgan Stefik[3], Richard Langford[1], Dominik Eder[2], Ulrich Wiesner[3], and Ullrich Steiner[1] — [1]Physics Department, Cavendish Laboratory, University of Cambridge, UK — [2]Materials Science Department, University of Cambridge, UK — [3]Materials Science Department, Cornell University, Ithaca, NY, USA

Mesoporous distributed Bragg reflectors (MDBRs) consist of a periodic lattice of alternating high and low refractive index, while exhibiting porosity on the sub-optical length scale. MDBRs have great potential as sensing materials in biology and chemistry, as adsorption and desorption of gas phase molecules lead to reversible changes in the refractive index of the stack. Optoelectronics is another promising field of applications. MDBRs can be used as light harvesting element in excitonic solar cells. When infiltrated with light emitting polymers, MDBRs have exhibited distributed feedback lasing.

We present a new route for the fabrication of MDBRs which relies on the self-assembling properties of the block copolymer PI-*b*-PEO in combination with sol-gel chemistry to finely tune porosity and pore size in the resulting inorganic material. Stacking-up multiple layers of alternating refractive index results in a fast and reliable assembly of a continuous network with well defined interfaces. The outcome are MDBRs of high quality optical properties even when built from a single material, in our case TiO_2.

HL 66.8 Wed 19:00 GER 38

Launching Surface Plasmons by Carbon Nanotube Photoluminescence — •Nicolai Hartmann[1], Johann Berthelot[2], Alexandre Bouhelier[2], and Achim Hartschuh[1] — [1]Department Chemie and CeNS, Ludwig-Maximilians-Universität München, Germany — [2]Département Nanosciences, Laboratoire Interdisciplinaire Carnot Bourgogne, Université de Bourgogne, Dijon, France

We report on the excitation of propagating surface plasmons in metal films and waveguides via photoluminescence emission from semiconducting single-walled carbon nanotubes. Upon excitation in the visible regime a single carbon nanotube acts as a directive near-infrared point dipole source for surface plasmons propagating along the direction of the nanotube axis. To investigate this behaviour we used leakage radiation microscopy [1,2]. The excitation of propagating surface plasmons manifests itself by a narrow emission of leakage radiation in Fourier space appearing at angles according to the surface plasmon resonance. In real space we observe the exponential decay of the intensity along the propagation direction of the plasmon. Propagation lengths between 11 and 13 μm could be extracted and supported by calculations, depending on the thickness of the dielectric spacer layer separating carbon nanotubes and metal film. Combining surface plasmon coupling with electroluminescence from carbon nanotubes [3] opens up the possibility to create an electrically driven plasmon source.

[1] B. Hecht, et.al., Phys. rev. Lett. 77, 1889 (1996) [2] M. Böhmler, et.al., Opt. Express 18, 16443 (2010) [3] P. Avouris, et.al., Nat. Photonics 2, 341 (2008)

HL 67: OLEDs and OFETs

Time: Wednesday 18:00–19:30 Location: FOE Anorg

HL 67.1 Wed 18:00 FOE Anorg

Band bending and energy-level alignment in organic semiconductors — Ilja Lange[1], James Blakesley[1], Johannes Frisch[2], Norbert Koch[2], and •Dieter Neher[1] — [1]Universität Potsdam — [2]Humboldt Universität Berlin

Energy level alignment at organic semiconductor / electrode interfaces has been the subject of intensive debate in recent years. In particular, the existence of band bending in undoped organic semiconductors is disputed. It has been proposed that strong band bending should be present due to electronic states within the energy gap of a disordered material. It is also known that such states dominate some crucial properties of organic semiconductor devices, such as charge injection and charge transport. Thus the elucidation of the distribution of these tail states provides a key to understanding fundamental processes in such devices and hence to increasing device efficiency. Unfortunately, the densities of the relevant states are often so low that they are difficult to detect directly. We use a Kelvin probe (KP) to study the energy level alignment of four undoped conjugated polymers deposited on various electrodes. Band bending is observed in all polymers when the substrate work function exceeds certain critical values. Through modeling, we show that the band bending is caused by charge transfer into a low-density population of states that extends several hundred meV into the band gap. KP can therefore be used as a tool to study the energetic distribution of such states. The energetic spread of these states is correlated with charge transport properties, suggesting that these states also determine relevant device properties.

HL 67.2 Wed 18:15 FOE Anorg

Optical Processes in OLEDs: Molecular Photonics — •Michael Flämmich, Dirk Michaelis, and Norbert Danz — Fraunhofer Institute for Applied Optics and Precision Engineering, 07745 Jena, Germany

Following the OLED display market take-off, huge world wide efforts are spent to develop OLEDs towards competitive sources for general lighting applications. In this context, the light outcoupling problem is well known as the key parameter to improve OLED efficiency in order to tackle existing lighting schemes. From the optical point of view, the device performance is driven (i) by the architecture of the OLEDs layered system and (ii) by the internal features of the emissive material. Studies in recent years have shown that the latter attributes (which

are the internal electroluminescence spectrum, the profile of the emission zone, the orientation of the transition dipole moments and the internal luminescence quantum efficiency q) can be determined in situ by measurements of the far-field emission pattern generated by active OLEDs (i.e. in electrical operation) and corresponding optical reverse simulations. Starting from basic considerations of the dipole radiation characteristics, we elaborate specifically how the orientation distribution of the dipole transition moments in the layered system can be analyzed in situ, providing insight into the internal photo-physical processes on the molecular scale of the emitter.

HL 67.3 Wed 18:30 FOE Anorg

Stability of Polarization in Organic Ferroelectric Metal-Insulator-Semiconductor (MIS) Structures — •Rene Kalbitz[1], Peter Frübing[1], Reimund Gerhard[1], and Martin Taylor[2] — [1]Department of Physics and Astronomy, University of Potsdam, Karl-Liebknecht-Straße 24-25, 14476, Potsdam, Germany — [2]School of Electronic Engineering, Bangor University, Dean Street, Bangor Gwynedd, LL57 1UT, UK

Ferroelectric field effect transistors (FeFETs) offer the prospect of an organic-based memory device. Since the charge transport in such devices is confined to the interface between the insulator and the semiconductor, the focus of the present study was on the investigation of this region. Capacitance-voltage (C-V) measurements of all-organic MIS devices with poly(vinylideneflouride- trifluoroethylene) (P(VDF-TrFE)) as gate insulator and poly(3-hexylthiophene)(P3HT) as semiconductor were carried out. When the structure was driven into depletion, a positive flat-band voltage shift was observed arising from the change in polarization state of the ferroelectric insulator. When driven into accumulation, the polarization was reversed. It is shown that both polarization states are stable. However, negative charge trapped at the interface during the depletion cycle masks the negative shift in flat-band voltage expected during the sweep to accumulation voltages. Measurements on P(VDF-TrFE)/P3HT based FeFETs yield further evidence for fixed charges at the interface. Output characteristics suggest the injection of negative charges into the interface region when a depletion voltage is applied between source and gate contact.

HL 67.4 Wed 18:45 FOE Anorg

Ambipolar organic field-effect devices using an aliphatic passivation layer — Michael Kraus, Matthias Horlet, Simon Haug, Stefan Richler, Wolfgang Brütting, and •Andreas Opitz — Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

In recent years electron and hole transport has been found to be an intrinsic feature for many organic semiconductors. The charge carrier type depends thereby on the injecting electrodes and the presence of interface traps.

In this contribution we demonstrate the application of the insulating long-chain alkane $C_{44}H_{90}$ tetratetracontane (TTC) as passivation layer, which has been shown to be highly suitable for the elimination of electron traps [1]. The analysis of its growth behaviour on silicon dioxide and of the subsequently deposited organic semiconductor will be shown for different molecular semiconductors like copper-phthalocyanine and diindenoperylene. The charge carrier transport in these semiconductor layers was analysed using top contact organic field-effect transistors. Thereby an asymmetry between electron and hole mobilities was found with diindenoperylene showing the better electron transport whereas copper-phthalocyanine has balanced mobilities at room temperature. The growth of the phthalocyanine gives crystalline needles up to 500 nm in length which improves the transport properties.

[1] M. Kraus et al., J. Appl. Phys. 107, 094503 (2010).

HL 67.5 Wed 19:00 FOE Anorg

Electrolyte-gated organic thin-film transistors for sensing applications — •Felix Buth, Deepu Kumar, Martin Stutzmann, and José Antonio Garrido — Walter Schottky Institut, Technische Universität München, Garching, Germany

Organic thin films can potentially be used in low-cost, disposable devices for chemical or bio-sensing. However, operating organic sensor devices in an aqueous environment raises difficulties when it comes to necessary operation voltages or device stability. One approach to reduce the gate voltage is increasing the capacitance of the gate dielectric. Electrolytic gates offer extraordinarily large capacitances, up to several $\mu F/cm^2$ at low frequencies. This high capacitance, which is the result of the formation of an electrical double layer at the electrolyte/semiconductor interface makes low-voltage operation possible, without high production costs. In this contribution, we investigate the behavior of polycrystalline α-sexithiophene (α6T) thin-film transistors with an aqueous electrolyte gate. Electrochemical impedance spectroscopy and CV measurements indicate a nearly perfectly polarizable interface with negligible parasitic Faradaic currents. For gate voltages below 1 V, a conductive channel is induced at the α6T/electrolyte interface via an electrical field effect. The transistor is stable for several hours and sensitive to changes in the pH or the ionic strength of the solution. The pH sensitivity arises from a shift in the threshold voltage of the transistor, and is not due to changes of the carrier mobility. The pH-dependent threshold voltage shift, in the range of 10 mV/pH, is caused by a change in the surface charge of the thin film.

HL 67.6 Wed 19:15 FOE Anorg

the origin of the short channel effect in organic field effect transistor. — •Ali Veysel Tunc[1], Elizabeth von Hauff[1], Ahmet Lütfi Ugur[2], Ali Erdogmus[2], and Jurgen Parisi[1] — [1]University of Oldenburg, Department of Physics, Energy and Semiconductor Research Laboratory (EHF) Carl-von-Ossietzky Str.9-11, 26129 Oldenburg, Germany — [2]Yildiz Technical University, Department of Chemistry, Davutpasa Campus, 34210 Esenler, Istanbul, Turkey

The origin of the short channel effect in polymer-based field effect transistors (FETs) was investigated. Here, we employed three different molecular weight poly [2-methoxy,5-(3',7'-dimethyl-octyloxy)]-p-phenylene vinylene (MDMO-PPV) and in blends with different ratios of 1-(3-methoxycarbonyl) propyl-1-phenyl[6,6]C61 (PCBM). In this work we demonstrate that the short channel effect is not only influenced by the device geometry but there is also a correlation between intrinsic material properties, the hole current, field effect mobility, contact resistance and short channel behavior in PPV based OFETs. Intrinsic properties, mobility or molecular weight, of the semiconductor influence the onset of the short channel effect. We observed that increasing the PCBM content in the blend leads to an increase in the hole current and field effect mobility, a decrease in the contact resistance, as well as a deviation from the saturation behavior of the output characteristics of the FET. This effect is attributed to a change in the polymer chain ordering in the source channel which in turn influences the charge transport properties in the polymer film.

HL 68: Photovoltaics: Chalcopyrites II

Time: Thursday 10:15–13:30 Location: FOE Anorg

HL 68.1 Thu 10:15 FOE Anorg

Radiative recombination of Cu_2ZnSnS_4 thin films and single crystals — •Steffen Kretzschmar[1], Justus Just[1], Björn Schubert[1], Susan Schorr[1], Thomas Unold[1], Serghei Levcenko[2], Victor E. Tezlevan[2], and Ernest Arushanov[2] — [1]Helmholtz Zentrum Berlin für Materialien und Energie, 14109 Berlin — [2]Institute of Applied Physics, Academy of Sciences of Moldova, Chisinau, MD 2028, Moldova

Cu_2ZnSnS_4 is an interesting absorber material for thin film solar cells, because it uses non-toxic and earth abundant elements. The best efficiencies reached so far are much lower than the record efficiencies of chalcopyrite thin film solar cells, 6.8% for Cu_2ZnSnS_4 and 9.6% for $Cu_2ZnSn(S,Se)_4$ have been reported in the literature. So far there is little knowledge about the optical and electronic properties of these materials. In this work Cu_2ZnSnS_4 thin films grown by coevaporation and Cu_2ZnSnS_4 single crystals grown by iodine transport chemical vapour deposition are investigated by photoluminescence spectroscopy. At low temperature shallow and deep transitions are observed. By temperature and intensity dependent measurements these transitions are

identified as excitons and free-bound transitions, respectively.

HL 68.2 Thu 10:30 FOE Anorg

Untersuchung der kristallographischen und elektronischen Struktur von Cu_2ZnSnS_4 mittels Röntgenabsorptionspektroskopie — •Justus Just[1,2], Thomas Unold[2], Dirk Lützenkirchen-Hecht[1], Hans-Werner Schock[2], Susan Schorr[2] und Ronald Frahm[1] — [1]Bergische Universität Wuppertal — [2]Helmholtz-Zentrum-Berlin, Institut für Technologie E-I3

Als alternatives Absorbermaterial für Dünnschichtsolarzellen im Vergleich zu herkömmlichen Chalkopyriten $Cu_2(In,Ga)(S,Se)_4$, bietet sich Cu_2ZnSnS_4 (CZTS) in chalkopyrit-verwandter Kesterit-Struktur an, und ist bislang kaum erforscht. Alle enthaltenen Elemente bzw. deren Verbindungen sind ungiftig und zu genüge in der Erdkruste enthalten, daher ist eine besonders kostengünstige Herstellung denkbar. Weiterhin hat CZTS eine zum Sonnenspektrum ideal angepasste Bandlücke von ca. 1,5eV und bietet einen hohen Absorptionskoeffizienten $\sim 10^4$/cm für sichtbares Licht. Somit eignet sich diese Verbindung ideal zur Herstellung von Dünnschichtsolarzellen. CZTS und dessen strukturverwandte Fremdphasen wurden mittels Röntgenabsorptionsspektroskopie bezüglich ihrer kristallografischen Struktur (EXAFS und Röntgenbeugung) und ihrer elektronischen Struktur nahe der Leitungsbandkante (XANES) untersucht. Die präsentierten Ergebnisse zeigen einen deutlichen Zusammenhang zwischen der aus theoretischen Kalkulationen bestimmten elektronischen Zustandsdichte unbesetzter Zustände und der gemessenen Röntgenabsorption. Dies ermöglicht eine quantitative Identifikation von Fremdphasen in den mittels Ko-Verdampfung hergestellten Dünnschichten.

HL 68.3 Thu 10:45 FOE Anorg

Ab initio based Monte Carlo studies of Cu-depleted CIS phases for solar cells — Christian Ludwig[1], •Thomas Gruhn[1], Claudia Felser[1], and Johannes Windeln[2] — [1]Institut für Anorganische and Analytische Chemie, Johannes Gutenberg-Universität Mainz, Deutschland — [2]IBM Mainz, Deutschland

Thin film solar cells with a $CuInSe_2$ (CIS) absorber layer have an increasing share of the solar cell market because of their low production costs and the high efficiency. One interesting aspect of CIS is the inherent resilience to defects and composition fluctuations. Beside the stable $CuInSe_2$ phase, there are various Cu-poor phases along the Cu_2Se–In_2Se_3 tie line, including the $CuIn_3Se_5$ and the $CuIn_5Se_8$ phase.

We have used ab initio calculations of Cu-poor CIS configurations to make a cluster expansion of the configurational energy. In the configurations, Cu atoms, In atoms, and vacancies are distributed over the Cu and In sites of a CIS cell with fixed Se atoms. With the resulting energy expression, $CuIn_3Se_5$ and $CuIn_5Se_8$ systems have been studied in the canonical ensemble. By analyzing the free energy landscape the transition temperature between a low-temperature ordered and a high-temperature disordered $CuIn_5Se_8$ phase has been determined.

Furthermore, grandcanonical ensemble simulations have been carried out, which provide the equilibrium Cu and In concentrations as a function of the chemical potentials μ_{Cu} and μ_{In}. Plateau regions for the $CuInSe_2$ and the $CuIn_5Se_8$ phases have been found and analyzed for different temperatures.

HL 68.4 Thu 11:00 FOE Anorg

The influence of sodium in $Cu(In,Ga)Se_2$ solar cells investigated by quantum efficiency measurements — •Stefan Puttnins[1,2], Hendrik Zachmann[1], Felix Daume[1,2], Andreas Rahm[1], and Marius Grundmann[2] — [1]Solarion AG, Ostende 5, 04288 Leipzig, Germany — [2]Institut für Experimentelle Physik II, Universität Leipzig, Linnéstr. 5, 04103 Leipzig, Germany

Thin film solar cells based on $Cu(In,Ga)Se_2$ (CIGSe) absorbers can be deposited on flexible plastic foils reaching efficiencies up to 17.6 %. The addition of sodium plays a key role for enhancing CIGSe solar cell perfomance.

As polyimide is a sodium free substrate (in contrast to soda-lime glass) extrinsic incorporation of sodium is indispensable to achieve high efficiencies.

The aim of this work is to analyze the influence of different sodium contents on photocurrent and defect characteristics by quantum efficiency (QE) measurements. We show that the sodium content influences the CIGSe bandgap, carrier collection in the long wavelength region of the QE spectra and the Urbach energy as a measure of structual disorder.

Furthermore, we show how luminescence spectra can be calculated from QE data and how the sodium content affects peak intensities and energetic peak positions in those spectra.

HL 68.5 Thu 11:15 FOE Anorg

Kathodolumineszenz-Mikroskopie von polykristallinen $Cu(In,Ga)Se_2$ -Absorberschichten — •Stefan Ribbe[1], Mathias Müller[1], Frank Bertram[1], Thomas Hempel[1], Wolfram Witte[2], Dimitrios Hariskos[2] und Jürgen Christen[1] — [1]Institut für Experimentelle Physik, Otto-von-Guericke Universität, Magdeburg, Deutschland — [2]Zentrum für Sonnenenergie- und Wasserstoff-Forschung, Baden Württemberg (ZSW), Stuttgart, Deutschland

Die Lumineszenzeigenschaften von $Cu(In,Ga)Se_2$-Schichten unterschiedlicher Schichtdicke als Absorber für hocheffiziente Dünnschichtsolarzellen wurden mittels hoch orts- und spektral-aufgelöster Kathodolumineszenz (KL) untersucht. Die Absorberschichten wurden in einem Durchlaufprozess mittels Koverdampfung auf Mobeschichtetes Kalk-Natron-Glas hergestellt. Unterschiedliche Schichtdicken von 1.0 und 3.0 μm wurden durch Variation der Durchlaufgeschwindigkeit realisiert. Auf den Oberflächen der polykristallinen Schichten ließen sich neben der typisch körnigen Struktur einzelne Facetten erkennen. Die ortsintegralen Tieftemperatur-KL-Spektren sind durch einen, für kupferarme Schichten typischen, breiten Peak um 1.13 eV (1.1 μm) gekennzeichnet. Durch Variation von Temperatur bzw. Anregungsdichte ließen sich DAP-Übergänge mit Beteiligung der Kupfervakanz und der Antisite-Defekt In_{Cu} identifizieren. Die laterale Lumineszenzverteilung ist sowohl hinsichtlich der Intensitäten als auch der Peakenergien mikroskopisch inhomogen. Hierbei sind sowohl Fluktuationen von Korn zu Korn, als auch eine Variation der Emissionswellenlänge innerhalb der einzelnen Partikeln zu erkennen.

HL 68.6 Thu 11:30 FOE Anorg

Investigations of lateral and vertical compositional gradients in $Cu(In,Ga)Se_2$ by highly spatially, spectrally and time resolved cathodoluminescence spectroscopy — •Mathias Müller[1], Stefan Ribbe[1], Thomas Hempel[1], Frank Bertram[1], Wolfram Witte[2], Dimitrios Hariskos[2], and Jürgen Christen[1] — [1]Institute for Experimental Physics, Otto-von-Guericke-University Magdeburg, Germany — [2]Zentrum für Sonnenenergie- und Wasserstoff-Forschung, Baden Württemberg (ZSW), Stuttgart, Germany

Luminescence properties of $Cu(In,Ga)Se_2$ (CIGS) layers with different thicknesses were investigated by means of highly spatially, spectrally and time resolved cathodoluminescence (CL) spectroscopy at low temperature (T = 5 K). A polycrystalline CIGS thin film with a thickness of 2.4 μm was grown using an in-line co-evaporation process with a final Cu-poor composition on top of a sputtered Mo layer on a soda lime glass substrate. The layer thickness was then reduced by highly controlled bromine methanol etching. The typical grainy ($d_{average}$ = 3 μm) structure of the untouched sample develops thin longish structures under the influence of the etchant. Integral CL spectra of the samples are dominated by donor-acceptor pair (DAP) luminescence. The peak energies of these spectra are ranging from 1.13 eV to 1.22 eV with decreasing layer thickness. The lateral distribution of the luminescence is inhomogeneous regarding the intensity as well as the peak energy. Time resolved CL shows a strong dependence of the initial lifetime from the emission energy.

15 min. break

HL 68.7 Thu 12:00 FOE Anorg

Band-lineup and junction formation between Zn-VI (VI = O, S, Se) and epitaxial $CuInSe_2$ — •Andreas Hofmann and Christian Pettenkofer — Helmholtz-Zentrum Berlin, Institut für Ladungsträgerdynamik, 12489 Berlin

The crucial interface in chalcopyrite-based solar cells is the one between $Cu(In,Ga)Se_2$ absorber and CdS buffer layer, where the p/n junction is situated and which should provide a beneficial energetic lineup among absorber and ZnO window. Due to its toxicity, Cd-free buffer layers are desirable.
Single-crystalline $CuInSe_2$(112) and (001) films were grown by molecular beam epitaxy as well-defined model systems to study the band alignment with alternative buffer layer materials. The Zn-VI layers were deposited stepwise with intermediate analysis by combined XPS/UPS and LEED, completely under UHV conditions. ZnO deposition by Metal-Organic MBE leads to the formation of an ultra-thin intrinsic ZnSe buffer layer (1-2 nm thickness), consistent with our

findings for $CuInS_2$(112) [1]. The valence band offset for the intrinsic buffer layer of 0.7 eV is conform with our result for the bulk and agrees well with theory [2]. On $CuInSe_2$(112) substrates, ZnO grows in registry with ZnSe(111) with its own lattice constant in the (0001) direction, as confirmed by the LEED pattern. From our measurements, the band alignment is largely independent on orientation.

[1] S. Andres *et al.*, Thin Solid Films **518**, 1032 (2009).
[2] W. Mönch, Appl. Phys. A **87**, 359-366 (2007).

HL 68.8 Thu 12:15 FOE Anorg

Band alignment of epitaxial ZnS on $CuInS_2$(001) and $CuInS_2$(112) — •Carsten Lehmann, Frank Kelleter, and Christian Pettenkofer — Helmholtz-Zentrum Berlin, Berlin, Deutschland

With respect to thin film solar cells based on $CuInS_2$ and ZnO ZnS is a promising alternative to CdS as buffer layer material [1,2]. We report on the band aligment of epitaxial ZnS prepared by molecular beam epitaxy (MBE) on $CuInS_2$ (001) and $CuInS_2$(112). The preparation and investigation of the samples were performed in an ultra high vacuum system at the Helmholtz-Zentrum Berlin. An alternating step-by-step growth and investigation by photoelectron spectroscopy (PES) and low energy electron diffraction (LEED) provided insight on the band line up of the $CuInS_2$-ZnS interface. The $CuInS_2$ substrates were prepared on GaAs by gas source molecular beam epitaxy (GSMBE) using di-tert butyl disulfide (TBDS) as sulfur precursor. Furthermore, the derived data were used to determine the band alignment of the corresponding $CuInS_2$-ZnS-ZnO interfaces prepared by metal organic molecular beam epitaxy (MOMBE) based on diethylzinc and water [2]. [1] M. Bär, et. al., Journal of Applied Physics 99 (2006) [2] S. Andres, et. al., Thin Solid Films 518 (2009)

HL 68.9 Thu 12:30 FOE Anorg

Spatially resolved photoluminescence studies on $CuGaSe_2$ and $CuInSe_2$ thin-films — •Christian Gutsche[1], Raquel Caballero[2], and Gottfried H. Bauer[1] — [1]Insitute of Physics, Carl von Ossietzky University Oldenburg, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie (HZB), Berlin, Germany

Chalcopyrite absorbers such as $Cu(In_{1-x}\ Ga_x)Se_2$ as convincingly promising candidates for solar light harvesting due to the grainy structure exhibit a high degree of compositional, optical and electronic inhomogeneities.

We have studied samples of the extreme values of stoichiometry, say x=0, and x=1 by steady state spectrally resolved photoluminescence with lateral resolution of ≤ 1 μm in a confocal cryostat setup. We compare the experimental observations of these two types of absorbers, $CuInSe_2$ with $CuGaSe_2$ with respect to laterally resolved luminescence yields, local splitting of quasi-Fermi levels, local absorption coefficients and local pseudo band gaps, as well as local recombination rates.

Furthermore we discuss the distribution of these magnitudes on the basis of histograms and Minkowski-operations like 'opening'-functions to extract lateral features and determine their pattern sizes.

HL 68.10 Thu 12:45 FOE Anorg

Cu(In,Ga)Se_2-based thin-film systems with different absorber thicknesses: spatially resolved photoluminescence and AFM measurements — •Oliver Neumann[1], Stephan J. Heise[1], Rudolf Brüggemann[1], Max Meessen[1], Wolfram Witte[2], Dimitrios Hariskos[2], and Gottfried H. Bauer[1] — [1]Institute of Physics, Carl von Ossietzky University Oldenburg, Germany — [2]Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg (ZSW), Stuttgart, Germany

Chalcopyrite absorbers exhibit spatial inhomogeneities in structural, optical and optoelectronic properties. We study the absorber thickness dependent behavior of the local properties such as the splitting of the quasi-Fermi levels, optical threshold energies and surface roughness of Cu(In,Ga)Se_2-based (CIGSe) thin-film systems with different absorber thicknesses, which are realized by etching traditionally prepared absorbers with nominal thicknesses of about 2 μm with bromine-methanol followed by a cadmium sulfide (CdS) passivation. AFM measurements reveal a decrease in the surface roughness with decreasing absorber thickness, i.e., increasing etching time. Photolumienscence experiments with high lateral resolution allow the extraction of the optical threshold energies and the splitting of the quasi-Fermi levels. Furthermore we verify a depth gradient of the gallium concentration and a variation of quasi-Fermi level splitting depending on the absorber thickness. Additionally, we show that the CdS/CIGSe junction formation of an unetched absorber in comparison to an etched absorber leads to higher quasi-Fermi level splitting.

HL 68.11 Thu 13:00 FOE Anorg

Photoelectric properties of variably RTP processed $CIGS_2$ solar cells — •Julia Riediger[1], Jörg Ohland[1], Martin Knipper[1], Jürgen Parisi[1], Ingo Riedel[1], Roland Mainz[2], Saoussen Merdes[2], and Joachim Klaer[2] — [1]Energy and Semiconductor Research Laboratory, Department of Physics, University of Oldenburg, 26111 Oldenburg, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie Berlin GmbH, Glienicker Straße100, 14109 Berlin, Germany

The open circuit voltage V_{oc} of $CuInS_2$ solar cells was found to improve via incorporation of gallium. The Cu(In,Ga)S_2 absorber of the samples studied in this work was prepared by sputtering (Cu,Ga) and In precursors subsequently sulfurized via rapid thermal processing (RTP) in sulfur vapor. Distinctive top/bottom $CuInS_2$/$CuGaS_2$ segregation has been observed which extent depends on the substrate temperature and holding time of the temperature during RTP-process. The insufficient gallium accumulation at the surface impedes high values of V_{oc}.We studied the consequences of RTP-process parameter variation in regard of the interdiffusion of $CuInS_2$ and $CuGaS_2$. Quantum efficiency (QE) and temperature-/illumination-dependent current-voltage (IV) profiling have been carried out for differently processed samples. These measurements provide the minimum band gap E_g of the graded absorber layer, the temperature dependent V_{oc} and the activation energy E_a for carrier recombination. Drive level capacitance (DLCP) profiling reveals the spatially resolved in-depth variation of the doping/defect concentration close to the space charge region.

HL 68.12 Thu 13:15 FOE Anorg

Comparison of Photovoltaic Parameters of Cu(In,Ga)Se2 Thin Film Solar Cells with Infrared Images Obtained with Lock-In Thermography — •Torben Klinkert[1], Jörg Ohland[1], Robin Knecht[1], Jürgen Parisi[1], Raymund Schäffler[2], and Bernhard Dimmler[2] — [1]Thin Film Photovoltaics, Energy- and Semiconductor Research Laboratory, University of Oldenburg, D-26111 Oldenburg — [2]Würth Solar GmbH & Co. KG, Alfred-Leikam-Straße 25, D-74523 Schwäbisch-Hall

The performance of photovoltaic modules comprised of monolithically series connected solar cells is basically determined by the weakest element in the circuit. In chalcopyrite thin film modules lateral film inhomogeneities and losses due to interconnection are likely to deteriorate the photovoltaic performance of individual cell stripes and, in consequence, to reduce the module efficiency. In this work we correlate microscopic features with the macroscopic device parameters of Cu(In,Ga)Se2 solar cells cut from large-area modules. Imaging of the film imperfections and regions of enhanced joule heating was realized by applying infrared Lock-In Thermography (LIT) with optical (I-LIT) and electrical (D-LIT) excitation of the sample. Via comparison of the infrared LIT images with the photovoltaic cell parameters obtained from STC current voltage profiling and quantum efficiency measurements we try to correlate macroscopic junction failure with microscopic disruptions of the film properties. These problems will also be discussed on the module level by analysis of D-LIT results obtained for individual cell stripes in an integrated series compound of a CIGSe-module.

HL 69: Nitrides: LEDs

Time: Thursday 10:15–11:30 Location: POT 51

HL 69.1 Thu 10:15 POT 51

Optical polarization of UV-A and UV-B (In)(Al)GaN multiple quantum well light emitting diodes — •Tim Kolbe[1], Arne Knauer[2], Joachim Stellmach[1], Chris Chua[3], Zhihong Yang[3], Sven Einfeldt[2], Patrick Vogt[1], Noble M. Johnson[3], Markus Weyers[2], and Michael Kneissl[1,2] — [1]Institute of Solid State Physics, TU Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, Gustav-Kirchhoff-Str. 4, 12489 Berlin, Germany — [3]Palo Alto Research Center, 3333 Coyote Hill Road, Palo Alto, CA 94304, USA

The optical polarization of the in-plane electroluminescence of (0001) oriented (In)(Al)GaN multiple quantum well light emitting diodes (LEDs) in the spectral range from 288 nm to 386 nm has been investigated. A decrease of the intensity of transverse-electric (TE) polarized light relative to transverse-magnetic (TM) polarized light with decreasing emission wavelength is found. This effect is attributed to rearrangement of the valence bands at the gamma-point of the Brillouin zone with changing aluminum and indium mole fractions in the (In)(Al)GaN quantum wells. For shorter wavelengths the crystal-field split-off hole band moves closer to the conduction band relative to the heavy and light hole bands. As a consequence TM polarized emission from the split-off hole band becomes more dominant for LEDs with a decreasing emission wavelength. A polarization of zero (that means that the intensities of the TE polarized light and the TM polarized light are the same) is found for LEDs emitting near 300 nm. For shorter wavelengths the emitted light is mainly TM polarized.

HL 69.2 Thu 10:30 POT 51

Processing of III-nitride thin film light emitting diodes via wafer bonding and laser lift-off — •Christian Gossler, Rüdiger Moser, Michael Kunzer, Klaus Köhler, and Ulrich Schwarz — Fraunhofer-Institut für Angewandte Festkörperphysik, Tullastraße 72, D-9108 Freiburg

High-brightness thin film (Al,In)GaN-based light emitting diodes are generally manufactured by wafer bonding and laser lift-off of the sapphire substrate. This technique is the key for a drastic improvement of light extraction efficiency due to the possibilities of roughening the outcoupling surface and employing a reflective backside contact.

We present the development of a rapid thin film process not using lithographic structuring. A novel bonding scheme based on the eutectic system Aluminium-Germanium is shown. The 2 inch GaN-on-sapphire epiwafers are prepared by depositing 1 μm Aluminium via electron beam evaporation in a shadow mask process. The bonding to a Germanium wafer occurs at high vacuum well above the eutectic temperature of $T = 693\,\mathrm{K}$. For laser lift-off we use an excimer laser work station emitting at $\lambda = 248\,\mathrm{nm}$ with a homogenized laser spot of up to $2\,\mathrm{mm} \times 2\,\mathrm{mm}$. Additionally, the GaN layer is separated into mechanically isolated areas prior to wafer bonding by fabricating trenches via picosecond laser processing to improve yield and process control. The thin film LEDs are characterised via electroluminescence and possible effects of the laser trenching are discussed.

HL 69.3 Thu 10:45 POT 51

Micromachining with picosecond laser pulses: A versatile tool for the fabrication of optoelectronic devices — •Rüdiger Moser, Michael Kunzer, Christian Gossler, Klaus Köhler, Ulrich Schwarz, and Joachim Wagner — Fraunhofer-Institut für Angewandte Festkörperphysik, Tullastrasse 72, D-79108 Freiburg, Germany

Picosecond (ps) lasers provide a universal tool for material processing. Due to the short laser pulses material is removed by a process called "cold ablation", with minimal thermal damage to neighbour regions. As a result, better defined structures with smother and cleaner side walls can be fabricated than with "long-pulse" lasers. This offers new possibilities for laser processing in semiconductor technology for both semiconductor materials and contact or bond metallizations. The fabrication of semiconductor devices typically requires lithography steps, which are time consuming and expensive. Therefore one would like to avoid these steps at least for development and prototyping. One way to do so is to replace lithography steps by direct laser writing. In this presentation we report on the development of ps laser processes to directly pattern the semiconductor surface with trenches and mesas for the fabrication of GaN-based LEDs. The laser processed devices are electrically and optically characterised and compared with conventionally fabricated test devices. Furthermore the realization and use of high quality shadow masks for e.g. deposition of ohmic contact metallizations is reported and compared with results obtained using nanosecond laser processing.

HL 69.4 Thu 11:00 POT 51

High n-type crack-free GaN layers on Si substrates by Ge doping — •Armin Dadgar, Jürgen Bläsing, Annette Diez, and Alois Krost — Institut für Experimentelle Physik, Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg

GaN based growth on silicon substrates usually requires strain-engineering methods to avoid tensile stress after cooling from growth temperature. Silicon doping required for contacting and current spreading is known to induce additional tensile stress during growth originating in edge dislocation climb. Consequently, the typically inferior material quality for GaN on Si in comparison to GaN grown on sapphire leads to high tensile stresses for highly Si doped layers, limiting freedom in device design and performance. We present that germanium doping enables the growth of thick highly n-type doped layers on silicon substrates not influencing strain evolution. By this, it enables a possible improvement of GaN-on-Si LEDs. We also conclude that the mechanism of dislocation climb in the case of silicon doping is not dominated by surface roughening but by silicon-nitride induced dislocation masking which does not apply for germanium.

HL 69.5 Thu 11:15 POT 51

All-optical determination of absolute quantum efficiency values of GaInN-based light-emitters — •Bastian Galler, Matthias Sabathil, Ansgar Laubsch, Tobias Meyer, Lutz Höppel, Gertrud Kräuter, Hans-Jürgen Lugauer, Asako Hirai, Martin Strassburg, Matthias Peter, Andreas Biebersdorf, Ulrich Steegmüller, and Berthold Hahn — OSRAM Opto Semiconductors GmbH, Leibnizstraße 4, 93055 Regensburg, Germany

The efficiency droop of GaInN-based light-emitting diodes (LEDs) gets more and more significant for increasing wavelengths and thus contributes to the well-known green gap [1]. A major reason for this behaviour is that multi-quantum-well (MQW) operation is harder to achieve under electroluminescence conditions for LEDs with high indium content due to higher transport barriers. A possibility to circumvent this difficulty is optical pumping of a large number of green-emitting quantum wells. Using a UV-LED as an electrically driven pump for a green 40x MQW glued directly on its top, we show that this system can outperform direct green LEDs at large current densities. In addition to that, the combination of LED and converter platelet allows for an absolute quantum efficiency determination of the converter structure in contrast to conventional photoluminescence experiments. We use this method to obtain further evidence that the droop is due to a QW-internal loss process. Furthermore, we propose this approach as a general tool for the evaluation of other light-emitting structures that cannot be pumped electrically.

[1] T. Mukai et al., Jpn. J. Appl. Phys., Part 1 38 (1999).

HL 70: Quantum Dots and Wires: Theory

Time: Thursday 10:15–13:45 Location: POT 151

HL 70.1 Thu 10:15 POT 151

Lasing and transport properties in a coupled dot-resonator system — •Peiqing Jin, Michael Marthaler, Jared Cole, and Gerd Schön — Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany

The study of the interaction between light and matter at the quantum level is of great interest for quantum information. We investigate a system consisting of double quantum dots coupled to an electrical resonator. A pumping scheme induced by the incoherent tunneling between electrodes and dots is considered. For small tunneling rates, the system reaches the non-classical regime where the radiation field exhibits sub-Poissonian statistics. In this regime, the peak of the current through the double dots, which appears at resonance, is almost the same at charge resonance.

The spin degree of freedom is involved when an external magnetic field is present. The difference between the effective magnetic fields provided by nuclear spins in each dot leads to an asymmetry between the two spin channels. Different behavior of the radiation field at the resonance of each spin channel is discussed.

HL 70.2 Thu 10:30 POT 151

Electronic properties of (111)-grown InGaAs/GaAs quantum dots — •Oliver Marquardt and Eoin O'Reilly — Tyndall National Institute, Lee Maltings, Cork, Ireland

InGaAs-QDs grown along the (111)-axis in GaAs exhibit electronic properties that are excellently suited to the generation of single and entangled photons, as required for quantum cryptography or quantum computing purposes.

We employ an eight-band $\mathbf{k}\cdot\mathbf{p}$ model to provide a theoretical study of these nanostructures. Strain and polarisation potentials that modify the bulk electronic properties of the system are calculated using second-order continuum elasticity theory. Moreover, we have taken second-order piezoelectric contributions into account in our calculations of the polarisation potential.

Our studies reveal that, for the case of (111)-grown zincblende InGaAs/GaAs quantum dots, second-order piezoelectric contributions have a significant influence on electron and hole eigenenergies and charge densities. In particular, such second-order contributions are found to significantly reduce the resulting polarisation potentials in comparison to potentials obtained from using only the first-oder piezoelectric constants. This reduction of the piezoelectric potential allows for better electron-hole overlap and thus higher recombination rates and is in much better agreement with recent experimental observations than calculations employing first-order piezoelectric constants only.

HL 70.3 Thu 10:45 POT 151

Spin blockade in the optical response of a charged quantum dot — •Eleftheria Kavousanaki and Guido Burkard — Department of Physics, University of Konstanz, Germany

We theoretically model the population dynamics in a semiconductor quantum dot charged with a single electron in an optical pump-probe setup when the two lowest quantum dot levels are photoexcited. We calculate the differential transmission spectrum as a function of the time delay between the two circularly polarized optical pulses by using a density matrix formalism and treating intraband relaxation with the Lindblad equation. Taking into account both spin conserving and spin-flip relaxation processes we investigate the possibility for spin-dependent blocking of intraband relaxation due to the presence of the ground state electron for zero and finite magnetic fields. We show that the differential transmission spectrum is initially dominated by the fast spin-conserving mechanism before the slower spin-flip processes start to contribute at longer time scales. As a consequence of spin conservation for short time scales, we find a spin blockade effect in the optical recombination process.

HL 70.4 Thu 11:00 POT 151

Monitoring the switching of a Mn spin in a quantum dot by optical signals — •Doris E. Reiter[1], Vollrath Martin Axt[2], and Tilmann Kuhn[1] — [1]Institut für Festkörpertheorie, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster — [2]Theoretische Physik III, Universität Bayreuth, 95440 Bayreuth

When a single Mn atom is embedded in a single quantum dot, in the photoluminescence spectrum the exciton line splits into a set of six lines even at zero magnetic field due to the strong exchange interaction between exciton and Mn spin. Each line corresponds to one of the six Mn spin states, such that if the Mn spin is in an eigenstate only a single line with a given spectral position appears. Recently we proposed a protocol to optically switch the Mn spin from a given initial state into all other states using a sequence of laser pulses [PRL **102**, 177403 (2009)]. To monitor the dynamics of the Mn spin state we here propose a pump-probe set-up, for which we calculate the optical signals. For the switching steps during the protocol different signatures in the spectrum appear and most remarkably the spectral position of the line in the probe spectrum shifts according to the Mn spin state. With a modified switching protocol superpositions of different Mn spin states can be generated. In the probe spectrum now instead of a single line two lines at the spectral position of the involved Mn spin states show up, while the line strengths correspond to the weights of the superposition. In this contribution we show how the Mn spin dynamics can be deduced from the optical signals.

HL 70.5 Thu 11:15 POT 151

Theory of exciton fine structure in cubic semiconductor quantum dots — •Erik Welander and Guido Burkard — Department of Physics, University of Konstanz, Konstanz, Germany

We theoretically investigate the radiative recombination of biexcitons in semiconductor quantum dots. The biexciton recombines via one out of two possible intermediate exciton states, causing two linearly photons to be emitted, $|X\rangle|Y\rangle$ or $|Y\rangle|X\rangle$. The order in which the photons are emitted depends on which exciton, $|X\rangle$ or $|Y\rangle$, mediates the recombination (which-way). If the intermediate state is energetically degenerate, a coherent superposition of the two double-photon states is possible, $(|X\rangle|Y\rangle + |Y\rangle|X\rangle)/\sqrt{2}$. This allows the biexciton cascade recombination to produce entangled photon pairs. The geometry dependent electron-hole exchange interaction is known to remove the degeneracy of the intermediate exciton states. Since the polarization of the light then would be entangled with the photon energy, the which-path information would be available via frequency measurements and thus the creation of polarization entangled photons would no longer be possible. We develop a model for the quantum dot exciton fine-structure and its dependence on geometry. The emerging photon states are studied and explicit results are presented for a spatially asymmetric, harmonically confined GaAs quantum dot surrounded by AlAs. Moreover, we examine the possibility of restoring the degeneracy by applying external electric and/or magnetic fields.

HL 70.6 Thu 11:30 POT 151

Interrelation of Biexciton Binding Energies and Structural Properties of GaN/AlN Quantum Dots — •Gerald Hönig, Christian Kindel, Momme Winkelnkemper, Andrei Schliwa, Sven Rodt, Irina Ostapenko, Axel Hoffmann, and Dieter Bimberg — Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstraße 36, D-10623 Berlin, Germany

Nitride-based quantum dots (QDs) are very promising candidates for high-temperature stable, entangled photon pair emitters. Tuning the biexciton energy (E^{xx}) by varying structural parameters [1] is of largest importance for QDs in microcavities, where the emission has to match the cavity-mode. The experimental observation of a sign change of the biexciton binding energy ($E^{bind} := 2E^x - E^{xx}$, with $E^x :=$ exciton energy) in GaN/AlN QDs [2], is theoretically not understood so far. We are able to investigate this feature by using a configuration interaction scheme (CI) based on self-consistent 8-band-$k\cdot p$ Hartree-Fock (HF) states. The self-consistency is crucial since built-in piezo- and pyroelectric fields (on the order of MV/cm) cause a spatial separation between electrons and holes within nitride-based QDs, making a CI basis of renormalised HF states superior to single particle wave functions. We take a close look on different structural parameters influencing E^{xx} as well as the quantity of correlation effects in GaN/AlN QDs. Both, positive and negative biexciton binding energies are possible for respective QD structures. Funded by SFB 787.

[1] A. Schliwa, et al., Phys. Rev. B 79, 075443 (2009)
[2] D. Simeonov, et al., Phys. Rev. B 77, 075306 (2008)

HL 70.7 Thu 11:45 POT 151

Carrier multiplication in quantum dots: Quantum optical emission dynamics — •Franz Schulze, Sandra Cecilia Kuhn, Andreas Knorr, and Carsten Weber — Institut f. Theoretische Physik, Technische Universität Berlin, Germany

Measurements of carrier multiplication in quantum dots based on excitonic and multiexcitonic decay dynamics [1] show potential for its utilization in photovoltaic conversion, but also contradicting results. Theoretical treatments of the process are typically based on stationary methods or simple Bloch equation approaches [2]. As a more fundamental approach to an unambiguous signal of carrier multiplication, we present a microscopically derived dynamical model of carrier multiplication in a single quantum dot. Within this model a time resolved quantum optical emission spectrum is investigated, which shows a behaviour characteristic of the carrier multiplication dynamics observed in the purely electronic system. Different paths in the electronic system leading from an initial optical excitation to the creation of multiple carriers are discussed.

[1] R. D. Schaller and V. I. Klimov, Phys. Rev. Lett. **92**, 186601 (2004)
[2] A. Shabaev, A. L. Efros, and A. J. Nozik, Nano Lett. **6**, 2856 (2006)

15 min. break

HL 70.8 Thu 12:15 POT 151

Reduction of the modulation bandwidth for high carrier scattering in semiconductor QD based laser devices — •Michael Lorke, Torben R. Nielsen, and Jesper Mørk — DTU Fotonik, Department of Photonics Engineering, Technical University of Denmark, 2800 Kgs. Lyngby, Denmark

Semiconductor lasers are central components of current optical technologies such as optical data storage and optical communications. To meet the continuously increasing need for progressively higher data transmission rates, a high modulation bandwidth of the underlying semiconductor device is required. The combination of quantum dots (QDs) with high-quality cavities, e.g. realized by photonic crystals, opens a multitude of possibilities for guiding and modifying the emission properties of QD-based devices via the Purcell effect.

We apply a microscopic theory to study dynamical properties of QD based nanocavity devices. Application relevant quantities such the modulation bandwidth as well as fundamental properties such as the laser linewidth and switch-on behavior are determined consistently from a microscopic semiconductor approach. Our theory predicts a reduction of the modulation bandwidth at high scattering rate allowing for optimization of QD based nanocavity devices. This behavior arises from a delicate balancing of the emission time and the photon lifetime in the cavity, as both the relaxation oscillation frequency and the damping of the relaxation oscillations grow with faster scattering.

HL 70.9 Thu 12:30 POT 151

Exciton fine structure splitting in self-assembled semiconductor QDs: Intrinsic and extrinsic effects — •Ranber Singh and Gabriel Bester — Max-Planck-Institut f\"{u}r Festk\"{o}rperforschung, Heisenbergstrasse 1, 70569 Stuttgart, Germany

There are ongoing efforts to understand excitonic fine structure splitting (FSS) in self-assembled strained (InGaAs/GaAs) and unstrained (GaAs/AlGaAs) quantum dots (QDs). We investigate the excitonic FSS in InGaAs/GaAs and GaAs/AlGaAs QDs of different shapes and sizes using the atomistic pseudopotential approach. We consider the effects of the growth direction, alloy ordering, charged point defects and uniaxial strain. We find that the growth direction, alloy ordering and uniaxial strain affect the FSS quite significantly. However, charged point defects have a rather small effect on the FSS. We obtain a large FSS in small QDs, when the single particle wavefunctions of electrons and/or holes spread into the interface regions between the QD and the barrier. In such a case a small elongation along [110] or [1$\bar{1}$0] in the circular QD base increases the FSS quite significantly. However, if the QD is large enough (which represents the "conventional" case) so that S single particle wavefunctions of electrons and holes are well confined in the center region of the QD, the elongation of the QD has a marginal effect on the FSS.

HL 70.10 Thu 12:45 POT 151

Semiconductor theory for single quantum dot emitters — •Matthias Florian[1], Paul Gartner[1,2], Christopher Gies[1], and Frank Jahnke[1] — [1]Institute for Theoretical Physics, University of Bremen, Germany — [2]National Institute of Materials Physics, Bucharest-Magurele, Romania

The controlled interaction of a single quantum-dot (QD) emitter with a single mode of the confined electromagnetic field is one of the recent remarkable achievements in cavity quantum-electrodynamics. The discrete level structure of QDs and the similarity to atomic systems has been widely used by invoking atomic models to describe QD-systems. But QDs are significantly different due to multiple carriers in the system and a reduced configuration interaction strength. This leads to several configurations, which are energetically close by and involved in the same interaction process. Moreover, typical excitation of carriers in the continuum states of the wetting layer or barrier material can introduce excitation-induced screening and dephasing. To analyze the quantum-mechanical interaction processes, we propose a microscopic theory based on a direct numerical solution of the von-Neumann equation for the coupled carrier-photon system. The Coulomb interaction as well as carrier scattering and dephasing processes are included and their influence on the statistical properties of the emitted photons like coherence, antibunching, and quenching are discussed.

HL 70.11 Thu 13:00 POT 151

Nonclassical light and stimulated emission in the strong coupling regime for single-quantum dot lasers — •Christopher Gies, Kolja Schuh, Matthias Florian, and Frank Jahnke — Institute for Theoretical Physics, University of Bremen, Germany

With a single quantum dot (QD) emitter in a high-quality cavity, the ultimate limit of miniaturization for a semiconductor laser has been reached and new physical effects emerge. Recent experiments on single-QD lasers exhibit an s-shaped input/output curve known from ensemble-based lasers. Also surprising is the transition from photon antibunching to bunching in the laser threshold region before coherent emission is reached. We present a microscopic theory and explain both effects in terms of competing contributions from multi-exciton states that start to contribute at elevated pumping conditions. Excitation-induced dephasing and screening facilitate the off-resonant coupling of multi-exciton transitions. Furthermore, we study stimulated emission in the presence of strong coupling. With increasing pump we can identify signatures of higher rungs of the Jaynes-Cummings ladder in the emission spectrum before excitation-induced dephasing carries the system into the weak coupling regime.

HL 70.12 Thu 13:15 POT 151

Microscopic description of the dynamics of luminescence and dephasing of semiconductor quantum dots — •Heinrich A.M. Leymann[1], Matthias Florian[2], Jan Wiersig[1], and Frank Jahnke[2] — [1]Institut für Theoretische Physik, Universität Magdeburg, 39016 Magdeburg — [2]Institut für Theoretische Physik, Universität Bremen, 28334 Bremen

Semiconductor quantum dots (QDs) are of considerable interest due to their potential for device applications such as lasers and non-classical light sources, as well as fundamental studies.

We present a microscopic theory for the photoluminescence of QDs based on an equation of motion technique. The influence of Coulomb- and carrier-photon interaction will be discussed in terms of correlation functions. A consistent treatment of pumping, scattering and dephasing will be presented that extends the cluster-expansion technique used in [1].

Furthermore results for a single QD emitter coupled to a single cavity mode will be discussed and compared to direct solutions of the von-Neumann equation of the statistical operator, showing excellent agreement.

[1] N. Baer et al., Eur. Phys. J. B 50 411 (2006).

HL 70.13 Thu 13:30 POT 151

Influence of LO-phonon collisions on robust adiabatic passage in semiconductor quantum dots — •Kolja Schuh[1], Michael Lorke[2], and Frank Jahnke[1] — [1]Institute for Theoretical Physics, University of Bremen, Germany — [2]DTU Fotonik, Department of Photonics Enginering, Technical University of Denmark

While Rabi-oscillations can be used to invert a system with a resonant optical pulse, the inversion is very sensitive to pulse parameters like frequency and pulse area. An inversion can also be achieved via an adiabatic passage using a chirped optical pulse. In contrast to a resonant pulse, this inversion is robust over a large parameter scale.

The influence of LO-phonon collisions on robust adiabatic passage in

self-assembled semiconductor quantum-dot (QD) systems is analyzed within a quantum-kinetic many-body theory including non-Markovian effects and quasi-particle properties [1]. For QD states the effective LO-phonon coupling is enhanced leading to pronounced dephasing as well as fast carrier scattering processes even in low polar semiconductors.

Numerical results are presented for different InGaAs QD systems including wetting layer contributions. While inversion can be achieved in QD systems with slow dephasing by a pulse length of several ps, this is not possible for systems with fast dephasing and scattering. Achieving inversion in such dots requires a tradeoff between keeping the adiabatic regime and minimizing dephasing and carrier scattering by short and strongly chirped pulses.

[1] K. Schuh et al., APL 94, 201108 (2009).

HL 71: Quantum Dots: Optical Properties

Time: Thursday 10:15–13:15 Location: POT 251

HL 71.1 Thu 10:15 POT 251

Simultaneous control of single self-assembled quantum dots by strain and electric fields — •Rinaldo Trotta, Paola Atkinson, Johannes D. Plumhof, Santosh Kumar, Roman Rezaev, Eugenio Zallo, Andreas Herklotz, Kathrin Dörr, Armando Rastelli, and Oliver G. Schmidt — Institute for Integrative Nanosciences, IFW Dresden, Helmholtzstrasse 20, D-01069 Dresden, Germany

The possibility to control the physical properties of semiconductor quantum dots (QDs) through external perturbations has led to an explosion of research interest from both fundamental and technological standpoints. Here we will report on the fabrication of a novel device, which allows applying strain and electric fields on a single QD simultaneously. Diode-like-nanomembranes containing quantum dots are integrated onto piezoelectric actuators via gold thermo-compression bonding. Different diode-like-structures (n-i-Schottky and p-i-n diodes) will be presented and the optical properties of embedded dots will be discussed. By applying biases to the piezoelectric actuator we can reversibly shift the emission energy of a single QD by more than 10 meV, while by applying a bias to the diode structure we can control the charge state of the QD or excite electroluminescence. The latter result represents the first demonstration of a strain-tuneable Light-Emitting Diode (LED) based on single quantum dots, a device which might be of high potential interest for quantum information technology.

HL 71.2 Thu 10:30 POT 251

Dynamic control of charge carrier injection into individual quantum dots and quantum posts by surface acoustic waves — •Florian J. R. Schülein[1], Stefan Völk[1], Florian Knall[1], Dirk Reuter[2], Andreas D. Wieck[2], Tuan A. Truong[3], Heejung Kim[3], Pierre M. Petroff[3], Achim Wixforth[1], and Hubert J. Krenner[1] — [1]Lehrstuhl für Experimentalphysik I, 86159 Augsburg, Germany — [2]Lehrstuhl für Angewandte Festkörperphysik, 44780 Bochum, Germany — [3]Materials Department, University of California, Santa Barbara, CA 93106, United States

We present a detailed study of the surface acoustic wave (SAW) power dependence on the carrier injection into and recombination in self-assembled quantum posts (QPs) and quantum dots (QDs). The matrix quantum well of QPs is a wide ($\sim$ 23nm) confinement potential, in contrast to the wetting layer of QDs. Thus, the energy levels of the thin ($\sim 1-2$nm) wetting layer is modulated by monolayer fluctuations giving rise to charge carrier traps and very low overall mobility. For both systems we observe a clear switching between different states (X^0 and $X^{+/-}$) with increasing SAW power. This switching is symmetric in SAW power for QPs and shows a broad hysteresis for QDs. This can be explained by SAW driven ionization of traps within the wetting layer during the up-sweep of the SAW power. With a laser excitation scheme for which the phase of the SAW is locked to the excitation laser, we are able to resolve the full phase information of this dynamically driven carrier injection.

HL 71.3 Thu 10:45 POT 251

Built-in dipole moments of InGaN/GaN single quantum dot excitons — •Irina A. Ostapenko, Christian Kindel, Gerald Hönig, Sven Rodt, André Strittmatter, Axel Hoffmann, and Dieter Bimberg — Institut für Festkörperphysik, TU Berlin, Hardenbergstr 36, 10623 Berlin, Germany

We report on direct determination of intrinsic dipole moments of excitonic complexes in InGaN/GaN quantum dots from cathodoluminescence experiments. Single nitride-based QDs show large potential as sources of entangled photon pairs at room temperature for quantum information processing and cryptography applications [1]. The built-in piezoelectric and pyroelectric fields tremendously affect electro-optical properties of nitride heterostructures [2]. The insight into interplay between confined charge carriers and electric fields is crucial for improvement and control of nitride QD-based devices. Only in cathodoluminescence we observe a re-occurring characteristic pattern in temporal traces of emission lines and explain this feature with a model of interaction between an exciton in a quantum dot and a gradually changing electric field of a charge carrier, moving through the material. We derive the magnitude of the built-in excitonic dipole moments as 0.7-7*10-28C*m*0.3-3 e*nm. These values are in good agreement with calculations based on 8-band k*p, extended by a self-consistent Hartree formalism. [1] C. Kindel, S. Kako, T. Kawano, H. Oishi, Y. Arakawa, G. Hönig, M. Winkelnkemper, A. Schliwa, A. Hoffmann, and D. Bimberg, Phys. Rev. B 81, 241309(R) (2010) [2] M. Winkelnkemper, A. Schliwa, and D. Bimberg, Phys. Rev. B 74,155322 (2006)

HL 71.4 Thu 11:00 POT 251

GaInN quantum dots as optochemical transducers — •Jörg Teubert[1], Sebastian Koslowski[1], Aparna Das[2], Eva Monroy[2], Philomela Komninou[3], and Martin Eickhoff[1] — [1]I. Physikalisches Institut, Justus-Liebig-Universität Gießen, Germany — [2]CEA-CNRS, INAC/SP2M/NPSC, CEA-Grenoble, France — [3]Department of Physics, Aristotle University of Thessaloniki, Greece

We report on the sensitivity of photoluminescence (PL) properties of polar InGaN/GaN quantum dot (QD) super-lattices to changes in the chemical environment. III-N QD structures arouse increasing interest e.g. as light emitters in optoelectronics and telecommunication. Here we address the potential of these nanostructures in the field of chemical sensing. We studied the PL response of III-N QDs upon pH-variations in liquid environment. The experimental results demonstrate that InGaN-quantum dot super-lattices (QDSL) are well suited for the fabrication of novel opto-chemical transducers. InGaN/GaN QDSLs were grown by plasma assisted molecular beam epitaxy on AlN-on-sapphire templates. Measurements in liquid environment were performed using a standard three electrode setup and PBS-buffer with HCl admixture as electrolyte. In order to obtain a deeper understanding of the underlying mechanisms, external electric fields were applied in liquid environment along the QDSL. They reveal a superlinear increase of the PL intensity by more than one order of magnitude when changing the bias voltage by only 600 mV. The underlying mechanism will be discussed in terms of an enhanced carrier confinement under applied bias using numerical simulations of the quantum confinement.

HL 71.5 Thu 11:15 POT 251

Observation of nuclear spin-polarization through electrical and optical injection of spin-polarized electrons in a spin-LED — •Pablo Asshoff, Gunter Wüst, Andreas Merz, Christoph Krämmer, Heinz Kalt, and Michael Hetterich — Karlsruhe Institute of Technology (KIT)

We present a detailed investigation of spin-polarization of quantum dot nuclei in a spin light-emitting diode by analyzing the Overhauser shift. Pumping of the nuclear spins is achieved with either electrical or optical excitation. Typical quantum dots exhibit a behavior where both excitation modes result in an asymmetrical Overhauser shift of comparable magnitude, which we analyze in a theoretical framework.

15 min. break

HL 71.6 Thu 11:45 POT 251

Off-resonant generation of electron spin coherence in InAs quantum dots — •Britt-Marie Meiners[1], Alexander Schwan[1], Stefan Spatzek[1], Steffen Varwig[1], Dmitri Yakovlev[1], Andre Henriques[2], and Manfred Bayer[1] — [1]Experimentelle Physik 2, U

Dortmund,D-44227 Dortmund, Germany — [2]Instituto de Física, Universidade de São Paulo, 05315-970 São Paulo, SP, Brazil

Studies of electron spin dynamics in solids have recently become a rapidly developing field of condensed-matter physics. We studied electron spin coherence in an inhomogeneous ensemble of singly charged (In,Ga)As/GaAs QDs by means of time-resolved techniques. The temporal evolution of the spin precession is measured by two-colour Faraday rotation and ellipticity.

Excitation energy was varied in an wide range up to 100 meV above the QDs resonances and even beyond the GaAs barrieer band gap, while the signal was detected on QD trion resonances. Surprisingly, we find that the electron spin coherence can be very efficiently excited even for strong detuning of the pump laser energy. This means that the electrons do not loose their spin coherence in the course of the energy relaxation of more than 100 meV.Also energy dispersion of the electron g-factors across the QD photoluminescence band has been measured and analyzed.

HL 71.7 Thu 12:00 POT 251

Faraday rotation and ellipticity signals of mode-locked spins in InGaAs quantum dots — •Steffen Varwig[1], Stefan Spatzek[1], Alexander Schwan[1], Mikhail M. Glazov[2], Irina A. Yugova[3], Dmitri R. Yakovlev[1], Dirk Reuter[4], Andreas D. Wieck[4], and Manfred Bayer[1] — [1]Experimentelle Physik II, TU Dortmund, D-44221 Dortmund, Germany — [2]A. F. Ioffe Physico-Technical Institute, 194021 St. Petersburg, Russia — [3]Institute of Physics, St. Petersburg State University, 198504 St. Petersburg, Russia — [4]Angewandte Festkörperphysik, Ruhr- Universität Bochum, D-44780 Bochum, Germany

We have studied the pump-probe Faraday rotation and ellipticity signals of electron spins in ensembles of singly charged (In,Ga)As/GaAs quantum dots.

For degenerate pump and probe we observe that the Faraday rotation signal amplitude first grows with increasing the time separation between pump and probe before a decay is observed for large temporal separations. The temporal behavior of the ellipticity signal, on the other hand, is regular: its amplitude decays with the separation. By contrast, for detuned pump and probe the Faraday rotation and ellipticty signals both exhibit similar and conventional behavior. The comparison between calculations and experimental data allows us to provide insight into the spectral dependence of the electron spin precession frequencies and extract the electron g factor dependence on energy [M. M. Glazov et al., Phys. Rev. B 82, 155325 (2010)].

HL 71.8 Thu 12:15 POT 251

Asymmetric optical nuclear spin pumping in a single uncharged quantum dot — •Florian Klotz[1], Vase Jovanov[1], Johannes Kierig[1], Emily Clark[1], Max Bichler[1], Gerhard Abstreiter[1], Heike Schwager[2], Geza Giedke[2], Martin Brandt[1], and Jonathan Finley[1] — [1]Walter Schottky Institut, Technische Universität München, Am Coulombwall 3, 85748 Garching — [2]Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Straße 1, 85748 Garching

We present the observation of a unipolar optically pumped dynamic nuclear polarization (DNP) in a single self assembled InGaAs quantum dot (QD). Electrons are resonantly excited in the QD and polarize the nuclear spin system via the hyperfine contact coupling, creating an Overhauser magnetic field. Remarkably, we observe a strong asymmetry in nuclear spin pumping for excitation of the two Zeeman-split neutral exciton states. Hereby, pumping the higher energy Zeeman branch effectively polarizes the nuclear spin system, whereas the lower energy branch does not. We also find a characteristic dependence of the observed DNP on the applied magnetic field where optically induced nuclear spin pumping is most efficient for an intermediate regime of 4 - 6 T, with a polarization of the nuclear spin bath of 53%. A theoretical model is developed that successfully explains the empirically found features based on the exciton level structure of the system.

HL 71.9 Thu 12:30 POT 251

Subnanosecond electrical charge control in a single InGaAs quantum dot — •Jörg Nannen[1], Wolf Quitsch[1], Sven Eliasson[1], Tilmar Kümmell[1], Karl Brunner[2], and Gerd Bacher[1] — [1]Werkstoffe der Elektrotechnik & CeNIDE, Universität Duisburg-Essen, Bismarckstr. 81, 47057 Duisburg — [2]Experimentelle Physik III, Universität Würzburg, Am Hubland, 97074 Würzburg

Single quantum dots (SQD's) are highly interesting candidates for future memory devices, which utilize single electrons or single holes as information carriers. The possibility to electrically and optically address SQD's in charge-tunable semiconductor heterostructures has led to different new concepts to inject, store and read-out the information of a single carrier in a SQD.

We use a high frequency adapted charge-tunable device in order to get electrical access to self-assembled single InGaAs quantum dots in the GHz regime [1]. Under high reverse bias we are able to optically prepare a single hole in the SQD. By the application of a subsequent high frequency voltage pulse, controlled electron tunneling into the SQD is achieved. We demonstrate that depending on the applied voltage either one or two electrons can tunnel into the SQD. It is shown that the electrons can be transported into and out of the quantum dot on time scales down to 300 ps.

[1] Nannen et al., Appl. Phys. Lett. 97, 173108 (2010)

HL 71.10 Thu 12:45 POT 251

Transient Differential Reflection Spectroscopy of Single Lateral InGaAs Quantum Dot Molecules — •Christian Wolpert[1,2], Lijuan Wang[3], Paola Atkinson[3], Armando Rastelli[3], Oliver G. Schmidt[3], and Markus Lippitz[1,2] — [1]Max-Planck Institut für Festkörperforschung, Stuttgart, Germany — [2]4. Physikalisches Institut, Universität Stuttgert, Germany — [3]Institut für Integrative Nanowissenschaften, IFW Dresden, Germany

We use a reflective all-optical pump-probe technique in order to characterize single lateral quantum dot molecules (QDMs), which are coupled by electron tunneling. By applying a bias voltage along the molecular axis one can control the coupling strength as well as the energies of the confined states. This becomes manifest in a strong dependence of the photoluminescence (PL) spectrum with respect to the bias voltage. The emission can be switched from one dot to the other as one passes the bias value at which the electron states are energetically aligned. Our interest lies in the understanding of this switching behavior. Differential reflection spectroscopy is well suited for this problem, as it does not depend on the emission of a photon but rather probes the QD's absorption directly. Furhermore one can capture the kinetics of the process by varying the delay time between pump and probe pulses and thus characterize the system beyond PL.

HL 71.11 Thu 13:00 POT 251

Time-resolved photoluminescence quenching measurements in InAs/GaAs quantum dots using terahertz laser pulses — •Jayeeta Bhattacharyya[1], Sabine Zybell[1], Martin Wagner[1], Manfred Helm[1], Mark Hopkinson[2], Luke R Wilson[2], and Harald Schneider[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]University of Sheffield, Sheffield, UK

Carrier dynamics and relaxation processes in self assembled quantum dots (QDs) are of fundamental interest due to their influences on the performances of optoelectronic devices. The intersublevel relaxation mechanisms influence the temporal response of the photoluminescence (PL). In this paper we present our work on time-resolved PL quenching measurements on QD ensembles using terahertz pulses. A Ti:Sapphire laser was used for interband excitation and the PL was measured by a streak camera. Terahertz pulses obtained from a Free Electron Laser were tuned to excite intersublevel transitions in the QDs which caused partial depletion of the electronic ground state resulting in quenching of the interband PL. The samples studied consisted of self-assembled InAs/GaAs QDs for which the intersublevel relaxation times varied from few ps to ns. Simultaneous time and wavelength resolved measurements enabled us to study the carrier redistribution by the terahertz pulse and their dynamics. The PL transients were fitted using exponential functions convoluted with a Gaussian system response and the PL quenching depth and recovery times were extracted. We will present a comparative analysis for different QD samples, with emphasis on the effect of intersublevel relaxation times on the carrier dynamics.

HL 72: Joint Session: Organic Electronics and Photovoltaics I

Time: Thursday 10:15–11:45 Location: GER 38

HL 72.1 Thu 10:15 GER 38

Structuring of Organic Conductors by Laser Ablation — •Alexander Esser, Moritz Schaefer, Jens Holtkamp, and Arnold Gillner — Fraunhofer ILT, Steinbachstraße 15, 52074 Aachen

PEDOT:PSS is a transparent organic polymer with a sheet resistivity of about 200ohm/sq. These attributes make it an ideal candidate for substituting ITO in organic LEDs and organic photovoltaic cells: making them fully organic, flexible, lightweight and cheap to produce. Organic thin-film photovoltaics are a low cost alternative to state of the art silicon and other inorganic semiconductor-based solar cells. OLEDs can be made more flexible without the use of transparent conducting oxides.

We present structuring of organic conductors by laser ablation from spin coated films of PEDOT:PSS. We have investigated ablation characteristics of PEDOT:PSS depending on laser wavelength in the deep UV and required fluence. The smallest structuring resolution by UV laser patterning has been found.

In further measurements we have determined the conductivity depending on layer thickness and structure size. Especially the influence of laser radiation on conductivity and electrical properties in the vicinity of the ablated area has been studied. Therefor we have performed AFM measurements as well as four-point probing.

HL 72.2 Thu 10:30 GER 38

Investigation of the origin of the memory effect in devices based on C_{60} — •Philipp Sebastian, Alexander Zakhidov, Björn Lüssem, and Karl Leo — Institut für Angewandte Photophysik, George-Bähr-Straße 1, 01069 Dresden, Germany

Besides their application in organic solar cells and organic light emitting diodes, organic semiconductors also show much potential in the field of flexible and lightweight electronics, such as organic memory. In particular, the development of organic memory devices has turned out to be challenging. So far, many different approaches for organic memory devices have been reported in literature [1].

In this contribution, we report on an organic memory device comprising SiO_2 layer on top of a indium tin (ITO) ground contact, followed by electron accepting C_{60} layer, a n-doped (Cs) 4,7-diphenyl-1,10-phenanthroline (BPhen) layer and an Al top electrode. IV measurements reveal a reproducible hysteresis of our devices with a maximum ON-OFF ratio of about one order of magnitude. The memory devices also demonstrate a remarkable switching cycle durability of more than 10^4 successfully applied write read erase read cycles, whereas the ON-OFF ratio remains constant at about 10. Retention times of several weeks underline a reasonable non-volatility. Further, the memory mechanism has been investigated by impedance spectroscopy. A hysteresis in capacitance-voltage measurements expresses the accumulation of electrons in the C_{60} and at the interface to the SiO_2 layer.

[1] J. Scott, L. Bozano, Advanced Materials 19, 1452 (2007)

HL 72.3 Thu 10:45 GER 38

Growth and morphology of aluminium contacts on P3HT films — •Gunar Kaune[1,2], Robert Meier[1], Ezzeldin Metwalli[1], Volker Körstgens[1], Kai Schlage[3], Sebastien Couet[3], Stephan V. Roth[3], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, Lehrstuhl für Funktionelle Materialien, James-Franck-Straße 1, 85747 Garching — [2]Martin-Luther-Universität Halle-Wittenberg, Institut für Physik, Fachgruppe Photovoltaik, Von-Danckelmann-Platz 3, 06120 Halle — [3]HASYLAB at DESY, Notkestraße 85, 22603 Hamburg

The characteristics of organic electronic devices are strongly influenced by the type and structure of the metal electrodes needed to inject or extract charge carriers. Therefore understanding of the metal growth process and its relation to the interactions at the metal-organic interface are necessary. We investigate the growth of an aluminium layer on the surface of a P3HT thin film by in-situ application of grazing incidence small-angle X-ray scattering (GISAXS). By subsequent modelling of the scattering data the structural parameters of the growing film are extracted and a growth process is found, which proceeds two-dimensional by stacking single atomic layers on top each other. This process results in a homogeneous film with a large contact area to the polymer and is explained by a strong chemical interaction between aluminium and P3HT, which suppresses clustering of the metal on the polymer surface. The diffusion of single aluminium atoms into the P3HT and the formation of an intermixing layer is revealed by X-ray reflectivity measurements.

HL 72.4 Thu 11:00 GER 38

Effect of high-k substrates on the photocurrent of organic semiconductors: Tailoring the Coulomb interaction — •Miriam Engel[1], Doru C. Lupascu[2], Niels Benson[1], and Roland Schmechel[1] — [1]Nanostrukturtechnik, Universität Duisburg-Essen, 47057 Duisburg — [2]Institut für Materialwissenschaft, Universität Duisburg-Essen, 45117 Essen

A major difficulty for organic photovoltaic cells is the dissociation of excitons into free charge-carriers. This is caused by high exciton binding energies, due to the low permittivity of the organic material. There are approaches to use acceptor-donator systems in the form of bulk-heterojunctions, which leads to successful exciton dissociations per volume. However, re-trapping may occur even after efficient charge-carrier separation due to Coulomb interaction (CI). Our aim is to use inorganic high-k materials to increase the exciton dissociation and to lower CI. In our proof of principle experiments devices are based on substrates with different permittivities. Pentacene is deposited as the active organic layer on them. Silver electrodes are used as top-contacts. For the electrical characterization we performed I(V) measurements in the dark and under illumination. Because of the known influence of the pentacene morphology on the mobility of the charge-carriers, we corrected the current under illumination by the dark current to obtain the pure contribution from the photo-effect. We obtained an improvement of the photocurrent using high-k substrates. The final goal is to transfer the layered system into an organic-inorganic composite system with high-k nanoparticles embedded in a photoactive organic matrix.

HL 72.5 Thu 11:15 GER 38

Organic pin-Diodes with Adjustable Current-Voltage Performance Applicable at Ultra-High-Frequencies — •Hans Kleemann, Christoph Schünemann, Paul Pahner, Alexander A. Zakhidov, Björn Lüssem, and Karl Leo — Institut für Angewandte Photophysik, Technische Universität Dresden, George-Bähr-Straße 1, 01069 Dresden, Germany

Organic diodes have been intensively studied during the past years and great progress has been achieved in the field of organic light-emitting diodes (OLEDs) and organic solar cells (OSC). Moreover, the development of other organic devices like thin film transistors, vertical transistors, memory arrays, and high-frequency diodes which are required for an electronic circuitry will allow the design and integration of complete organic electronics. In this contribution we present organic *pin*-diodes with adjustable forward and reverse current-voltage performance applicable in the ultra-high-frequency region. Key parameters to design these diodes are the doping concentration, the intrinsic interlayer thickness and the material properties. In this way the reversible backward breakdown can be shifted from $-3V$ to more than $-20V$ independently of the forward performance [1]. Due to the high rectification ratio (10^5) and since the diodes contain high mobility materials like pentacene and C_{60} we present high-frequency properties of these pin-diodes above 13.56MHz required for RFID-tags.

[1] H. Kleemann et al., Organic Zener Diodes: Tunneling across the Gap in Organic Semiconductor Materials, Nano Letters 2010, published online.

HL 72.6 Thu 11:30 GER 38

Photoinduced degradation process of Fir6 emitter molecules: a laser desorption/ionization time-of-flight mass spectrometry investigation — •Ines Rabelo de Moraes[1], Ruben Seifert[1,2], Sebastian Scholz[1,3], Björn Lüssem[1], and Karl Leo[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, George-Bähr-Str. 1, 01062 Dresden, Germany — [2]Von Ardenne Anlagentechnik GmbH, Plattleite 19/29, 01324 Dresden, Germany — [3]Fraunhofer-Institut für Keramische Technologien und Systeme, Winterbergstraße 28, 01277 Dresden, Germany

Phosphorescent Organic Light Emitting diodes (OLEDs) have attracted much interest for their potential application in the field of full color displays and as next generation of lighting sources. One of

the major problems related to the OLED technology is the short lifetime of the blue phosphorescent emitters. For improving the lifetime of the OLEDs a deep understanding of the intrinsic chemical degradation is required. Our work is focused on the photoinduced degradation process of single layer of the Fir6 molecule used as blue phosphorescent emitter by laser desorption/ionization time-of-flight mass spectrometry (LDI-TOF-MS). The LDI-TOF spectra collected at the laser intensity of 114 μJ/pulse indicate that the Fir6 molecule dissociates into [Ir(F2ppy)2]+ and [Fir6-(pyrazole)1]+. The reaction between the Fir6 fragments and the Fir6 molecule itself resulting in the formation of [Fir6+(pyrazole)1]+, and [Fir6-(pyrazole)1+Ir(F2ppy)2]+ could be observed as well. Additionally, the degradation processes of full processed OLEDs based on Fir6 emitter will be presented.

HL 73: Joint Session: Organic Electronics and Photovoltaics II

Time: Thursday 12:00–13:00 Location: GER 38

HL 73.1 Thu 12:00 GER 38

Improving the performance of phosphorescent light-emitting electrochemical cells without sacrificing stability — •Sebastian Meier[1,2], Wiebke Sarfert[2], David Hartmann[2], and Albrecht Winnacker[1] — [1]University of Erlangen-Nuremberg, Department of Materials Science, Chair VI: Materials for Electronics and Energy Technology, Martensstr. 7, 91058 Erlangen, Germany — [2]Siemens AG, Corporate Technology, GTF ORE, Günther-Scharowsky-Str. 1, 91058 Erlangen, Germany

Within the past few years a novel class of solution-processable solid-state organic light-emitting devices referred to as light-emitting electrochemical cells (LECs) has attracted considerable interest. Key feature of these devices is the existence of mobile ions within the active layer, which enable in-situ electrochemical doping with subsequent formation of a light-emitting p-n-junction. Due to their simple architecture and the use of air-stable electrodes LECs are regarded as an attractive approach for flexible large area lighting applications.

To compete with state of the art lighting technologies, however, the overall device performance of LECs has to be improved. For this purpose, an optimization of the device configuration and processing conditions as well as the use of a proper driving mode can be helpful. We show that the performance can be significantly enhanced due to modifications in the stack configuration (e.g. interfaces, layer thickness, cathode), processing conditions and by an adequate mode of operation without any losses in the device stability.

HL 73.2 Thu 12:15 GER 38

OLEDs under high current densities – transient electroluminescence turn-on dynamics and singlet-triplet quenching — •Daniel Kasemann, Hartmut Fröb, and Karl Leo — Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden, Germany

Organic solid state lasers have been intensively studied during the last decade due to the promising combination of versatile organic materials with the advantages of solid state emitters. Even though various optically pumped devices comprising different resonator types and material combinations have been shown, direct electrical pumping has not been achieved yet. The high excitation density needed in the active layer to achieve inversion is easily created by pulsed optical pumping, but additional losses prevent the excitation to reach the critical point when driven electrically.

To estimate the dimensions of these additional losses, we investigate full pin-OLEDs comprising the singlet emitter system DCM doped into Alq3 under high current densities. With the OLED active area reduced to $100x100\mu m^2$, these devices sustain current densities in the order of kA/cm^2 in pulsed operation. The results of time resolved electroluminescence (EL) measurements as well as power dependent emission spectra give promising insight into the behaviour of OLEDs under these extreme excitation conditions. Intense EL transient turn-on peaks on the nanosecond time scale can be explained by modelling the singlet and triplet population taking into account singlet-triplet and triplet-triplet quenching in the emission layer.

HL 73.3 Thu 12:30 GER 38

Investigation of the chemical and electronic structure of F_{16}CoPc from Monolayer to thick films by photoemission spectroscopy — •M. Grobosch and M. Knupfer — IFW Dresden, D-01069 Dresden, Germany

We have grown F_{16}CoPc with different film thickness under ultra high vacuum conditions on polycrystalline Au surfaces. By means of combined X-ray and ultraviolet photoemission spectroscopy (XPS, UPS) we have investigated the chemical and electronic structure of the F_{16}CoPc films. Within the first monolayers we could identify a charge transfer from the substrate on the F_{16}CoPc molecules. Our results indicate a clear difference in the valence band spectra for submonolayer thin and several nm thick F_{16}CoPc films. Furthermore, for F_{16}CoPc the ionization potential can be changed by the fluorination of the molecules from 4.8 eV for CoPc to 6.5 eV for F_{16}CoPc. The investigated heterointerface CoPc/F_{16}CoPc can be characterized as free from chemical reactions.

HL 73.4 Thu 12:45 GER 38

Influence of sample geometry and contact metal on the characterictics of organic field-effect transistors — •Dominik Klaus, Christopher Keil, Jan Hartel, and Derck Schlettwein — Institute of Applied Physics, Justus-Liebig-University Giessen, Germany. email:schlettwein@uni-giessen.de

Thin films of $F_{16}PcCu$ were prepared by physical vapor deposition on μ-structured electrode arrays of different contact metals. I/V-measurements of structures with various channel lengths showed a nonlinear injection of charge carriers for low Source-Drain-Voltages V_{DS}. Such behavior was especially found for μ-structures of small channel length indicating an influence of the contact behavior at the interface between metal electrode and organic semiconductor channel. A model was developed based on different aspects of an injection barrier, channel resistance and a parameter characterizing the geometry of the conducting channel which were separately used in the literature before. The model was used to determine the charge carrier mobility also for low values of V_{DS} and consistent values with those from typically evaluated large V_{DS} in the saturation regime were obtained. Implications for technical applicability of such transistors and general validity of such model are discussed.

HL 74: Joint Session: Quantum Optics of Solid State Photon Sources

Time: Thursday 10:30–13:00 Location: HSZ 02

HL 74.1 Thu 10:30 HSZ 02

Solid state single photon sources based on color centers in diamond — •Elke Neu[1], David Steinmetz[1], Christian Hepp[1], Janine Riedrich-Möller[1], Roland Albrecht[1], Jan Meijer[2], Martin Fischer[3], Stefan Gsell[3], Matthias Schreck[3], and Christoph Becher[1] — [1]Universität des Saarlandes, FR 7.2 Experimentalphysik, D-66123 Saarbrücken — [2]RUBION, Ruhr-Universität Bochum, D-44780 Bochum — [3]Universität Augsburg, Lehrstuhl für Experimentalphysik 4, D-86135 Augsburg

Color centers in diamond are promising candidates for practical single photon sources due to room temperature operation and superior photostability. We observe single photon emission from various color centers, produced either by ion-implantation or in-situ doping during CVD-growth. Optimum results are obtained from Silicon-Vacancy (SiV)-centers in isolated nano-diamonds grown on Iridium layers. These centers feature emission predominantly (80-90 %) into the narrow (0.7 nm) zero-phonon-line and high brightness with up to 4.8 Mcps at saturation, thus being the brightest single color centers to date [1]. We observe for the first time the fine structure of a single SiV-center at

cryogenic temperatures and perfom detailed spectroscopy investigating level structures, polarization and the influence of spectral diffusion. We discuss strategies for enhancing spectral and spatial emission properties by coupling color centers to micro-cavities e.g. fiber-based or photonic crystal cavities.

[1] E. Neu et al, ArXiv 1008.4736 accepted for publication in *New J. Phys.*

HL 74.2 Thu 11:00 HSZ 02

Quantum Light from a Whispering Gallery Resonator — •Josef Fürst[1], Dmitry Strekalov[2], Dominique Elser[1], Ulrik L. Andersen[1,3], Andrea Aiello[1], Christoph Marquardt[1], and Gerd Leuchs[1] — [1]Max Planck Institute for the Science of Light, Institute for Optics, Information and Photonics, University Erlangen-Nuremberg, Erlangen, Germany — [2]Jet Propulsion Laboratory, California lnstitute of Technology, Pasadena, USA — [3]Department of Physics, Technical University of Denmark, Kgs. Lyngby, Denmark

Optical subharmonic generation, also referred to as parametric down-conversion (PDC) is mediated by an optically nonlinear dielectric medium and connects an optical field to its subharmonic. In this process, one pump photon is converted to two subharmonic photons, called signal and idler. Enclosing the nonlinear medium in a cavity, the setup is called an optical parametric oscillator (OPO). We use a whispering gallery mode (WGM) resonator for our OPO. These WGM cavities offer high quality factors, that enhance the conversion efficiency of the nonlinear process. With a WGM resonator made from Lithium Niobate, we were able to show extremely efficient PDC in our WGM OPO. As the signal and idler photon pairs originate from one pump photon in PDC, they are strongly correlated in photon number. Investigating the quantum properties of the interacting light fields, while driving the OPO above the pump threshold, we observed nonclassical parametric light [1]. We plan to further investigate these quantum properties and will present the latest results.

[1] J. U. Fürst et al., arXiv:1008.0594v6 (2010)

HL 74.3 Thu 11:15 HSZ 02

Studying Photon Number Distributions of (NV-) Single-Photon Centres — •Waldemar Schmunk[1], Marco Gramegna[3], Giorgio Brida[3], Ivo P. Degiovanni[3], Marco Genovese[3], Helmuth Hofer[1], Stefan Kück[1], Lapo Lolli[3], Matteo G.A. Paris[4], Silke Peters[1], Mauro Rajteri[3], Mark Rodenberger[1], Andras Ruschhaupt[2], Emanuele Taralli[3], and Paolo Traina[3] — [1]Physikalisch-Technische Bundesanstalt, 38116 Braunschweig, Germany — [2]Leibniz Universtität Hannover, 30167 Hannover, Germany — [3]L'Istituto Nazionale di Ricerca Metrologica INRIM, 10135 Torino, Italy — [4]Universita degli studi di Milano, 20122 Milano, Italy

Reconstruction of the optical density matrix provides information on photon number distributions of unknown quantum states. In the present work we focus on the photon statistics of different nitrogen vacancies centres in diamond. For that purpose, the diagonal elements of the density matrix were experimentally determined by using a transition-edge sensor (TES), which produces an output pulse proportional to the number of photons absorbed and is therefore capable to resolve the photon number. Additional measurements were performed by on/off-statistics using avalanche photodetection assisted by a maximum likelihood estimation. From the data of the two photon number resolving techniques, values of the second order correlation function $g^{(2)}(t = 0)$ were determined and compared with the corresponding values measured by a Hanbury-Brown-Twiss interferometer. In the presentation, the three methods will be described and discussed in detail.

HL 74.4 Thu 11:30 HSZ 02

Realization of photonic crystal microcavities in single crystal diamond — •Janine Riedrich-Möller[1], Laura Kipfstuhl[1], Christian Hepp[1], Martin Fischer[2], Stefan Gsell[2], Matthias Schreck[2], and Christoph Becher[1] — [1]Universität des Saarlandes, Fachrichtung 7.2 (Experimentalphysik), Campus E2.6, 66123 Saarbrücken — [2]Universität Augsburg, Experimentalphysik IV, 86159 Augsburg

Microcavities in two-dimensional photonic crystal slabs allow to strongly confine light in volumes of about one cubic wavelength. They are expected to enable the realization of highly efficient emitters and control of spontaneous emission. Such photonic crystal microcavities are routinely fabricated in semiconductor materials. On the other hand, in recent years diamond has attracted significant interest as material for quantum information processing due to the extraordinary properties of optically active defect centers. These so called colour centers can be employed e.g. for cavity enhanced single photon sources that operate at room temperature or cavity-based atom-photon interfaces. We here investigate the fabrication of photonic crystal cavities in single crystalline diamond grown on an Iridium layer. We produce free-standing diamond membranes by dry-etching techniques and pattern them by focussed ion beam milling (FIB). We both realize 1D nanobeam cavities etched in a freestanding waveguide and 2D cavities with several missing holes in a triangular lattice. For the 2D cavities we experimentally obtain quality factors of Q = 300.

HL 74.5 Thu 11:45 HSZ 02

Photon blockade in a strongly coupled quantum-dot cavity system — •Thomas Volz, Andreas Reinhard, and Atac Imamoglu — Institute of Quantum Electronics, ETH Zurich, 8093 Zurich, Switzerland

A long-standing goal in the field of mesoscopic cavity quantum electrodynamics is the demonstration of photon blockade in a strongly coupled quantum-dot cavity system. While signatures of quantum correlations in resonant scattering have been observed previously, here we demonstrate for the first time strong photon blockade in such a device. Our system consists of a single self-assembled InGaAs quantum dot positioned at the field maximum of a photonic crystal L3 cavity (Q≈24000), leading to a coupling strength of g ≈ 150 μeV. In order to tune the cavity in resonance with the neutral quantum dot transition we employ a nitrogen tuning technique. We then probe the strongly coupled device with a resonant laser employing a cross-polarization technique to suppress the excitation-laser light. Due to strong classical blinking dynamics of the quantum dot we additionally use a repump laser to enhance the polariton signal. The photons scattered from the strongly-coupled system are analysed in a standard Hanbury-Brown-Twiss correlation setup. Due to the fast decay dynamics of the polaritons we carry out the experiment in pulsed mode. When the laser is resonant with the polaritons we observe strong antibunching - clear signature of photon blockade. Our results pave the way for the realization of non-linear photonic devices, such as a single-photon transistor or the quantum optical Josephson interferometer.

HL 74.6 Thu 12:00 HSZ 02

Deterministic Coupling of Individual Quantum Systems to Photonic Crystal Structures — Janik Wolters[1], •Andreas W. Schell[1], Günter Kewes[1], Nils Nüsse[2], Max Schoengen[2], Bernd Löchel[2], Michael Barth[1], and Oliver Benson[1] — [1]Nano-Optics, Institute of Physics, Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin — [2]Operator Centre Microtechnology, Helmholtz-Centre Berlin for Materials and Energy, Albert-Einstein-Straße 15, 12489 Berlin

The controlled and scaleable coupling of single quantum emitters to photonic crystal structures is one of the main challenges on the way towards integrated solid-state devices for optical quantum information processing. We tackle this problem by using a hybrid approach, which combines lithographic fabrication techniques with nanomanipulation methods, allowing the deterministic coupling of arbitrary emitters or other nanoscopic objects to the optical modes of photonic crystal cavities. Here we present recent experimental results on the controlled coupling of the zero phonon line emission from a single NV-center in a nanodiamond to such cavities. Our approach is well suited for the creation of improved single photon sources and also complex photonic devices with several emitters coupled coherently via shared cavity modes.

HL 74.7 Thu 12:15 HSZ 02

Deterministic Coupling of Single Nitrogen Vacancy Centres in Diamond Nanocrystals to Bowtie Nanoantennas — •Günter Kewes, Andreas Schell, Thomas Aichele, and Oliver Benson — Humboldt-Universität zu Berlin, Institut für Physik, Nanooptik

Surface plasmons polaritons provide the opportunity to concentrate electromagnetic energy in volumes much smaller than the wavelength of a photon with equal frequency, i.e. focussing beyond Abbe's limit, therefore giving large interaction between light and matter. This can be exploited in the construction of optical antennas which are designed to concentrate excitation energy at an emitter's location and further enhance the emitters output.

We present the coupling of single nitrogen vacancy (NV) centres in nanodiamond with a gold nanoantenna. The NV centres were systematically rearranged through AFM nanomanipulation around the

nanoantenna, resulting in maps of excited state lifetime reduction. These maps can give great insight into the near-field properties of such structures allowing for optimization of hybrid emitter-antenna systems. We observe that this reduction is not solely a fluorescence quenching effect, and an overall enchancement of the photon rate by a factor 2.2 was found.

HL 74.8 Thu 12:30 HSZ 02

Quantum key distribution using electrically triggered quantum dot-micropillar single photon sources — •Tobias Heindel[1], Markus Rau[2], Christian Schneider[1], Martin Fürst[2,3], Sebastian Nauerth[2,3], Matthias Lermer[1], Henning Weier[2,3], Stephan Reitzenstein[1], Sven Höfling[1], Martin Kamp[1], Harald Weinfurter[2,4], and Alfred Forchel[1] — [1]Technische Physik and Wilhelm Conrad Röntgen Research Center for Complex Material Systems, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Fakultät für Physik, Ludwig-Maximilians-Universität, 80799 Munich, Germany — [3]qutools GmbH, 80539 Munich, Germany — [4]Max-Planck-Institut für Quantenoptik, 85748 Garching, Germany

In 1984, Bennett and Brassard proposed a secret key-distribution protocol (BB84) that uses the quantum mechanical properties of single photons to avoid the possibility of eavesdropping on an encoded message. Due to the lack of efficient single photon sources however most quantum key distribution (QKD) experiments have been performed with strongly attenuated lasers. First experiments utilizing optically pumped solid state based single photon sources affirmed the great potential of QKD but still suffered from the drawbacks of this excitation scheme.

In this work we report on a QKD experiment using highly efficient electrically triggered quantum dot - micropillar single photon sources with $g^{(2)}(0)$-values below 0.5 and sifted key rates in the range of 10 kBit/s.

HL 74.9 Thu 12:45 HSZ 02

Generation of entangled photon pairs from the polariton ground state in a switchable optical cavity — •Adrian Auer and Guido Burkard — Department of Physics, University of Konstanz, D-78457 Konstanz, Germany

Intersubband cavity polaritons are the fundamental excitations of a planar microcavity embedding a sequence of doped quantum wells [1]. They arise from the interaction of cavity photons with intersubband excitations in the quantum wells. The ground state of the system, the polariton vacuum, contains a finite number of photons and, moreover, correlations of two photons having opposite in-plane wave vectors. It was proposed that these photons can be released by a non-adiabatic tuning of the light-matter interaction [1,2]. We theoretically investigate the polariton vacuum state in order to determine the entanglement between two photons, where we restrict our analysis to only two different modes. This could be carried out experimentally by a post-selective measurement. In this case we find that there is some entanglement for photon pairs having exactly opposite in-plane wave vectors which we quantify by the concurrence C. The amount of entanglement depends on the frequency of each photon and can be as high as $C = 0.7$ for experimentally reasonable values. The probability for a successful post-selection is determined to be on the order of 10^{-5}.

[1] C. Ciuti, G. Bastard and I. Carusotto, Phys Rev. B **72**, 115303 (2005).

[2] S. De Liberato, C. Ciuti and I. Carusotto, Phys. Rev. Lett. **98**, 103602 (2007).

HL 75: Joint Focussed Session: Theory and Computation of Electronic Structure: New Frontiers V

Time: Thursday 11:15–13:00 Location: TRE Phy

Topical Talk HL 75.1 Thu 11:15 TRE Phy

Electronic excitations in thin-film materials for solar cells: beyond standard density functional theory — •Silvana Botti — LSI, École Polytechnique, CNRS, CEA-DSM, Palaiseau, France — LPMCN, Université Claude Bernard Lyon 1, CNRS, Villeurbanne, France — European Theoretical Spectroscopy Facility

$Cu(In,Ga)(Se,S)_2$ (CIGS) thin-film solar cells have emerged as a technology that can challenge the current hegemony of silicon solar panels. CIGS conserve to a very high degree their electronic properties in a large non-stoichiometric range and are remarkably insensitive to radiation damage or impurities. Kesterites $Cu_2ZnSe(S,Se)_4$ have very similar electronic properties. Unlike CIGS, they are composed of abundant, non-toxic, less expensive chemical elements.

The origin of the exceptional electronic properties of these complex materials is still not completely understood, despite the large amount of experimental and theoretical work dedicated to that purpose. In particular, standard density functional theory (DFT) yields band structures in quantitative and qualitative disagreement with experiments. This is a serious problem when it comes to designing new materials for more efficient photovoltaic energy conversion.

I will discuss which theoretical approaches beyond standard DFT are reliable at a reasonable computational cost, together with the new physical insight that they allow to obtain.

HL 75.2 Thu 11:45 TRE Phy

What is the G^0W^0 band gap of ZnO? — Martin Stankovski[1], •Gabriel Antonius[2,1], David Waroquiers[1], Anna Miglio[1], Hemant Dixit[3], Patrick Rinke[4], Hong Jiang[4], Matteo Giantomassi[1], Xavier Gonze[1], Michel Côté[2], and Gian-Marco Rignanese[1] — [1]IMCN-NAPS, Université catholique de Louvain,B-1348 Louvain-la-Neuve, Belgium — [2]Département de physique, Université de Montréal , Montréal, Canada — [3]CMT-EMAT, Departement Fysica, Universiteit Antwerpen, Groenenborgerlaan 171, B-2020, Antwerpen, Belgium — [4]Fritz-Haber-Institut, Berlin-Dahlem, Germany

Zinc oxide is known to be a challenging system for G^0W^0 calculations. Its theoretical description has been widely discussed recently, and authors do not agree on the value of the band gap one should obtain from the G^0W^0 method. In an attempt to clarify the situation, we study the accuracy and the convergence properties of many schemes or approximations used at each level of the calculation, and show how different procedures may lead to very different conclusions. We first invest the sensitivity of the final band gap on the initial exchange-correlation potential used to generate the Kohn-Sham structure. We then study the behaviour of various plasmon pole models used to reproduce the dynamical properties of the dielectric matrix and discuss their validity for this particular system. Finally, the pseudopotential approach is compared to the PAW formalism, equivalent to an all-electrons calculation.

HL 75.3 Thu 12:00 TRE Phy

Global exploration of the energy landscape of solids on the ab initio level — •Klaus Doll[1,2], Aniket Kulkarni[1], Dejan Zagorac[1], J. Christian Schön[1], and Martin Jansen[1] — [1]Max Planck Institute for Solid State Research, D-70569 Stuttgart — [2]Institut für Math. Phys., TU Braunschweig, D-38106 Braunschweig

In the first step of rational synthesis planning, one needs to identify targets, i.e. (meta)stable crystal structures [1]. Simulated annealing has been shown to be one possibility to explore the respective energy landscape [2]. Our approach consists of a global search for structure candidates based on (up to very recently) empirical potentials, and subsequently a high accuracy local optimization. In order to overcome the limitation of employing potentials, ab initio energies are now used in all the stages [3-7].

After LiF [4] and BN [5], GeF_2 has been studied as an example of a system with stereochemically active lone pairs. Chain-like structures have been found. Further examples include CaC_2 with newly predicted structures at zero pressure as well as at high pressure [6], and PbS [7].

[1] M. Jansen, Angew. Chem. Int. Ed. 41, 3746 (2002); [2] J. C. Schön and M. Jansen, Angew. Chem. Int. Ed. 35, 1286, (1996); [3] J. C. Schön, K. Doll, M. Jansen, Phys. Status Solidi (b) 247, 23 (2010); [4] K. Doll, J. C. Schön, M. Jansen, Phys. Chem. Chem. Phys. 9, 6128 (2007); [5] K. Doll, J. C. Schön, M. Jansen, Phys. Rev. B 78, 144110 (2008); [6] A. Kulkarni, K. Doll, J. C. Schön, M. Jansen, J. Phys. Chem. B 114, 15573 (2010); [7] D. Zagorac, K. Doll, J. C. Schön, M. Jansen, in preparation

HL 75.4 Thu 12:15 TRE Phy

Ab initio calculations of electronic excitations: Collapsing spectral sums — •Arjan Berger[1,2], Lucia Reining[1,2], and Francesco Sottile[1,2] — [1]Laboratoire des Solides Irradiés, Ecole Polytechnique, CNRS, CEA-DSM, 91128 Palaiseau, France — [2]European Theoretical Spectroscopy Facility (ETSF)

We present a method for the evaluation of electronic excitations of advanced materials by reformulating spectral sum-over-states expressions such that only occupied states appear. All empty states are accounted for by one effective energy. Thus we keep the simplicity and precision of the sum-over-states approach while speeding up calculations by more than an order of magnitude. We demonstrate its power by applying it to the GW method, where a huge summation over empty states appears twice (screening and self-energy). We show the precision bulk silicon and argon. We then use it to determine the band structure and optical spectrum of the technologically important oxide SnO2. We will also show how our approach can be used to develop exchange-correlation kernels for time-dependent density-functional theory that are both accurate and computationally efficient.

HL 75.5 Thu 12:30 TRE Phy

Oxides – a challenge for (theoretical) spectroscopy — •Patrick Rinke[1], Hong Jiang[1], Matthias Scheffler[1], Andreas Greuling[2], Michael Rohlfing[2], Anderson Janotti[3], Emmanouil Kioupakis[3], and Chris G. Van de Walle[3] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Universität Osnabrück, Osnabrück — [3]University of California at Santa Barbara, CA

Oxides are of tremendous technological importance, yet challenging materials to characterize. In many cases the agreement between experimental and theoretical spectroscopy observed for other material classes has not been attained. We use rutile TiO_2 as an example to illustrate some of the problems. Many-body perturbation theory in the G_0W_0 approach based on density-functional theory in the local-density approximation gives a fundamental band gap of 3.3 eV in seemingly good agreement with the 3.3±0.5 eV measured in direct and inverse photoemission [1]. However, the lowest exciton computed in Bethe-Salpeter calculations for the optical spectrum is found at an energy of 3.21 eV, while optical experiments only give 3.03 eV [2]. Polaronic effects, i.e. the renormalization of the band edges due to electron-phonon coupling, reduce the band gap, but it remains a challenge to include the ionic contribution to the dielectric function, which can be substantial in oxides, in the G_0W_0 calculations and to incorporate both effects consistently into Bethe-Salpeter calculations. Another aspect to consider is the role of electron correlations. [1] Y. Tezuka *et al.*, J. Phys. Soc. Jpn.**63**, 347 (1994). [2] J. Pascual *et al.*, Phys. Rev. B **18**, 5606 (1978).

HL 75.6 Thu 12:45 TRE Phy

The surprising accuracy of semilocal functionals within density functional theory (DFT): A study of systems involving point defects — •Rampi Ramprasad[1], Patrick Rinke[2], and Matthias Scheffler[2] — [1]University of Connecticut, Storrs, USA; Fritz-Haber-Institut der MPG, Berlin, Germany — [2]Fritz-Haber-Institut der MPG, Berlin, Germany

The use of screened nonlocal exchange functionals within hybrid DFT computations is becoming practical, providing improved electronic structure descriptions [1]. However, the appropriate amount of nonlocal exchange (α) and the extent of screening (ω) to be used are still being explored. Here, we will focus on two properties relevant for systems containing point defects: charge transition levels and defect formation energies. By making the α and ω as variables, it will be shown that semilocal treatments of the exchange interaction for defects in Si and ZrO_2 yield charge transition levels that are quantitatively competitive with more involved nonlocal treatments, extending notions presented recently [2]. This implies that the difference in formation energies of neutral and charged defects remains a constant, although the formation energy itself may vary with the type of treatment. We have identified correlations between defect formation energies and features of the electronic structure of the defect-free parent material, allowing for extrapolations of the formation energy to the "correct" values.

[1] A. V. Krukau, et al, J. Chem. Phys. 125, 224106 (2006). [2] H. Komsa, et al, Phys. Rev. B 81, 205118 (2010).

HL 76: Nitride-based Green Lasers

Time: Thursday 11:45–13:15 Location: POT 51

HL 76.1 Thu 11:45 POT 51

Dynamics of (Al,In)GaN-based laser diodes — •Christian Hornuss, Wolfgang G. Scheibenzuber, Ulrich T. Schwarz, and Joachim Wagner — Fraunhofer-Institut für Angewandte Festkörperphysik, Tullastraße 72, D-79108 Freiburg

Understanding the dynamics of (Al,In)GaN-based laser diodes is essential for realizing ultra-short pulse lasers for biomedical imaging. We investigate the dynamic behavior of violet laser diodes above and below laser threshold. Relaxation dynamics above threshold are analyzed with high temporal and spectral resolution, as well as electroluminescence decay below threshold to determine the charge carrier lifetime. The experimental results are compared with rate equation simulations.By comparison of experimental and theoretical data we derive the carrier lifetime at threshold and the differential gain.

HL 76.2 Thu 12:00 POT 51

The loss mechanisms in green-emitting laser diodes — •Andreas Kruse[1], Moritz Brendel[1], Uwe Rossow[1], Hyonju Chauveau[2], Jean-Yves Duboz[2], and Andreas Hangleiter[1] — [1]Institut für Angewandte Physik, TU Braunschweig — [2]CRHEA-CNRS, Valbonne, France

While GaInN violet-blue laser diodes with high output power and long lifetimes are already commercially available, strong decrease in power performance by extending the emission wavelength beyond to 500 nm is observed. The aim of our investigations is to understand the limits of optical gain for green-emitting LDs. For this purpose we carried out optical gain measurements by using the variable stripe length method on laser structures grown on c-plane sapphire and GaN bulk substrates, in which various parameters such as number and thickness of quantum well(QW) as well as indium content in QW up to ca. 30% were varied. We focus our studies on two aspects: (1) the impact of defects on gain amplitude as well as inhomogeneous broadening of the gain spectra and (2) the influence of AlInN and AlGaN lower cladding layers on the optical confinement properties due to their different refractive index contrast. Our SQW laser structures emitting at longer wavelength show a net optical gain with internal optical losses smaller than $30cm^{-1}$. Moreover, an increase of the inhomogeneous broadening with increasing number of QWs is observed. For the laser structures with AlInN as lower cladding layer very high net optical gain is achieved compared to those with AlGaN cladding layers.

HL 76.3 Thu 12:15 POT 51

Growth and characterization of AlInN for cladding layers in long wavelength GaN based laser structures — •Ernst Ronald Buss[1], Heiko Bremers[1], Uwe Rossow[1], Egidijus Sakalauskas[2], Rüdiger Goldhahn[3], and Andreas Hangleiter[1] — [1]Institute of Applied Physics, TU Braunschweig, Mendelssohnstraße 2, Braunschweig — [2]Institute of Physics, TU Ilmenau, Weimarer Straße 32, Ilmenau — [3]Institute of Experimental Physics, Otto-von-Guericke-University Magdeburg, Universitätsplatz 2, Magdeburg

Cladding layers in actual GaN based laser structures usually consist of AlGaN, or AlGaN/GaN superlattices. Alloying GaN with AlN does always lead to strain in the whole compositional range, and the difference of the refractive indices of GaN and AlGaN is very small. In contrast AlInN can be grown matched to the a-lattice constant of GaN, so the stress in these structures can be minimized. Furthermore, the refractive index contrast is about 0.08 at 530 nm resulting in a better optical confinement in green laser structures.

The samples are grown by low pressure MOVPE. To optimize growth conditions parameters like temperature, reactor pressure and source fluxes has been varied. HRXRD measurements on samples with $x_{In} \approx 0.179$ show pseudomorphic growth and lattice matching for 845°C and 50mbar. Investigations by AFM exhibit smooth surfaces with low RMS roughnesses built up of small domains surrounding pits generated by crystal defects. The refractive index and the band gap energy are obtained from spectroscopic ellipsometry. Optical gain has

already been shown and first laser structures are realized.

HL 76.4 Thu 12:30 POT 51

Strain Relaxation Mechanisms in Green Emitting GaInN/GaN Laser Diode Structures — •Lars Hoffmann[1], Heiko Bremers[1], Holger Jönen[1], Uwe Rossow[1], Johannes Thalmair[2], Josef Zweck[2], Marco Schowalter[3], Andreas Rosenauer[3], and Andreas Hangleiter[1] — [1]TU Braunschweig, Institute of Applied Physics, Braunschweig, Germany — [2]Universität Regensburg, Institut für Experimentelle und Angewandte Physik, Regensburg, Germany — [3]Universität Bremen, Institute of Solid State Physics, Bremen, Germany

While GaN-based blue light emitting devices exhibit exceptionally large internal quantum efficiencies (up to 80% at room temperature) their green counterparts quickly become less efficient at longer wavelength ("green gap"). Green emitting laser diodes based on polar as well as non- and semipolar planes have also been demonstrated, but it remains increasingly difficult to push the emission to longer wavelength. Using Transmission Electron Microscopy (TEM) and X-ray diffraction (XRD) we have studied ultrathin (< 2nm) high indium content quantum well (QW) structures suitable for blue-green laser diodes. We investigate the mechanisms of relaxation and possible misfit dislocation generation in c-plane LD structures, partial relaxation and thermal degradation. We observe threading dislocations (TD) bending by several degrees at highly strained interfaces. The results indicate that larger lattice mismatch strain leads to larger bend angles. Furthermore, if two of those TDs are crossing each other, they could annihilate and reduce the TD density.

HL 76.5 Thu 12:45 POT 51

Growth of AlGaN stripes with semipolar side facets as waveguide claddings for semipolar laser structures — •Robert Anton Richard Leute[1], Kamran Forghani[1], Frank Lipski[1], Ferdinand Scholz[1], Ingo Tischer[2], Benjamin Neuschl[2], and Klaus Thonke[2] — [1]Institut für Optoelektronik, Universität Ulm — [2]Institut für Quantenmaterie / Gruppe Halbleiterphysik, Universität Ulm

Selective area growth of group III nitrides allows the epitaxy of semipolar facets with reduced piezoelectric field on 2-inch sapphire substrates. Additionally, the 3D growth of stripes, pyramids or the like enables us to manipulate the extraction and propagation of light by changing the surface topology. LEDs grown on GaN stripes with $\{11\bar{2}2\}$ facets and GaN stripes with $\{10\bar{1}1\}$ facets have been published. The fabrication of laser structures with resonators along the stripes depends critically on the controlled growth of a waveguide cladding for optical confinement, typically realized by AlGaN layers. However, the growth parameters of AlGaN are challenging for selective epitaxy. The high growth temperature promotes lateral growth, leading to the emergence of an undesirable c-plane facet, whereas the reduced selectivity of the mask material for Al atoms leads to polycrystalline growth on masked areas. We investigate the selective growth of AlGaN with Al contents up to 10% with structured SiO_2 and SiN_x masks. The influence of mask geometries (stripes $\parallel m$ and $\perp m$, variable opening sizes and periods) on topology, material quality and Al incorporation is examined. Therefore, we present SEM investigations, spatially resolved cathodoluminescence as well as low temperature photoluminescence.

HL 76.6 Thu 13:00 POT 51

Electroluminescence from InGaN quantum dots in a monolithically grown GaN/AlInN cavity — •Heiko Dartsch[1], Christian Tessarek[1], Stephan Figge[1], Timo Aschenbrenner[1], Carsten Kruse[1], Marco Schowalter[2], Andreas Rosenauer[2], and Detlef Hommel[1] — [1]University of Bremen, Institute of Solid State Physics - Semiconductor Epitaxy — [2]University of Bremen, Institute of Solid State Physics - Electron Microscopy

InGaN quantum dots (QDs) and their implementation into the micro cavity of a vertical distributed Bragg reflector (DBR) resonator are the key elements to achieve single photon emission required for quantum cryptography. However, the epitaxial overgrowth of InGaN QDs is challenging because they are easily destroyed by elevated temperatures. For this reason a common approach is the fabrication of a hybride cavity structure by non epitaxial deposition of a dielectric top DBR.

We will present the first successful implementation of electrically driven InGaN QDs into a monolithic GaN/AlInN cavity structure fully epitaxial grown by metal organic vapor phase epitaxy. Therefore a single layer of InGaN QDs has been embedded in a n- and p-type doped 5λ GaN cavity surrounded by a 40 fold bottom- and a 10 fold GaN/AlInN top-DBR. Electroluminescence of the InGaN QDs was achived by the application of intra cavity contacts. Optical and structural properties of the device will be discussed.

HL 77: Joint Session: Organic Electronics and Photovoltaics III

Time: Thursday 14:00–16:00 Location: GER 38

HL 77.1 Thu 14:00 GER 38

Influence of the thickness dependent structural order on the electrical potential distribution in the channel of OFET's — Richa Sharma, Benedikt Gburek, •Torsten Balster, and Veit Wagner — School of Engineering and Science, Jacobs University Bremen, Campus Ring 1, 28759 Bremen

Soluble organic semiconductors often exhibit a charge carrier dependent mobility and energetic disorder, which typically vary with layer thickness. In this study, organic field effect transistors (OFET) with different thicknesses of regio-regular P3HT as semiconductor and PMMA as gate-insulator on PET foils are investigated and analyzed statistically.

The mobility, which is very low for layers up to 10 nm, increases with the thickness over two orders of magnitude and saturates after 30 nm. This behavior is analyzed according to the Vissenberg-Matters model (VM) of the charge carrier density dependent mobility $\mu = \mu_0((V_{GS} - V_{th})/V_{aa})^{\gamma}$, where the disorder parameter γ decreases from 1.7 to 0.8 over the examined thicknesses proving the higher energetic disorder for thinner films. Increasing domain sizes in phase contrast AFM pictures confirm these findings.

The potential distribution within the channel, which has been measured by additional sense electrodes, is used to determine the potential steps at source and drain contact applying the VM model. The influence of the disorder parameter on the potential distribution is elucidated.

HL 77.2 Thu 14:15 GER 38

Local analysis on organic field effect transistors — •Harald Graaf[1], Franziska Lüttich[1], Daniel Lehmann[2], Dietrich R.T. Zahn[2], and Christian von Borczyskowski[1] — [1]Optische Spektroskopie und Molekülphysik, Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz — [2]Halbleiterphysik, Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz

Within the last decade the interest on organic electronics increased tremendously and reaches even industrial applications. Nevertheless, there are still a lot of open questions concerning e.g. the charge transport in the organic materials especially on a local scale. Here the focus is on the influence of trap states at interfaces and within the bulk provided e.g. by grain boundaries. By the combination of diverse measurement techniques a deeper insight and a better understanding of the local properties of the materials can be obtained.

We will present recent results on organic materials gained by electrical DC-measurements, Kelvin probe force microscopy on operating devices, optical and topographical investigations. By the results one obtain on the one hand information about the orientation and the coupling of the chromophoric systems (which is responsible also for the charge transport) within the film. On the other hand the electrical and electronical characterizations permit insight in the properties especially at the relevant interfaces (electrode/semiconductor and semiconductor/isolator) and on the local transport characteristics of the charges.

HL 77.3 Thu 14:30 GER 38

Dynamics of optically induced instabilities in P3HT field-effect transistors — •Lorenz Kehrer, Christian Melzer, and Heinz von Seggern — Electronic Materials Department, Institute of Materials Science, TU Darmstadt, Petersenstr. 23, 64287 Darmstadt

The development of stable printed organic electronic circuits for every-

day use remains a great challenge. Under ambient conditions electrical instabilities may be driven by external influences such as gases, humidity or light. Here, we report on a light induced instability of state of the art poly(3-hexylthiophene) field-effect transistors under ambient atmosphere. By illuminating p-type, top-gate poly(3-hexylthiophene) field-effect transistors in depletion mode with visible light a substantial shift of the threshold-voltage and an increase in the off-current by three orders of magnitudes has been observed. Both phenomena, the threshold-voltage shift and the increase of the off-current, require the presence of oxygen and are persistent for days at room temperature. The origin of this long lasting instability is attributed to traps which are induced in the semiconductor by oxygen incorporation and subsequent optical filling of these traps by electrons. This charge trapping shifts the threshold voltage and increases the doping level. The temporal evolution of the optically induced changes in the OFET characteristics under different thermal conditions will be highlighted. Such an instability is crucial for logic elements where OFETs are normally hold in the off-state, thus in depletion. Under these operational conditions light induces the aforementioned change in the OFET characteristics affecting the functionality of the employed logic circuit substantially.

HL 77.4 Thu 14:45 GER 38

Towards a biosensing device based on pentacene transistors — •Martin Göllner, Martin Huth, and Bert Nickel — Department für Physik und CeNS, Ludwig-Maximilians-Universität, Geschwister-Scholl-Platz 1, 80539 München, Deutschland

Organic semiconductors can be processed on flexible, biocompatible plastic substrates and offer a soft and non-toxic ambience to living cells (e.g. neurons). Therefore organic thin film transistors (OTFTs) are considered as promising candidates for the next generation of biosensing devices. However, most high mobility organic semiconductors have a limited lifetime in physiological aqueous conditions. For a stable device operation it is necessary to suppress redox reactions with the electrolyte and so called leakage currents.

For this purpose we recently used a thin alkane layer to passivate a pentacene thin film transistor, enabling the operation in an aquatic environment for many hours [1]. A transducer based on a capped OTFT should be sensitive to subtle changes of the charges at the interface to the electrolyte. Ongoing measurements indicate that it is possible to change the source-drain current of the transistor by changing the electrochemical potential of the electrolyte by a few mV. This suggests that the device should also be sensitive to the adsorption of charged molecules and the activity of cells. The sensing mechanism is discussed.

[1] M. Göllner, M. Huth, B. Nickel, Advanced Materials 22, 4350-4354 (2010)

HL 77.5 Thu 15:00 GER 38

Electronic properties of spiro-compounds: A combined photoelectron spectroscopy and energy-loss spectroscopy study — •B. Mahns[1], M. Grobosch[1], T. Saragi[2], J. Salbeck[2], and M. Knupfer[1] — [1]IFW Dresden, Helmhotzstrasse 20, 01069 Dresden, Germany — [2]Macromolecular Chemistry and Molecular Materials, Institute of Chemistry, Department of Science and Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, Heinrich-Plett-Strasse 40, 34132 Kassel, Germany

The electronic properties of three different spiro-compounds have been investigated using a combination of photoelectron spectroscopy and electron energy-loss spectroscopy. The compounds are characterized by parts with different electron affinity, and we demonstrate their variation in ionization potential and optical gap. Moreover, our data give a measure of the occupied density of states as well as the dielectric properties in a wide energy range.

HL 77.6 Thu 15:15 GER 38

Spatially resolved photoresponse of pentacene thin film transistors: slow component by trap release — •Christian Westermeier, Matthias Fiebig, and Bert Nickel — Department für Physik und CeNS, Ludwig-Maximilians-Universität München

Organic thin film transistors (OTFTs) have witnessed continuous improvement over the past years and become suited for widespread application. Small organic molecules, such as pentacene, are often used for OTFTs, since their ordered thin-film structures result in high charge carrier mobilities. Although pentacene has attracted high interest of research, the electronic transport and photoresponse mechanisms and their relation to the morphology and trap densities of the polycrystalline film are not well understood.

We perform spatially and time resolved photoresponse measurements of pentacene TFTs using a laser scanning setup for local illumination with varying laser frequencies and a photon energy of 1.96 eV. The excitation corresponds to the upper Davydov component of the S_1 state of pentacene. Besides the absorption in the 50 nm pentacene film, a significant fraction of the laser light is absorbed in the Si wafer upon reflection. Since the excitons in pentacene decay mostly radiationless, both contributions result in local heating. We argue that heat assisted detrapping results in the release of holes from trap states, thus the effective charge carrier mobility increases locally. These bolometric effects are associated with a slow contribution to the photoresponse on a millisecond timescale and with an inhomogeneous structure presumably corresponding to the trap density distribution in pentacene.

HL 77.7 Thu 15:30 GER 38

Contact properties of organic PCBM field effect transistors analyzed by combined photoemission spectroscopy and electrical measurements — •M. Grobosch[1], I. Hörselmann[2], J. Bartsch[2], S. Scheinert[2], M. Knupfer[1], and G. Paasch[1] — [1]IFW Dresden, D-01069 Dresden, Germany — [2]Technical University Ilmenau, D-98684 Ilmenau, Germany

Source/drain contacts in OFETs based on a solution prepared modified PCBM were characterized by combined X-ray and ultra violet photoemission spectroscopy (XPS, UPS) and electrical measurements of the OFET. Thereby the sample preparation for the different measuring principles has been realized in parallel, differing only in the layer thickness of the polymer. By means of UPS a reduced work function could be demonstrated for differently prepared, sputtered, and as-received Au and Al contacts in agreement with previous publications [1]. On top of the Al contacts a natural AlO_x layer could be identified. For both the PCBM/Au and PCBM/Al systems from UPS a hole injection barrier of 1.8 eV has been determined. Considering the gap of 2.0 eV [2] the electron injection barrier would be the same of 0.2 eV. In contrast to these identical barriers as following from UPS, the OFET currents with Au and Al contacts differ by more than two orders of magnitude. A possible origin of this striking discrepancacy will be presented. [1] M. Grobosch et al., Adv. Mater. 19 (2007) 754. [2] Z.-L. Guan et al., Organic Electronics 11 (2010) 1779.

HL 77.8 Thu 15:45 GER 38

Dye directed changes in ZnO matrices in organic/inorganic photovoltaic systems — •Harald Graaf[1], Franziska Lüttich[1], Mirko Kehr[1], Christian Dunkel[2], and Torsten Oekermann[2] — [1]Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz — [2]Institut für Physikalische Chemie und Elektrochemie, Leibniz Universität Hannover, 30167 Hannover

Dye-sensitized photovoltaic cells with zinc oxide (ZnO) as the inorganic semiconductor and organic dye molecules as the sensitizer are well-known devices with high efficiency. Such cells are prepared by electrochemical deposition of an aqueous zinc salt solution including dye molecules. After deposition the dye is desorbed to obtain a porous ZnO network followed by re-adsorption of the dye as a sensitizer. The dye molecules influence the crystal orientation of the ZnO as they tend to physisorb on different crystal surfaces.

We will present recent results on as-deposited and desorbed dye/ZnO films obtained by different analytic methods: X-ray investigations, Scanning Electron Microscopy, Atomic and Kelvin probe force microscopy and optical spectroscopy. This allows a deep insight into the dye/semiconductor system, which is necessary to improve the efficiency of such devices. Here the focus is on crystal orientation, morphology and work function of the ZnO matrix. Also the arrangement of the dye molecules in as well as on top of the as-deposited films and the band edge of the zinc oxide is accessible.

HL 78: Joint Session: Organic Electronics and Photovoltaics IV

Time: Thursday 16:15–17:45 Location: GER 38

HL 78.1 Thu 16:15 GER 38

Energy level alignment at polymer/PCBM heterojunctions under operating conditions in an organic photovoltaic cell structure — •Johannes Frisch[1], Andreas Wilke[1], Patrick Amsalem[1], Jens Niederhausen[1], Antje Vollmer[2], and Norbert Koch[1] — [1]Humboldt-Universität zu Berlin, Institut für Physik, Brook-Taylor-Str. 6, D-12489 Berlin, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie - Speicherring BESSY II, Berlin, Germany

For heterojunction organic photovoltaic cells (OPVCs) generally vacuum level alignment at the donor/acceptor interface is assumed. In contrast, it has been shown that interface dipoles might occur at organic/organic heterojunctions, which questions the assumption of vacuum level alignment at OPVC interfaces. Therefore, we investigated the energy level alignment at the poly(3-hexylthiophene)/1-(3-methoxycarbonyl)propyl-1-phenyl[6.6]C61 (P3HT:PCBM) heterojunctions with ultraviolet photoelectron spectroscopy (UPS). The valence band of P3HT shifted to higher binding energy by 0.45 eV after deposition of PCBM, while vacuum level alignment was found. This observation would imply an increase of the P3HT ionization energy upon interface formation, which is usually not considered in simple models. The observed phenomenon can be explained either by a structural rearrangement of the donor polymer layer upon acceptor deposition or by surface photovoltage effects that occur during photoemission, which charges the P3HT layer positively whereas negative charges are collected in the PCBM layer.

HL 78.2 Thu 16:30 GER 38

New Imaging Approach for Organic Bulk Heterojunction Solar Cells Using Selective Dissolution — •Bettina Friedel, Bruno Ehrler, and Neil C. Greenham — University of Cambridge, Cavendish Laboratory, JJ Thomson Avenue, CB30HE Cambridge, United Kingdom

Morphology in organic photovoltaic devices is one of the most vital and most studied issues for optimum functionality, especially concerning bulk heterojunctions. However, it is always a challenge to control its microscopic structure towards improved exciton dissociation and charge transport. To get an insight into this microstructure usually a combination of various imaging techniques together with spectroscopic methods is used. Unfortunately imaging on all-organic structures is rather challenging since the high similarity of the carbon-based materials gives low contrasts and makes them hard to distinguish. We will present a new imaging approach for organic blends, based on a temperature controlled selective dissolution technique. We will demonstrate on two systems (polymer-polymer and polymer-PCBM) that this technique allows to selectively remove one of the components from a bulk heterojunction, leaving a scaffold of the other component, which can be easily characterized by high resolution imaging, due to the higher air-material contrast. Further the technique allows us to quantify the disordered fraction of semicrystalline components in a blend structure, which is valuable information for matters of charge transport. These new structural insights help understanding the changes in PV performance e.g. following thermal treatments or using solvent additives.

HL 78.3 Thu 16:45 GER 38

improvement of the CdSe/P3HT solar cells efficiency due to surface modification of the CdSe nanoparticles by alkylamine treatments — •nikolay radychev, irina lokteva, holger borchert, joanna kolny-olesiak, and jürgen parisi — institute of physics, energy and semiconductor research laboratory, university of oldenburg,oldenburg,germany

Semiconductor quantum dots (QDs) continue to attract immense attention because of their size-dependent optical, physical, and chemical properties which causes them to be a promising material for hybrid solar cell applications. Meanwhile QDs in a polymer matrix have to be stabilized by organic ligands that show significant influence on the charge transport and charge separation processes. Surface modification procedures such as stabilizing ligand exchange or crosslinking the QDs can enhance the efficiency of the hybrid blends. In the present work, as-synthesized QDs, initially capped with oleic acid, were subjected to ligand exchange procedures with the intention to obtain nanoparticles capped by butylamine ligands. Detailed characterisations of the butylamine stabilized QDs based on thermogravimetric analysis, nuclear magnetic resonance and transmission electron microscopy are shown. Laboratory solar cells with blends of the butylamine capped CdSe QDs and poly-3-hexylthiophene (P3HT) as active layer were prepared and investigated by current-voltage and external quantum efficiency measurements. Energy conversion efficiency of about 2% was obtained. The fundamental reasons of the efficiency enhancement were analyzed

HL 78.4 Thu 17:00 GER 38

Comparison of the operation of standard and inverted P3HT:PCBM solar cells — •Thomas J.K. Brenner, Yana Vaynzof, Zhe Li, Dinesh Kabra, Richard H. Friend, and Christopher R. McNeill — Cavendish Laboratory, Department of Physics, University of Cambridge, JJ Thomson Ave., Cambridge CB3 0HE, United Kingdom

Inverted organic solar cells have attracted recent attention due to their enhanced environmental stability compared to the standard device architecture. However to date inverted cells have shown poorer efficiencies compared to the standard geometry. To clarify the origin of this behaviour, we have investigated inverted (ITO/ZnO/P3HT:PCBM/ WO3/Ag) and regular (ITO/PEDOT:PSS/P3HT:PCBM/Al) P3HT:PCBM solar cells with different active layer thickness. Using white light bias external quantum efficiency and photocurrent transient measurements, we propose an explanation for the reduced performance of inverted cells. Whereas for inverted devices high EQEs of up to 68% are measured under low light intensities (3 mW/cm^2), EQE drops with increasing white light bias (up to 140 mW/cm^2) down to 20%. This drop is accompanied by a severe distortion of the spectra. For increased thickness (from 90 nm to 550 nm), the drop and shape change can be seen at lower intensities. For regular devices we also observe a drop in EQE, however they still resemble the absorption spectrum showing minor distortion. Unbalanced charge transport and/or unfavourable vertical phase separation in inverted devices are presented as likely causes of the observed behaviour.

HL 78.5 Thu 17:15 GER 38

Organic Photovoltaic Cells with Pentacene Nanocolumn Arrays — •Shuwen Yu, Peter Schäfer, Jürgen P. Rabe, and Norbert Koch — Institut für Physik, Humboldt-Universität zu Berlin, Brook-Taylor-Str. 6, 12489 Berlin, Germany

Highly ordered pentacene nanocolumn arrays were fabricated by glancing angle deposition (GLAD) on indium tin oxide (ITO) substrates. The nanocolumn diameter was set to 100-150 nm as revealed by scanning electron microscopy and atomic force microscopy. Interdigitated bulk heterojunction photovoltaic cells (OPVCs) were formed by spincoating [6,6]-phenyl-C61-butyric acid methyl ester (PCBM) as the acceptor material onto the pentacene nanocolumn film. Bathocuproine (BCP) was deposited on top of PCBM as exciton blocking layer. The conversion efficiency of nanocolumn-based OPVCs was significantly higher compared to planar heterojunction OPVCs of the same materials. Further device performance improvement was achieved through employing a thin pentacene seed layer before GLAD, which promoted PCBM solution infiltration between pentacene nanocolumns.

HL 78.6 Thu 17:30 GER 38

Performance and stability of P3HT/PCBM bulk heterojunction organic solar cells — •Nivedita Yumnam, Sidhant Bom, and Veit Wagner — School of Engineering and Science, Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

Organic photovoltaic cells are promising candidates for large-area, low-cost production of solar cells. However, the low stability in conjunction with their medium performance is one of the major drawbacks in comparison to their inorganic counterparts. In this investigation environmental conditions for degradation of bulk heterojunction P3HT/PCBM solar cells are systematically analyzed over a period of one week. Devices were prepared by spin coating from different compositions of P3HT and PCBM in Chlorobenzene (C_6H_5Cl). Performance parameters, efficiency and I-V characteristics were determined in a N_2 glove box showing optimized efficiency for a 1:1 ratio. Degradation behavior in N_2 atmosphere, vacuum and solvent-enriched atmosphere (Chlorobenzene) showed best results for vacuum stored solar cells while

for solvent-enriched atmosphere rapid degradation was observed. Remarkable degradation (open-circuit voltage and short-circuit current reduced to 90% and 60% after one week) was also found for N_2 atmosphere of the glove box used for the solar cell production. Residual solvent vapor left dispersed in the atmosphere of the glovebox after the spin coating process is identified as an important parameter of this degradation.

HL 79: Photovoltaics: Mainly Silicon

Time: Thursday 14:30–17:15 Location: FOE Anorg

HL 79.1 Thu 14:30 FOE Anorg

Microstructuring of silicon with femtosecond laser pulses — •Waldemar Freund, Jan P. Richters, Tobias Voss, and Jürgen Gutowski — Institute of Solid State Physics, Semiconductor Optics Group, University of Bremen

Silicon structured with ultrashort laser pulses which is called "black silicon" due to its dark appearance has been a field of intense studies in recent years. It exibits a nearly uniform absorptivity beyond 90% in the whole visible to near-infrared spectral region. Therefore, it is a promising material for applications in solar cells and photo diodes.

In this talk a brief introduction of microstructuring of silicon with ultrashort laser pulses will be given. Structuring is carried out in a sulfurhexafluoride (SF_6) atmosphere, which simultaneously allows doping of the silicon with sulfur far above the solubility limit. The structuring leads to a specific quasiperiodic surface morphology at which incident light is reflected multiple times. Thus light absorption in the silicon is considerably enhanced. The extremely high doping with sulfur results in the formation of a distinct defect band which is the origin of high absorptance in the near infrared. Furthermore, sulfur acts as a donor in silicon. Hence, microstructuring of p-doped silicon in SF_6 atmosphere leads to the formation of a p-n^+ junction. This is an important step towards the fabrication of efficient solar cells and photo diodes with increased infrared sensitivity on base of easy-to-produce black silicon.

HL 79.2 Thu 14:45 FOE Anorg

Potential of silicon nanoparticles for photovoltaic applications — •Martin Meseth[1], Pawel Ziolkowski[2], Nils Petermann[3], Gabi Schierning[1], Niels Benson[1], Hartmut Wiggers[3], and Roland Schmechel[1] — [1]University of Duisburg-Essen, Nanostrukturtechnik, 47057-Duisburg — [2]DLR (German Aerospace Center), Institute of Materials Research, 51147-Köln — [3]University of Duisburg-Essen, Institut für Verbrennung und Gasdynamik, 47057-Duisburg

To reduce costs per watt of commercial photovoltaics (PVs) silicon nanoparticles are considered as an interesting alternative to conventional PV thin films. To proof the principle concept a pn-junction is created by spark plasma sintering of highly p- and n-doped ($\approx 10^{20} cm^{-3}$) Si nanoparticles with diameters in the range of $10nm$ to $50nm$. While SEM-investigations of these sintered samples show still a nanocrystalline structure, density measurements result in a high compaction value of up to 95% of crystalline Si. The structural formation of a pn-junction is proven using microscopic Seebeck-coefficient- and EDX-measurements, each showing a clear separation of the respectively doped materials and a sharp interface in between. Furthermore electrical DC-characterization is done showing a clearly rectifying behaviour. This leads to the conclusion that this pn-junction behaves also electrically as a diode. Further, a small photovoltaic effect under illumination with a $1000W$-tungsten lamp indicates the presence of a built-in field between the p- and n-region.

HL 79.3 Thu 15:00 FOE Anorg

Simulation of polycrystalline silicon thin film solar cells - model calibration and sensitivity analysis — •Ana-Maria Teodoreanu, Caspar Leendertz, Tobias Sontheimer, and Bernd Rech — Helmholtz-Zentrum Berlin, Kekuléstr. 5. 12489 Berlin

To gain a better insight into the efficiency-limiting processes in polycrystalline silicon (poly-Si) thin film solar cells, we developed a simulation model for the J-V characteristics and minority carrier lifetime based on experimental results using the numerical 1D simulation program AFORS-HET. The calibration of the model has been achieved through simultaneously fitting the measured dark and light J-V curves of twelve poly-Si thin film minimodules with dissimilar thickness and absorber doping concentration. Effective defect density, capture cross section products of $10 \ldots 100 cm^{-1}$ have been determined in the poly-Si absorber by this procedure. Transient photoconductance decay measurements of the poly-Si absorbers have also been conducted in the low injection regime ($4.5 \cdot 10^{14} cm^{-3}$). High lifetimes of $100\mu s$ have been found which can be explained within our simulation model by field effect passivation. Furthermore simulations indicate that this field effect leads to a strong injection-dependence of carrier lifetime in the operation range of the solar cell. The sensitivity analysis performed with our calibrated model shows that the defects in the absorber layer are crucial for the cell efficiency. Thus, the improvement of the emitter and back surface field layers becomes important only if the absorber itself is of better quality. Moreover we discuss the optimum absorber thickness subject to different doping levels and absorber defect densities.

HL 79.4 Thu 15:15 FOE Anorg

Numerical 3D-Simulation of Micromorph Silicon Thin Film Solar Cells — •Stefan Geissendörfer, Jürgen Lacombe, Karsten von Maydell, and Carsten Agert — EWE-Forschungszentrum für Energietechnologie e.V. NEXT ENERGY, Carl-von-Ossietzky-Str. 15, 26129 Oldenburg

In this contribution 3-dimensional simulations of micromorph silicon thin film solar cells, which have a tandem structure consisting of amorphous and microcrystalline subcells, will be presented. The variety of different active layers leads to a very complex structure. Additionally, randomly textured surfaces and interfaces have to be taken into account. Our goal is to create physical models to describe the coupled optical and electrical behaviour of the whole structure in three dimensions to determine the theoretical limits and dominant material parameters. To simulate solar cells with rough interfaces, the surfaces topography was measured via atomic force microscopy (AFM) and transferred to the commercial software Sentaurus TCAD from the company Synopsys. The virtual structure includes layer thicknesses and optoelectronic parameters. Results of the space resolved optical generation rates by using the optical solver "Raytracer" will be presented. The space resolved optical generation rate inside the semiconductor layers depends on the structure of the TCO interface. Therefore, regions with higher charge charrier densities can be observed which has an influence on the current transport through the stack. These investigations and the influence to the IV characteristic will be presented.

HL 79.5 Thu 15:30 FOE Anorg

Modulated photoluminescence studies for lifetime determination in amorphous-silicon based passivation of crystalline-silicon wafers — •Florian Effenberg, Rudolf Brüggemann, and Gottfried H. Bauer — Institute of Physics, Carl von Ossietzky University Oldenburg, Germany

Efficient passivation of interface defects is crucial in the development of efficient amorphous silicon / crystalline silicon heterojunction solar cells. Pre-treatment of the crystalline silicon wafer prior to the amorphous-silicon deposition determines the density of interface defects to a large degree. In addition, the deposition of the passivation layer itself determines the density of interface defects. By modulated photoluminescence, we study the influence of these interface defects on the recombination of excess carriers in wafers with different passivation schemes. Emphasis is laid on the deposition of amorphous-silicon passivation layers, which will also be part of the final solar cell. The analysis of modulated photoluminescence shows that the effective lifetime can be determined from the frequency response of the photoluminescence signal. For the modulated photoluminescence measurements at room-temperature we detail the excitation-density dependence of the excess-carrier lifetime and compare its variation for different passivation schemes. From the excitation-density dependence we draw conclusions on the energetic variation in the density-of-states of the interface defects and the absolute density.

15 min. break

HL 79.6 Thu 16:00 FOE Anorg

Shunts in Thin-Film Photovoltaics — •Stephanie Malek[1], Uli

F. Wischnath[2], Juan Rechid[3], Ingo Riedel[1], and Jürgen Parisi[1] — [1]Energy and Semiconductor Research Laboratory, Department of Physics, University of Oldenburg, 26111 Oldenburg, Germany — [2]aleo solar Deutschland GmbH, 26122 Oldenburg, Germany — [3]CIS Solartechnik GmbH & Co. KG, 20539 Hamburg, Germany

Shunts can lead to severe performance reduction in thin film solar cells. This work reports on a microscopic approach to locate and characterize the details of shunts in order to reveal their origin. Localization of hot spots and film disruptions is commonly addressed by lock-in infrared thermography (LIT) through visualization of the Joule heating. The resolution of this method is restricted to the μm-range. We use different methods of LIT for the fast localization of local-lateral peculiarities in order to identify positions of interest. For a more detailed analysis of these features we use high resolution microscopy like Scanning Electron Microscopy (SEM) and AFM-based methods. These small-scale investigations can for example reveal whether areas of high heat dissipation are rather related to the inner structure of the involved thin films or to accidentally incorporated imperfections.

HL 79.7 Thu 16:15 FOE Anorg

Scanning Spreading Resistance Microscopy for Characterization of Laser Doped Selective Emitter Structures in Solar Cells — •Stefan Doering[1], Stefan Jakschik[1], Thomas Mikolajick[1,2], Jens Krause[3], Rico Böhme[3], and Marc Petri[3] — [1]NaMLab gGmbH, Dresden, Germany — [2]TU Dresden, Dresden, Germany — [3]Roth & Rau AG, Hohenstein-Ernstthal, Germany

Focus of our work is the visualization of local heavily laser doped selective emitter (LDSE) structures with a self-aligned metallization via plating in mono crystalline silicon solar cells. The LDSE process was developed at the University of New South Wales (UNSW) and enables high conductive metal fingers with a low contact resistance to the emitter, thus allowing the finger dimensions to be reduced significantly. As a result, the amount of light per area that is used for energy conversion is increased, leading to an increase in cell efficiency. The lower doped full area emitter leads to a better blue response and contributes to cell efficiency improvements, too.

Scanning Spreading Resistance Microscopy (SSRM) is known as a powerful tool for quantitative visualization of activated dopants in semiconductor materials. In this work we present SSRM measurements, showing the laser doped selective emitter diffusion into the bulk silicon. Dimensions of the LDSE as width and length can be extracted from the measured data. To our knowledge it is the first time the lateral dimensions of selective emitter activated dopants fabricated by laser annealing are visualized by SSRM in high lateral resolution.

HL 79.8 Thu 16:30 FOE Anorg

Comparison of the annealing treatments of PVD and ALD Al_2O_3 passivated silicon for solar cell applications — •Frank Benner[1], Maria Tarasova[1,3], Steve Kupke[1], Stefan Jakschik[1], and Thomas Mikolajick[1,2] — [1]NaMLab gGmbH, Dresden, Germany — [2]Lehrstuhl für Nanoelektronische Materialien, TU Dresden, Germany — [3]Institut für Elektronik- und Sensormaterialien, TU Bergakademie Freiberg, Germany

One reason for the electrical losses in solar cells is surface recombination, which decreases the effective carrier lifetime. A highly p-doped area is commonly used for the passivation of silicon solar cell rear surfaces. Alternatively, an electric field can be established to prevent the carriers from diffusing towards the surface. Negative charges need to be near the silicon surface in the passivation layer to repel the minority carriers in the p-doped silicon. We have investigated Al_2O_3 layers to determine the density of interface states and fixed charges. Different annealing times, temperatures and process gases were investigated and their impact on the electrical characteristics and carrier lifetimes compared. Annealing in forming gas (N_2/H_2) was preferable to nitrogen. Moderate temperatures decreased the density of interface states, increased the density of fixed charges and, therefore, increased the carrier lifetime. A high temperature treatment degraded the passivation layers significantly. Al_2O_3 layers deposited with ALD were superior to PVD in carrier lifetimes even though the internal charge characteristics are similar. Our results indicate a higher concentration of impurities and a thicker interface layer.

HL 79.9 Thu 16:45 FOE Anorg

Estimation of the excess carrier concentration from the spectral photoluminescence yield — •Sebastian Knabe and Gottfried H. Bauer — Carl von Ossietzky Universität Oldenburg, Institut für Physik, Oldenburg, Deutschland

The photoluminescence emitted from excited semiconductors provides access to parameters like splitting of quasi-Fermi-levels, optical absorption, etc. and it is furthermore based on the recombination of excess carriers. In this study we show one option to estimate from photoluminescence measurements parameters, such as recombination lifetime, surface recombination velocity of the excess carriers for crystalline silicon. Therefore we simulate the spectral photoluminescence emitted from an excited silicon wafer with consideration of the excess carrier concentration mostly governed by surface recombination velocities, excess carrier lifetimes, diffusion lengths, as well as by optical absorption and reflection; the simulated PL fed to the detector also contains propagation of pl-photons across surfaces and according phase accumulation through layers formulated by a matrix transfer approach. The input parameters determining the excess carrier concentration are optimized with a generic algorithm to minimize the differences in numerically simulated spectral response and experimentally recorded photoluminescence using different functions to calculate the differences between simulation and measured spectrum. The application of this approach yields excess carrier depth profiles and according influences on spectral luminescence.

HL 79.10 Thu 17:00 FOE Anorg

Charakterisierung von WS_2-Korngrenzen mit ortsaufgelösten Rasterkraftmikroskopietechniken (CAFM, KPFM) — •Roman Mankowsky, Klaus Ellmer und Stephan Brunken — Helmholtz-Zentrum, Berlin, Germany

Wolframdisulfid ist wegen seiner direkten Bandlücke von 1,8eV und dem hohen Absorptionskoeffizienten von $10^5 cm^{-1}$ ein interessantes Material für Absorberschichten in Dünnschichtsolarzellen. Zudem kommt WS_2 mit einem Anteil von $6 \cdot 10^{-3}$% in der Erdkruste sehr viel häufiger vor als andere für Dünnschichtsolarzellen verwendete Materialien. Aus diesen Gründen bietet es sich an zu untersuchen, ob WS_2 für die Produktion von Solarzellen in großem Umfang geeignet ist.

In vorangehenden Arbeiten wurde demonstriert, wie mit nickelinduzierter Kristallisation amorpher WS_{3+x}-Schichten photoaktive WS_2-Schichten auf einem metallischen Rückkontakt aus Ti(N,O) hergestellt werden können. Dennoch konnten wegen Kurzschlüssen in den WS_2-Schichten bisher keine Solarzellen präpariert werden.

Zur Bestimmung der elektrischen Eigenschaften der mikroskopischen Strukturen wurden ortsaufgelöste Leitfähigkeitsmessungen (CAFM) und Austrittsarbeitsmessungen (KPFM) kombiniert. Die Kombination von KPFM- und CAFM-Messungen erlaubt einen tiefen Einblick in die elektrischen Eigenschaften von Strompfaden mit nm Auflösung.

Mit diesen Techniken wurden Strompfade an WS_2-Korngrenzen und Fremdphasen in den WS_2-Schichten untersucht und mit Messungen an CdTe- und Cu(In,Ga)S_2-Schichten verglichen.

HL 80: Focussed Session: Novel Green Laser Diodes

Time: Thursday 14:30–17:15 Location: POT 51

Invited Talk HL 80.1 Thu 14:30 POT 51

GaN-based green laser diodes grown on c-plane GaN substrate — •Shinichi Nagahama — Nitride Semiconductor Research Laboratory, Nichia Corporation, 491 Oka, Kaminakacho, Anan, Tokushima 774-8601, Japan

We have succeeded in developing the GaN-based green laser diodes (LDs) with an emission wavelength of 510-515 nm and output power of 50 mW for the green light source in the small laser projectors.The green LDs structures were grown on conventional c-plane GaN substrates by metal organic chemical vapour deposition. The operating current and threshold voltage with an output power of 50mW were 200 mA and 5.0 V, respectively. The lifetime test of these LDs was carried out under high driving temperature up to 60 °C in cw operation. Lifetime was estimated to be over 10,000 h with an optical output power of 50mW. These results ensure that GaN-based LDs is the best candidate

for the green light source in the future small laser display applications.

Invited Talk HL 80.2 Thu 15:00 POT 51
Room-temperature CW operation of BeZnCdSe green laser diode — •SHIGEHISA TANAKA[1], JUN-ICHI KASAI[2], SUMIKO FUJISAKI[1], RYOUICHI AKIMOTO[2], TAKESHI KIKAWA[1], SHINJI TSUJI[1], HARUHIKO KUWATSUKA[2], TOSHIFUMI HASAMA[2], and HIROSHI ISHIKAWA[2] — [1]Hitachi Central Research Laboratory, Kokubunji-shi, Tokyo, Japan — [2]National Institute of Advanced Industrial Science and Technologies, Tsukuba-shi, Ibaraki, Japan

Recently, green laser diodes have been received much attention because they enable novel devices such as micro-projectors or vivid color displays when used in combination with red and blue laser diodes. Although several approaches using III-nitride-based semiconductors and their successful laser operations with wavelength of over 500 nm have already been reported, their threshold currents still increase as their lasing wavelengths approach to the pure green region. ZnSe based compound semiconductors are also promising materials for the green laser diodes. In particular, Be containing ZnSe based mixed crystals are expected to overcome the problem of limited lifetime of II-VI-based laser diodes.

In this study, a room temperature continuous-wave operation at 545 nm was demonstrated with a BeZnCdSe quantum-well laser diode. Its threshold current density was as low as 1.7 kA/cm2. This result indicates this material system is advantageous in realizing a green laser diode with low power consumption.

Invited Talk HL 80.3 Thu 15:30 POT 51
Growth and properties of semi-polar GaN on patterned silicon substrate — •NOBUHIKO SAWAKI — Aichi Institute of Technology, Yakusa, Toyota 470-0392, Japan

Growth and properties of semi-polar and non-polar GaN on Si substrate is reviewed. Particular attention is paid on selective MOVPE on patterned substrates. By tilting the c-axis of the GaN on the silicon surface, the thermal expansion coefficient mismatch and the threading dislocation density were much reduced to improve the crystalline quality. By the virtue of self-organized growth mode on a facet, we achieved excellent surface morphology. The incorporation of carbon and magnesium were investigated in (1-101)GaN which is terminated by nitrogen. We found that the sample doped with carbon shows p-type conduction. Optical spectra and Hall measurements suggested the formation of shallow acceptor levels in the sample.

Coffee Break

Invited Talk HL 80.4 Thu 16:15 POT 51
Advantages of Using Semipolar Orientation for Making Green InGaN QW Laser Diodes. — •DMITRY SIZOV, RAJARAM BHAT, KECHANG SONG, and CHUNG-EN ZAH — Corning Incorporated, One Science Center Dr., Corning, NY, 14831, USA

During recent years, several research groups demonstrated a steady progress in increasing InGaN quantum well (QW) laser diode lasing wavelength. Using c-plane substrates has been a preferred approach for it, thanks to established growth and fabrication techniques and available 2-inch substrates. More lately, semipolar substrates became available enabling faster progress in this field. Theoretical and experimental studies show that in green spectral range, because of lower built-in electric fields, the differential gain of semipolar QW is much higher than in c-plane if the stripe direction is properly chosen. For this, one needs to take into account that emission polarization depends not only on QW plane orientation, but also on pumping level. Another advantage of semipolar orientation is easier carrier transport in green semipolar multiple-QWs due to smoother band profile resulting from reduced pizeoelectrical effect, allowing uniform carrier injection among QWs when using more QWs to increase net optical gain. While having the improved optical gain, we found that the internal optical losses are not a strong function of substrate orientation, but rather depend on acceptor concentration in p-layers. Both quantum efficiency and optical gain can however be altered by strain relaxation, which is prone in the semipolar system, but can be avoided via proper strain management.

Invited Talk HL 80.5 Thu 16:45 POT 51
Optical gain of green (Al,In)GaN laser diodes — •ULRICH SCHWARZ — Fraunhofer IAF, Freiburg, Germany — IMTEK, University of Freiburg, Germany

To achieve lasing in the green spectral region with group III-nitrides, InGaN quantum wells with Indium content larger than 25% are necessary. It is extremely difficult to find growth conditions which are producing homogeneous InGaN quantum wells without dark spots at this high Indium content. Both, the density of nonradiative recombination centers and the width of inhomogeneously broadened photoluminescence spectra increase with Indium content. The consequences are broadened optical gain spectra and lower differential gain. For green laser diodes amplified spontaneous emission sets in far below lasing threshold due to the low differential gain. Going from c-plane to semi- and non-polar oriented quantum wells the differential gain as function of carrier density increases. However, the carrier liefetime decreases, lowering the differential gain as function of current density. The orientation of the quantum well has also an impact on the width of the gain spectra, both through intrinsic band structure effects and through dependency of the growth conditions and Indium fluctuations on the individual growth plane. For semipolar quantum wells also the effect of birefringence on the waveguide modes and optical gain has to be considered.

HL 81: Graphene: Transport

Time: Thursday 14:30–17:15 Location: POT 151

HL 81.1 Thu 14:30 POT 151
Acoustic phonons and spin coherence in graphene nanoribbons — •MATTHIAS DROTH and GUIDO BURKARD — University of Konstanz, 78457 Konstanz, Germany

A spintronics approach to quantum information science is considered promising due to the readily available expertise in solid state physics and possibly long coherence times [1]. We investigate a qubit implementation as real electron spin in graphene nanoribbon quantum dots. This system is particularly interesting because it allows for non-local coupling of qubits [2]. Spin coherence is determined by the coupling to nuclear spins and the lattice and the relaxation time T_1 only depends on interaction with phonons. Starting from a continuum model, we derive a full phonon field theory for acoustical phonon modes in a graphene nanoribbon and at the center of the Brillouin zone. We consider fixed boundary conditions at the edges of the quasi-one-dimensional nanoribbon as well as open boundaries. In the latter case, the usual q^2-dependence for out-of-plane modes in bulk is cut off at the zone center (near $q = 0$), where we find a linear dispersion. The transverse and longitudinal sound velocities of the in-plane modes match the literature values for comparable systems [3] and, as expected, all modes approach bulk behavior for wavelengths much smaller than the ribbon width.

[1] D. Loss and D. P. DiVincenzo, Phys. Rev. A **57** (1998).
[2] B. Trauzettel et al., Nature Physics **3** (2007).
[3] L. A. Falkovsky, Phys. Lett. A **372** (2008).

HL 81.2 Thu 14:45 POT 151
p-type doping in graphene nanostructures and electron-phonon coupling of LO-LA phonons in graphene identified by Raman spectroscopy — •STEFANIE HEYDRICH, MICHAEL HIRMER, CHRISTOPH PREIS, DANIEL HUTZLER, JONATHAN EROMS, DIETER WEISS, TOBIAS KORN, and CHRISTIAN SCHÜLLER — Institut für Experimentelle und Angewandte Physik, Universität Regensburg, 93040 Regensburg

We present recent results on graphene etched with antidot lattices and an analysis of the LO-LA phonon around the K-point and its electron-phonon coupling constant.

We utilize fast, high-resolution scans to map graphene antidot flakes on Si/SiO2-substrates. The Raman spectrum is evaluated and height, position and FWHM of the characteristic G (1580 cm^{-1}), D (1350 cm^{-1}) and 2D (2700 cm^{-1}) peaks are plotted for each point.

In flakes patterned with antidot lattices, we find a stiffening of the G-peak on the structured areas compared to unstructured parts, which is due to a p-type doping in the patterned areas [1].

Additionally, we studied the LO-LA mode at the K-point in plain graphene. When exciting with higher laser energies, the peak softens and acquires a pronounced triangular shape. We also extracted the electron-phonon coupling constant [2], which yields an experimental value of about $7x10^{-3}$.

[1] S. Heydrich, M. Hirmer, C. Preis et al., Appl. Phys. Lett. **97**, 043113 (2010)

[2] V. Fal′ko, private communication

HL 81.3 Thu 15:00 POT 151

Spin Transport and Spin Precession in Bilayer Graphene with Transparent and Tunneling Ferromagnetic Contacts — •Bastian Birkner, Jonathan Eroms, and Dieter Weiss — Institut für Experimentelle und Angewandte Physik, Universität Regensburg, 93040 Regensburg, Germany

We achieved electrical spin injection with a DC current from a ferromagnetic material (Co) into bilayer graphene with transparent and with tunneling contacts. The approximately 1.4 nm thick AlOx tunnel barrier is produced by depositing Al over the entire sample at 180 K and subsequent oxidation at room temperature. AFM pictures reveal that the Al deposition at low temperature leads to a homogenous tunnel barrier. The I-V-characteristics of the Co/AlOx/graphene junction show non-linear behavior suggesting the absence of pinholes. For both, transparent and tunneling contacts we obtain a clear spin signal in a non-local four terminal scheme whose sign depends on the magnetization orientation (parallel/antiparallel) of the ferromagnetic electrodes. By applying a perpendicular magnetic field we also detect spin precession (Hanle effect) which confirms that the non-local spin signal originates from spin injection and spin transport. Fitting of these Hanle curves yields the spin relaxation time and length as well as the spin injection efficiency. By comparing the results for transparent and tunneling contacts we find that the tunnel barrier enhances the spin signal by a factor 100 and the spin injection efficiency from 1.7 percent to 5 percent.

HL 81.4 Thu 15:15 POT 151

Dynamic Hall effect driven by circularly polarized light in graphene — •J. Karch[1], P. Olbrich[1], M. Schmalzbauer[1], C. Zoth[1], C. Brinsteiner[1], M. Fehrenbacher[1], U. Wurstbauer[1], M. M. Glazov[2], S. A. Tarasenko[2], E. L. Ivchenko[2], D. Weiss[1], J. Eroms[1], R. Yakimova[3], S. Lara-Avila[4], S. Kubatkin[4], and S. D. Ganichev[1] — [1]Terahertz Center, Regensburg, Germany — [2]Ioffe Institute, St. Petersburg, Russia — [3]Linköping University, Linköping, Sweden — [4]Chalmers University of Technology, Göteborg, Sweden

We report the observation of the circular ac Hall effect where the current is solely driven by the crossed ac electric and magnetic fields of circularly polarized radiation [1]. To demonstrate the existence of this effect we studied monolayer graphene sheets. We show that illuminating an unbiased sample with circularly polarized terahertz radiation at room temperature generates - under oblique incidence - an electric current perpendicular to the plane of incidence, whose sign is reversed by switching the radiation helicity. Alike the classical dc Hall effect, the voltage is caused by crossed electric and magnetic fields which are, however, rotating with the light's frequency. The effect is studied in both exfoliated graphene on SiO_2 substrates and epitaxial samples thermally grown on SiC. The photocurrent experiments are carried out using a cw and a high power pulsed terahertz laser. Besides the circular ac Hall effect we observe helicity dependent currents at normal incidence stemming from the illumination of the graphene edges.

[1] J. Karch et al., Phys. Rev. Lett. **105**, 227402 (2010).

HL 81.5 Thu 15:30 POT 151

Magnetotransport property of multigraphene in pulsed magnetic fields up to 62 T — José Luis Barzola Quiquia[1], Humberto Peredo[1], Srujana Dusari[1], •Prasanta Kumar Muduli[1], Carsten Putzke[2], and Thomas Herrmannsdörfer[2] — [1]Institut für Experimentelle Physik II, Universität Leipzig, Linnéstraße 5, D-04103 Leipzig, Germany — [2]Hochfeld-Magnetlabor Dresden (HLD), Forschungszentrum Dresden-Rossendorf, D-01314 Dresden, Germany

Many properties of the graphene like Dirac fermions, quantum Hall effect and fractional quantum Hall effect can be also observed in few-layers graphene or multigraphene samples. Therefore, magnetotransport study in multigraphene is an interesting area of research. In particular, the high-field properties of multigraphene are rather unknown. Most of the previous studies at high magnetic field were done on bulk graphite. However, those measurements do not reflect the intrinsic properties of graphite due to the influence of lattice defects and impurities. In order to investigate many aspects of high-field phenomena, we have made a detailed study of magnetic field-dependent longitudinal and Hall resistance in micrometer-sized and 30 nm thick multigraphene samples in pulsed magnetic field up to 62 T. We found that most of the features observed in the longitudinal and Hall resistance can be explained in a simple two-band model with nearly compensation of electrons and holes. The magnetoresistance and Hall resistance was found to saturate at high fields as expected within the two-band model. At low temperature, however, the magnetoresistance does not saturate above 20 T.

15 min. break

HL 81.6 Thu 16:00 POT 151

Scanning irradiation of polymers by low-energy ions — •Stefan Lücken, Yuri Koval, and Paul Müller — Department of Physics and Interdisciplinary Center for Molecular Materials (ICMM), Universität Erlangen-Nürnberg, Germany

We have already shown that nearly any polymer can be graphitized by low-energy ion irradiation. The surface consists of nanometer-sized graphite/graphene flakes [1]. In order to increase the size of these flakes and to enhance the conductivity of the graphitized surface, we introduce a new method of irradiation. A narrow ion beam is scanned gradually across the polymer surface. Using conductivity vs. temperature measurements, we compare samples produced with different parameters of irradiation, like fluence of ions, speed of scanning, and temperature of the samples. We have observed that a decreased width of the beam correlates to an enhanced conductivity of the surface both at room temperature and at 4.2 K. Compared to flood irradiation the conductivity becomes significantly less temperature dependent. We expect further improvements by optimizing beam width and scanning speed.

[1] I. Lazareva, Y. Koval, M. Alam, S. Strömsdörfer, P. Müller, Appl. Phys. Lett. 90, 262108 (2007).

HL 81.7 Thu 16:15 POT 151

Transport measurements on twisted graphene monolayer systems — •Hennrik Schmidt, Thomas Lüdtke, Patrick Barthold, and Rolf J. Haug — Institut für Festkörperphysik, Leibniz Universität Hannover, D-30167 Hannover, Germany

A system of two stacked graphene monolayers which are rotated with respect to Bernal stacking exhibits electrical properties quite different to samples of single monolayers or single crystal bilayer systems(1)(2). Magnetotransport measurements at different carrier concentrations are performed on decoupled monolayers being jointly contacted. Two superimposed Shubnikov-de Haas oscillations are observed with a Berrys phase of π each, indicating parallel transport through two graphene monolayers. In the Hall resistance plateaus are observed according to the minima of these oscillations. The bottom layer screens the other one both from backgate voltage and substrate influence leading to a lower carrier concentration but also significantly increased mobilities and scattering times in the upper layer. From temperature dependent measurements the cyclotron masses are obtained showing higher values than expected for a single monolayer. This indicates a reduced Fermi velocity and therefore an interaction of the two layers. In the vicinity of the charge neutrality point an asymetric temperature damping is observed.

(1)H. Schmidt, T. Lüdtke, P. Barthold, E. McCann, V. I. Fal'ko, and R. J. Haug, Appl. Phys. Lett. 93, 172108 (2008)

(2)H. Schmidt, T. Lüdtke, P. Barthold, and R. J. Haug, Phys. Rev. B, 81, 121403(R) (2010)

HL 81.8 Thu 16:30 POT 151

Investigating Aharonov-Bohm oscillations in a monolayer graphene ring structure — •Dmitri Smirnov, Hennrik Schmidt, and Rolf J. Haug — Institut für Festkörperphysik, Leibniz Universität Hannover, D-30167 Hannover, Germany

We analyse the electronical properties of a monolayer graphene ring. Graphene is obtained by micromechanical cleavage of natural graphite and is placed on a silicon substrate with a 285nm thick silicon dioxide. Monolayer graphene is found and identified via the optical microscope. The ring is formed using plasma etching and has an average radius of 280nm. After that the sample is contacted using standard electron beam lithography. Magnetotransport measurements are performed in a He3 cryostat with a base temperature of 0.5 Kelvin by varying the magnetic field up to 13 Tesla and the charge carrier concentration

using an applied back gate voltage. Shubnikov-de-Haas oscillations and Quantum-Hall measurements through the ring show characteristic properties of monolayer graphene. We also observe Aharonov-Bohm oscillations for various charge carrier concentrations for both electron and holes with a period in magnetic field that fits the size of the ring.

HL 81.9 Thu 16:45 POT 151

Graphene solution-gated field effect transistor arrays for sensing applications — •Lucas H. Hess, Pardis Ratsami, Max Seifert, Moritz Hauf, Markus Dankerl, Ian D. Sharp, Martin Stutzmann, and Jose A. Garrido — Walter Schottky Institut, Technische Universität München, Germany

Biosensing and bioelectronic applications have enormously profited from employing field effect transistors (FETs) as transducing devices, mainly due to their intrinsic amplification capability and the high integration offered by semiconductor technology. The sensitivity of so-called solution-gated FETs (SGFETs) largely depends on the charge carrier mobility and the distance between the conductive channel and the surface. On both counts, graphene appears as an ideal candidate for the development of highly sensitive SGFETs. In this work, microscopic graphene SGFET arrays are fabricated on large-scale graphene samples and characterized in aqueous environments. Both, in the electron and hole regime, the measured transconductances are significantly higher than in comparable devices based on silicon or group-III nitride transistors. The low-frequency noise of graphene SGFETs is investigated, revealing an effective gate noise of tens of μV, which compares very well with low-noise silicon devices currently used in bioelectronic applications. An on-chip structure is used for Hall-effect measurements allowing the direct determination of carrier concentrations and mobilities under electrolytic gate control. In combination with a model for the microscopic structure of water at the interface, the effect of the gate potential on charge transport in the graphene layer is analyzed.

HL 81.10 Thu 17:00 POT 151

Polymer Brushes on Graphene — •Max Seifert[1], Marin Steenackers[1,2], Alexander Gigler[3], Ning Zhang[2], Frank Deubel[2], Candy Xuan Lim[4], Kiang Loh[4], José Garrido[1], Rainer Jordan[2,5], Martin Stutzmann[1], and Ian Sharp[1] — [1]Walter Schottky Institut, TU München, Germany — [2]Wacker-Lehrstuhl für Makromolekulare Chemie, TU München, Germany — [3]CeNS and Department of Earth and Environmental Sciences, LMU München, Germany — [4]Department of Chemistry, National University of Singapore, Singapore — [5]Professur für Makromolekulare Chemie, Department Chemie, TU Dresden, Germany

We show that the direct photografting and photopolymerization of styrene yields polystyrene brush layers covalently bound to graphene. The broad applicability of this technique is demonstrated via polymerization on CVD grown graphene on Cu, epitaxial single and few layer graphene on SiC, and reduced graphene oxide. Scanning confocal Raman spectroscopy reveals that photopolymerization results in no significant disruption of the basal plane conjugation of graphene. Atomic force microscopy on few layer graphene reveals delamination due to intercalative polymerization. Finally, direct photopolymerization was attempted with a range of other vinyl monomers, none of which exhibited reactivity with graphene. However, in an alternative route we demonstrate that unreactive monomers can be locally grafted via an intermediate carbon layer formed by electron-beam-induced carbon deposition on the graphene surface.

HL 82: Ultrafast Phenomena

Time: Thursday 14:30–17:15 Location: POT 251

HL 82.1 Thu 14:30 POT 251

Interaction of intersubband transitions and ponderomotive responce in doped GaAs/AlGaAs multiple quantum wells at the THz regime — •Matthias Baudisch, Martin Wagner, Manfred Helm, and Dominik Stehr — Institute for Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf (HZDR), P.O. Box 510119, 01314 Dresden, Germany.

In the present work we investigate the line shape of the broadband terahertz (THz) response in doped multiple quantum wells by means of field-resolved detection. In an optically excited structure we recently observed a Fano-like shape of the THz response [1]. This results from the superposition of the broad continuous ponderomotive response and the sharp intersubband transition. The first originates from the force that takes effect on carriers in an oscillating electromagnetic field.

The applied spectroscopy technique is time-resolved ultrabroadband THz spectroscopy. The THz radiation is generated by phase-matched optical rectification of 10 fs near-infrared pulses in 50 μm thin GaSe crystals. The pulses are tuneable in a range from 15 to 40 THz with a width (FWHM) of up to 15 THz. The field-resolved detection is done by phase-matched electro optic sampling. The applied detection method is crucial for observing the effect since the ponderomotive current can only be seen as a lossless phaseshift of the transmitted THz radiation while the intersubband transition leads to an absorption. Thus we are able to observe directly the superposition of ponderomotive current and intersubband transition in the time-domain.

[1] D. Golde et al., Phys. Rev. Lett. 102, 127403 (2009).

HL 82.2 Thu 14:45 POT 251

Ultrafast Dynamics of ZnO and ZnO-BaTiO3 thin films — •Snigdhatanu Acharya[1], Sumedha Chouthe[1], Tammo Böntgen[2], Rüdiger Schmidt-Grund[2], Marius Grundmann[2], and Gerhard Seifert[1] — [1]Institute of Physics, Martin-Luther-University, Halle-Wittenberg, Von-Danckelmann Platz 3, D-06120, Halle, Germany. — [2]Institute for Experimental Physics-II, University of Leipzig, Linnestraße 5, D-04103 Leipzig, Germany.

Femtosecond pump-probe spectroscopy was performed at room temperature on ZnO thin film and a double layer thin film structure of BaTiO3/ZnO, to investigate coupling between the layers via the charge carrier dynamics. Frequency-doubled Ti:Sa laser pulses (150fs, 400nm) were used as pump; induced transmission changes were probed by supercontinuum (320-600nm) fs pulses. For ZnO, two photon absorption as well as direct excitation to the trap states close to the conduction band edge leads to transfer of carriers to the conduction band. The displaced carriers relax rapidly to the bottom of conduction band, and bleaching at 375nm attributed to population of discrete exciton A is observed. Further increase in the density at exciton levels lead to a stimulated emission at ~390 nm due to exciton-exciton scattering. Changes in refractive index induced by pump-pulse generates interferometric transmission changes between 400-600 nm. Similar contributions to the transient spectra are observed in BaTiO3/ZnO. BaTiO3 does not show any femtosecond response. Difference in the dynamical behaviour of the contributions in ZnO and BaTiO3/ZnO gives an indication of coupling between ZnO and BaTiO3.

HL 82.3 Thu 15:00 POT 251

Time-resolved photoluminescence from GaAs/AlGaAs multiquantum wells quenched by pulsed mid-infrared radiation — •Sabine Zybell, Harald Schneider, Stephan Winnerl, and Manfred Helm — Helmholtz-Zentrum Dresden-Rossendorf, Germany

Several groups have demonstrated the suppression of photoluminescence (PL) from semiconductor quantum wells (QWs) by intense mid-infrared radiation (MIR). Since most of the previous studies are done on time-integrated PL the ultrafast changes in the radiative state population are not well understood. We present a detailed study on time-resolved PL from an undoped GaAs/AlGaAs QW sample quenched by MIR pulses from a free-electron laser, which was tuned to the intersubband transition (ISBT) energy. At the arrival time of the MIR pulse a clear sharp dip appears in the PL transient. Free carrier absorption and ISBT are the two processes that take place under MIR excitation and result in an abrupt drop of the radiative state population and consequently in an ultrafast quenching of the PL. Performing polarization sensitive measurements, we were able to discriminate the contributions of free carrier absorption from that of ISBT. A quantitative analysis of the PL dip depth and recovery time as a function of MIR fluence was done using a model based on rate equations.

HL 82.4 Thu 15:15 POT 251

Coherent Lattice Vibrations in TiO_2 — •Elisabeth Bothschafter[1,2], Alexander Paarmann[3], Nicholas Karpowicz[2], Reinhard Kienberger[1,2], Ralph Ernstorfer[1,2,3],

and Ferenc Krausz[2,4] — [1]Fakultät für Physik, TUM, Garching — [2]Max-Planck-Institut für Quantenoptik, Garching — [3]Fritz-Haber-Institut der MPG , Berlin — [4]Department für Physik, LMU, Garching

Ultrafast time-resolved reflectivity measurements with femtosecond pulses allow investigations of the fast interplay between electronic and structural dynamics triggered by nonequilibrium electron distributions (e.g. [1]).

Here we study the ultrafast optical reflectivity changes of the rutile $TiO_2(110)$ surface with sub-5-fs ultraviolet pump and probe pulses centered at 5 eV. At the overlap of pump and probe the reflected intensity drops by 3.5% and is subsequently modulated at the frequency of the A_{1g} phonon at 18.1 THz [2]. The above bandgap excitation represents an effective charge transfer within the unit cell as the valence band density of states (DOS) is dominated by O_{2p} states whereas the conduction band has mainly Ti_{3d} character [3]. We assume that the abrupt change in the potential energy surface upon excitation induces the observed coherent lattice oscillation.

[1] M. Hase, M. Kitajima, A. M. Constantinescu, H. Petek, Nature 426(6), 51 (2003). [2] C. Lee et al., Phys. Rev. B 50, 13379 (1994). [3] H. Wang, J.P. Lewis, J. Phys., Condens. Matter 18, 421-434 (2006).

HL 82.5 Thu 15:30 POT 251

Modulation of photoluminescence kinetics of InGaAs quantum dots embedded into a microcavity using picosecond acoustics — •C. Brüggemann[1], T. Berstermann[1], A.V. Scherbakov[2], M. Bombeck[1], S. Höfling[3], C. Schneider[3], A. Forchel[3], A.V. Akimov[2], D.R. Yakovlev[1,2], and M. Bayer[1] — [1]Experimentelle Physik 2a, Technische Universität Dortmund, 44227 Dortmund, Germany — [2]A.F. Ioffe Physical Technical Institute, Russian Institute of Sciences, 194021 St. Petersburg, Russia — [3]Lehrstuhl für Technische Physik, Universität Würzburg, 97074 Würzburg, Germany

We use picosecond acoustics to modulate the photoluminescence (PL) kinetics of quantum dots (QDs) embedded into a microcavity (MC).

The distributed bragg reflector MC with a layer of $In_{0.3}Ga_{0.7}As$ QDs at the center is grown on a GaAs(100) substrate. An Al-film has been evaporated on the backside. It is used to excite and inject a picosecond strain-pulse into the substrate, by illumination of the film with an intense femtosecond laser pulse. The strain pulse propagates through the substrate and reaches the cavity structure at a specific time after the PL excitation, which can be variably delayed. While the strain-pulse propagates through the MC the PL kinetics are perturbated, which is monitored by a streak camera in the time- and spectral domain.

We observe a strong modulation of the PL intensity under pulsed and steady state PL excitation conditions, due to the strain-pulse perturbation. In the latter case we are able to decrease the PL intensity by a factor of 20 and later increase it up to a factor of 6 for ∼100 ps.

15 min. break

HL 82.6 Thu 16:00 POT 251

Extreme Nonlinear Optics in Semiconductors with Shaped Laser Pulses — •Matthias Reichelt[1], Andrea Walther[2], and Torsten Meier[1] — [1]Department of Physics and CeOPP, University of Paderborn, Warburger Str. 100, D-33098 Paderborn, Germany — [2]Institut für Mathematik, Universität Paderborn, Warburger Str. 100, D-33098 Paderborn, Germany

If a two-level system is excited with an intense light field of several times the Rabi frequency, the well-known Mollow triplets appear in the emitted radiation spectrum. [1] We show that the pattern of the emission spectrum can be changed by using appropriately shaped [2] laser pulses. The effect is also observable for a more realistic description of a semiconductor system [3].

[1] B.R. Mollow, Phys. Rev. **188**, 1969 (1969).
[2] M. Reichelt and T. Meier, Opt. Lett. **34**, 2900 (2009).
[3] D. Golde, T. Meier, and S.W. Koch, Phys. Rev. B **77** (2008).

HL 82.7 Thu 16:15 POT 251

Coulomb-induced relaxation dynamics in single-walled carbon nanotubes — •Eike Verdenhalven, Andreas Knorr, and Ermin Malić — Institut für Theoretische Physik, Technische Universität Berlin, Germany

We investigate the ultrafast Coulomb-induced relaxation dynamics of optically excited charge carriers in arbitrary single-walled carbon nanotubes. Using a density-matrix formalism we derive a corresponding Boltzmann equation in Born-Markov approximation. The bandstructure is obtained using the zone-folded tight-binding wave functions of graphene. Complying with the low dimensionality of nanotubes the Coulomb interaction is treated by a parametric interaction potential. Our approach allows to track (time- and momentum resolved) the relaxation paths of non-equilibrium electrons in metallic and semiconducting nanotubes of arbitrary chirality.

HL 82.8 Thu 16:30 POT 251

Microscopical calculation of non-linear polarization spectra of light-harvesting complexes — •Mario Schoth[1], Marten Richter[1], Thomas Renger[2], and Andreas Knorr[1] — [1]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Germany — [2]Institut für Theoretische Physik, Theoretische Biophysik, Johannes Kepler Universität Linz, Austria

Ultrafast spectroscopic techniques, such as nonlinear polarization spectroscopy [1], are used to investigate photosynthetic systems of higher plants. Performed in the frequency domain, non-linear polarization spectroscopy (NLPF) permits simultaneous measurements of dephasing and energy relaxation rates down to tens of femtoseconds. Within a Bloch equation approach [2], we calculate NLPF spectra of light-harvesting complexes such as the water-soluble chlorophyll binding protein complex (WSCP) microscopically. Hereby, we include self-consistently structural data for the excitonic couplings of pigments and the spectral density of exciton-vibrational coupling [3]. Furthermore we show that NLPF is suited to compensate effects of inhomogeneous broadening.

[1] W. Beenken, V. May, J. Opt. Soc. Am. B. 14, **11**, 2804 – 2810 (1997)
[2] M. Richter, T. Renger, G. Renger, A. Knorr, J. Chem. Phys. **127**, 075105 (2007)
[3] T. Renger et al., J. Phys. Chem. B, **111**, 10487 – 10501 (2007)

HL 82.9 Thu 16:45 POT 251

First principles of phonon squeezing in silicon — •Tobias Zier, Eeuwe S. Zijlstra, and Martin E. Garcia — Theoretische Physik, Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany

When silicon is excited by an intense ultrashort laser pulse, an extreme nonequilibrium state is induced, which consists of hot electrons (several 1000 K) and cold ions (near room temperature). The excited carriers change the potential energy surface seen by the ions, leading to a softening of the phonon modes and phonon squeezing. On the basis of density functional theory we perform a study of these effects, treating the phonons both quantum mechanically and classically, including anharmonic effects in the latter case by means of large-scale molecular dynamics simulations. Our results indicate that the initial ionic temperature before the laser excitation should not exceed approximately 77 K in order to observe quantum effects. At higher temperatures the anharmonicities amplify the classical phonon squeezing and cannot be ignored.

HL 82.10 Thu 17:00 POT 251

Intensity dependence of optically induced electron charge currents in quantum wells — •michał pochwała, huynh thanh duc, jens förstner, and torsten meier — Department of Physics and CeOPP, University of Paderborn, Warburger Str. 100, D-33098 Paderborn, Germany

We numerically investigate the intensity dependence of electron charge currents generated by perpendicular circularly polarized femtosecond laser pulse in (110)-grown semiconductor quantum wells GaAs/AlxGa1-xAs. Our analysis is based on a 14 band kp model [1] in combination with multisubband semiconductor Bloch equations [2-4]. The analysis shows that the generated electron charge currents depend on the intensity of the incident laser pulse in a highly nonlinear fashion. Oscillatory behavior of the electron charge current transients is predicted and explained.

[1] R. Winkler, Spin-Orbit Coupling Effects in Two Dimensional Electron and Hole Systems (Springer, Berlin, 2003).
[2] B. Pasenow, H. T. Duc, T. Meier, and S. W. Koch, Solid State Commun. 145, 61 (2008).
[3] H. T. Duc, J. Förstner, and T. Meier, Phys. Rev. B. 82, 115316 (2010).
[4] S. Priyadarshi, A. M. Racu, K. Pierz, U. Siegner, M. Bieler, H. T. Duc, J. Förstner, and T. Meier, Phys. Rev. Lett. 104, 217401 (2010).

HL 83: Joint Focussed Session: Theory and Computation of Electronic Structure: New Frontiers VI

Time: Thursday 15:00–16:30 Location: TRE Phy

HL 83.1 Thu 15:00 TRE Phy

Excited States from *GW*: the role of self-consistency — •Fabio Caruso[1], Xinguo Ren[1], Patrick Rinke[1], Angel Rubio[1,2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut, Faradayweg 4-6, Berlin, Germany — [2]Universidad del Pais Vasco, San Sebastian, Spain

The *GW* approximation offers an accurate framework to study *ab-initio* electronic excitations in molecules and solids. However, due to its numerical cost, *GW* is mostly introduced perturbatively following a density-functional theory (DFT) calculation (G_0W_0). We have implemented a fully self-consistent *GW* scheme based on the iterative solution of Dyson's equation in the all-electron localized basis set code FHI-*aims* [*http://www.fhi-berlin.mpg.de/aims*]. The self-consistent treatment corrects several pathologies of the G_0W_0 scheme, such as the violation of particle number conservation and the dependence on the starting point. Our self-consistent *GW* total energies are in good agreement with available literature values [Stan *et al*, JCP **130**, 114105 (2009)]. From the *GW* spectral function we extracted the ionization energies of a set of small molecules. The values are close to experimental results, but exhibit a slight tendency to underestimate. Building on this we apply self-consistent *GW* to charge-transfer systems. At large separation between the molecular fragments time-dependent DFT in (semi-)local approximations underestimates the charge-transfer energy. This error can be traced back to the wrong description of the HOMO-LUMO gap and its evolution with intermolecular distance. This error is capture by *GW* as it properly accounts for the difference between the donor ionization potential and acceptor electron affinity.

HL 83.2 Thu 15:15 TRE Phy

Electronic excitations from a perturbative LDA+*GdW* approach — •Michael Rohlfing — Fachbereich Physik, Universität Osnabrück, Germany

We discuss an efficient approach to excited electronic states within ab-initio many-body perturbation theory (MBPT). Quasiparticle corrections to density-functional theory result from the difference between metallic and non-metallic dielectric screening. They are evaluated as a small perturbation to the DFT-LDA band structure, rather than fully calculating the self energy and evaluating its difference from the exchange-correlation potential. The dielectric screening is desribed by a model, which applies to bulk crystals, as well as, to systems of reduced dimension, like molecules, surfaces, interfaces, and more. The approach also describes electron-hole interaction. The resulting electronic and optical spectra are slightly less accurate but much faster to calculate than a full MBPT calculation. We discuss results for bulk silicon and argon, for the Si(111)-(2×1) surface, the SiH_4 molecule, an argon-aluminum interface, and liquid argon.

[1] M. Rohlfing, Phys. Rev. B 82, 205127 (2010).

HL 83.3 Thu 15:30 TRE Phy

First-principles study (GW+PAW) on new phosphors for white LED — •Bruno Bertrand[1,2], Masayoshi Mikami[3], Martin Stankovski[1], and Xavier Gonze[1] — [1]European theoretical spectroscopy facility (ETSF), Université Catholique de Louvain, Louvain-la-Neuve, Belgium — [2]CERDECAM, Institut Supérieur Industriel ECAM, Bruxelles, Belgium — [3]Mitsubishi Chemical Group Science and Technology (S&T) Research Center, Inc., Yokohama, Japan

White-LEDs will be one of the major actor involved in the future generations of eco-friendly light sources. For novel types of white LEDs, an optimal combination of two green- and red-emitting phosphors absorbing partly the blue light from the InGaN LED is mandatory to obtain a white light source by post recombination of the light.

We have theoretically studied two oxynitride phosphors, one is an efficient green phosphor $Ba_3Si_6O_{12}N_2$:Eu developed at the Mitsubishi Chemical Group (S&T) Research Center, and the other is a bluish-green phosphor $Ba_3Si_6O_9N_4$:Eu that exhibits little luminescence at room temperature. Our results rely on many body perturbation approach (GW+PAW) applied to the two hosts : $Ba_3Si_6O_{12}N_2$ and $Ba_3Si_6O_9N_4$. The calculation shows a slightly narrower energy gap for $Ba_3Si_6O_9N_4$, that is 0.33 eV. Yet such a result provides keys to understand the thermal quenching mechanism, by comparing materials with a similar chemical composition, but different thermal behaviour. Then a deeper analysis with Eu-doped models sheds new light onto the relationship between emission/excitation colors from the Europium luminescent centers, and the properties of their complex ligands.

HL 83.4 Thu 15:45 TRE Phy

First principle calculation on the Fermi contact shift of lithium ion in paramagnetic battery materials — •Yuesheng Zhang[1], Florent Boucher[1], Aurore Castets[2], Dany Carlier[2], and Michel Ménétrier[2] — [1]IMN, Nantes, France — [2]ICMCB, Pessac, France

Solid state NMR in materials for lithium-ion batteries is considerably developing. In paramagnetic materials, the NMR shift of lithium is mainly contributed by the Fermi contact that can be qualitatively interpreted using chemical intuition and the concept of delocalization or polarization mechanisms. In this paper, with accurate first principle methods implemented into WIEN2k, we have obtained the spin density at the nucleus of lithium ions, and then calculated the contact shifts of lithium in several selected transition metal oxides or phosphates. The results show that the calculated values are sensitive to the exchange/correlation potential used in calculation. GGA or LDA generally overestimate the shifts, the calculated values being always shifted along positive direction comparing to the experimental ones. Adding orbital potential "U" or exact exchange on transitional metal ions can improve the results, but still some differences are found with experiments for some cases. The best agreement can be obtained when partial exact exchange potential is applied to both transitional metal and oxygen ions. This means that appropriate exchange correlation potential for transitional metals and oxygen ions is really crucial to calculate the contact shift of lithium ions. This work is funded by Agence Nationale de la Recherche (ANR-09-BLAN-0186-01)

HL 83.5 Thu 16:00 TRE Phy

First-principle approach to the temperature dependence of electronic energies. — Paul Boulanger[1,2], Michel Cote[2], and •Xavier Gonze[1] — [1]ETSF / IMCN, Université Catholique de Louvain, 1 Place Croix du Sud, B-1348 Louvain-la-Neuve, Belgium — [2]Département de physique, Université de Montréal, C.P. 6128, succ. Centre-ville, Montréal (Québec) H3C 3J7, Canada

The energy bands of semiconductors exhibit significant shifts with temperature, due to electron-phonon interactions. In search of an efficient first-principle approach to this effect, we have found that formulas derived by Allen, Heine and Cardona in a semi-empirical context cannot be transposed to Density-Functional Theory or to Many-Body Perturbation Theory without critical reexamination. For these theories, the correct formulation includes a extra term, the non-site-diagonal Debye-Waller term, which is dependent on second-order derivatives of the self-consistent electron-lattice potential with respects to atomic displacements. We have studied the importance of this extra term for diatomic molecules and found that it partially cancels the standard Debye-Waller and Fan terms leading a decrease by 52% for H2, 10% for N2 and 37% for LiF. For CO it adds about 15% to the temperature dependence. The lack of this term might explain the discrepancy found between previous theory and experiment for solids. Furthermore, the slow convergence of the sum-over-states approach of Allen-Heine-Cardona approach can be avoided in a new formalism proposed here, based on Density-Functional Perturbation Theory, leading to a dramatic decrease of calculation times.

HL 83.6 Thu 16:15 TRE Phy

Quasiparticle calculations of core levels — •Arno Schindlmayr and Dominik Biffart — Department Physik, Universität Paderborn, 33095 Paderborn, Germany

Electrons that occupy core orbitals are tightly bound to the atomic nucleus and do not participate in chemical bonding. Nevertheless, their binding energies are sensitive to the chemical environment, because the redistribution of the valence electrons due to bond formation strongly influences the interaction with the nucleus. For this reason, core-level spectroscopy is an important tool to clarify the atomic structure of materials, such as the geometry of surfaces, interfaces or defects, which can be used even when direct imaging techniques are not applicable. Theoretical calculations of core levels are typically based on density-functional theory. Although these often show the correct

trends, they are plagued by the well known deficiencies of common exchange-correlation functionals as well as technical difficulties, especially in the prevalent pseudopotential approximation. As an alternative, we employ many-body perturbation theory, where the quasiparticle correction to the Kohn-Sham eigenvalues provides a formally exact description of dynamical screening around the core hole in the final state. Our implementation is based on the full-potential linearized augmented-plane-wave (FLAPW) method and employs the *GW* approximation for the electronic self-energy. The calculated core levels of selected systems, such as silicon in various crystalline materials with differing local environments, are in very good quantitative agreement with experimental data from X-ray photoemission measurements.

HL 84: Joint Focussed Session: Theory and Computation of Electronic Structure: New Frontiers VII

Time: Thursday 17:15–19:15 Location: TRE Phy

Topical Talk HL 84.1 Thu 17:15 TRE Phy

Continuum mechanics for quantum many-body systems: the anti-adiabatic approximation — •Giovanni Vignale[1], Xianlong Gao[2], Jianmin Tao[3], Stefano Pittalis[1], and Ilya Tokatly[4] — [1]Department of Physics, University of Missouri, Columbia, MO 65211, USA — [2]Department of Physics, Zhejiang Normal University, Jinhua, Zhejiang Province, 321004, China — [3]Department of Chemistry, Rice University, 6100 Main Street Houston, TX 77005, USA — [4]ETSF Scientific Development Centre, Dpto. Fisica de Materiales, Universidad del Pais Vasco, Centro de Fisica de Materiales CSIC-UPV/EHU-MPC, Av. Tolosa 72, E-20018 San Sebastian, Spain

Classical continuum mechanics is a theory of the dynamics of classical liquids and solids in which the state of the body is described by a small set of collective fields, such as the displacement field in elasticity theory; density, velocity, and temperature in hydrodynamics. A similar description is possible for quantum many-body systems. In this talk I show how the exact Heisenberg equation of motion for the current density of a many-body system can be closed by expressing the quantum stress tensor as a functional of the current density. I then introduce an "anti-adiabatic" approximation scheme for this functional. The anti-adiabatic scheme allows us to bypass the solution of the time-dependent Schroedinger equation, resulting in an equation of motion for the displacement field that requires only ground-state properties as an input. I illustrate the formalism by applying it to the calculation of excitation energies in a few model systems.

HL 84.2 Thu 17:45 TRE Phy

Discontinuities of the Exchange-Correlation Kernel and Charge-Transfer Excitations in TDDFT — •Maria Hellgren and Eberhard K.U. Gross — Max-Planck-Institute of Microstructure Physics, Weinberg 2, Halle, Germany

An intriguing consequence for density functional theory (DFT) arises when considering ensembles with densities integrating to fractional particle number. The total ground-state energy as a function of particle number consists of straight-line segments and, consequently, the corresponding exchange-correlation (XC) potential jumps discontinuously. This feature of the exact theory turns out to be a key property to incorporate in approximate functionals in order to obtain, e.g, accurate band-gaps of solids and correct molecular dissociation limits.

It has been demonstrated that the discontinuous nature of the static XC potential naturally carries over to the XC potential of time-dependent density functional theory (TDDFT) appearing in, e.g., time-resolved ionization processes. How the same property is reflected in the XC kernel, defined as the functional derivative of the XC potential with respect to the density, has, so far, not received any attention. The XC kernel is of fundamental importance in TDDFT as it gives access to the particle conserving excitation spectrum. In this work we have investigated the discontinuities of the XC kernel and found them to be crucial for the description of long-range charge-transfer excitations.

HL 84.3 Thu 18:00 TRE Phy

Insights in the T-matrix formalism — •Pina Romaniello[1,4], Friedhelm Bechstedt[2,4], and Lucia Reining[3,4] — [1]Université Paul Sabatier, Toulouse, France — [2]Friedrich-Schiller-Universitaet Jena, Jena, Germany — [3]École Polytechnique, Palaiseau, France — [4]European Theoretical Spectroscopy Facility

In many-body perturbation theory the self-energy $\Sigma = GW\Gamma$ plays a key role since it contains all the many body effects of the system. The exact self-energy is not known and approximations are needed. As first approximation one can neglect the vertex Γ and obtain the GW approximation. In some cases this is not sufficient, and one needs to go beyond this approximation. In this work we elucidate the concept of T-matrix [1] and its relation with Hedin's equations [2]. Starting from the exact definition of self-energy we illustrate several aspects of the T-matrix formalism: i) which approximations to the self-energy yield the T-matrix formulation, in comparison with those that, instead, yield GW and beyond; ii) the role of the particle-particle and electron-hole contributions to the T-matrix; iii) a screened version of the T-matrix; iv) an approximate vertex that produces the same self-energy as the screened T-matrix. Tests are done on the exactly solvable Hubbard molecule [3].

[1] L. P. Kadanoff and G. Baym, Quantum Statistical Mechanics, W. A. Benjamin, Inc. New York, (1962).

[2] L. Hedin, Phys. Rev. 139, A796 (1965).

[3] P. Romaniello, S. Guyot, and L. Reining, J. Chem. Phys. 131, 154111 (2009); P. Romaniello, F. Bechstedt, L. Reining, in preparation.

HL 84.4 Thu 18:15 TRE Phy

Stochastic current DFT for periodic systems — •Heiko Appel — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin, Germany

Recently we have introduced stochastic current density functional theory (SCDFT) which is an approach that allows to describe decoherence and dissipation from first principles [1,2]. So far the method has been applied to finite systems only. In this talk I will present an extension of SCDFT to periodic systems. In particular I will discuss a scheme for the stochastic real-time propagation of the Kohn-Sham orbitals in extended systems and also address possible choices for the bath operators that appear in the SCDFT formalism. (Work supported in part by Lockheed Martin, DOE and MPG).

[1] Massimiliano Di Ventra and Roberto D'Agosta, Phys. Rev. Lett. 98, 226403 (2007).

[2] Heiko Appel and Massimiliano Di Ventra, Phys. Rev. B 80, 212303 (2009).

HL 84.5 Thu 18:30 TRE Phy

Wave function based treatment of electronic correlation in solids — •Andreas Grüneis[1], George H. Booth[2], James Spencer[3], Martijn Marsman[1], Ali Alavi[2], and Georg Kresse[1] — [1]University of Vienna, Faculty of Physics and Center for Computational Materials Science, Sensengasse 8/12, A-1090 Vienna, Austria — [2]University of Cambridge, Chemistry Department, Lensfield Road, Cambridge CB2 1EQ, U.K. — [3]Department of Physics and Thomas Young Centre, Imperial College London, Exhibition Road, London SW7 2AZ, U.K.

The use of wave function based methods to treat electronic correlation, such as Møller-Plesset perturbation theory, coupled-cluster theory, and full configuration interaction (CI) is common practice in the field of computational quantum chemistry. Due to the computational cost involved, however, these methods have rarely been applied to extended systems. We have implemented the second-order Møller-Plesset perturbation theory and coupled-cluster singles and doubles (CCSD) theory within the framework of the Projector-Augmented-Wave method, using periodic boundary conditions and a plane wave basis set in VASP.[1] Moreover, an interface between VASP and the full CI quantum Monte Carlo (FCIQMC) code presented in Ref.[2] has been developed. We have tested our implementations on small molecules and solids. We outline techniques that reduce the computational effort of CCSD and FCIQMC calculations, such as the use of natural orbitals and progressive downsampling. [1] A. Grüneis et al. JCP 133, 074107 (2010). [2] G. H. Booth et al. JCP 131, 054106 (2009).

HL 84.6 Thu 18:45 TRE Phy

Finite temperature reduced density matrix functional theory (FT-RDMFT) A novel approach to the description of quantum systems in thermal equilibrium. — •Tim Baldsiefen and E.K.U. Gross — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

Despite the big success of DFT for the description of groundstate properties of quantum mechanical systems, the finite temperature extension FT-DFT showed only little success in a restricted field of research. We develop the theoretical foundation for an alternative description of equilibrium properties, by employing the one-reduced density matrix (1RDM) rather than the density as central variable. The zero-temperature version of this theory proved to be quite successful in the last years, allowing for the description of groundstate properties of a wide class of systems (e.g. small molecules [1] and solids [2]). This sparks the hope, that a description of finite temperature ensembles by means of the 1RDM will succeed on fields of research formerly inaccessible by FT-DFT.

In this framework of FT-RDMFT we are able to employ methods from many body perturbation theory to develop approximate free-energy functionals. An application to the groundstate of the electron gas shows, that FT-RDMFT is able to significantly improve the groundstate energy compared to a strictly perturbative treatment.

[1] N. N. Lathiotakis et al., Phys. Rev. A, 79, 040501 (2009)

[2] S. Sharma et al., Phys. Rev. B 78, 201103(R) (2008)

HL 84.7 Thu 19:00 TRE Phy

Spin spirals in the uniform electron gas: Towards a new functional in SDFT — •F. G. Eich[1,2] and E. K. U. Gross[1] — [1]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany — [2]Freie Universität Berlin, Berlin, Germany

Based on our studies of the spin-spiral state of the uniform electron gas [1], we present a novel exchange-correlation functional for Spin-Density-Functional Theory (SDFT).

Much like in the well known local-density approximation (LDA) the local exchange-correlation energy is approximated by the exchange-correlation energy of the uniform electron gas. In contrast to the standard LDA the state of the electron gas is not only specified by its density but furthermore by its spin magnetization and spin-spiral wave vector. We show that, in order to determine a local spin-spiral wave vector, gradients of the spin magnetization have to be included in the functional.

As a first step towards application for real materials we obtain the energy of the spin-spiral electron gas using the random-phase approximation.

[1] F.G. Eich, S. Kurth, C. R. Proetto, S. Sharma, and E. K. U. Gross, Phys. Rev. B 81, 024430 (2010)

HL 85: Poster Session II

Time: Thursday 18:00–21:00 Location: P4

HL 85.1 Thu 18:00 P4

Quasiparticle wave functions in alloys — •Alexander Müller, Marko Stölzel, Gabriele Benndorf, and Marius Grundmann — Universität Leipzig, Institut für Exp. Physik II, Abteilung Halbleiterphysik, Linnéstr. 5, 04103 Leipzig

The effective mass approximation is a powerful tool to understand many effects in semiconductors such as the transport properties of electrons and holes, bound states at impurities as well as multi-particle complexes such as excitons. However, up to now this model has mainly been applied to elemental/compound semiconductors or virtual crystals. For alloys, there exist a number of methods to estimate the band gap or effective carrier masses such as the virtual crystal approximation or local density approximations on supercells. However, the applicability to very large cells to investigate localization effects is limited.

In this contribution we investigate the suitability of the effective mass approximation for alloys to include localization effects in this theory. Calculated envelopes of electron and hole wave functions are compared to wave functions determined using a 1D Kronig–Penney-like model. Indeed, we observe a good agreement between both models. The effective mass model is applied to excitons and the numerical accuracy of the found energy states is discussed.

HL 85.2 Thu 18:00 P4

Empirical band gap corrected local density approximation study — •Roby Cherian and Gabriel Bester — Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, D-70569 Stuttgart, Germany.

We have developed empirical pseudopotentials directly from ab-initio methods, in the local density approximation (LDA), keeping the empiricism at the lowest possible level. Major problems of the LDA calculation for the electronic band structure is the severe underestimation of the electron band gap and the electron effective mass. We have implemented and tested different empirical schemes such as different modifications of the semi-local and the local potentials. We discuss limitations of this approach, e.g., the band gap and the effective mass cannot be corrected simultaneously. On the other hand we demonstrate the quality of the obtained potential by comparing deformation potentials for valence and conduction band with experiment and density functional theory.

HL 85.3 Thu 18:00 P4

Modelling Hertzian Point Dipoles Using the Fourier Modal Method — •Benjamin Lutz, Thomas Zebrowski, Sabine Essig, and Kurt Busch — Institut für Theoretische Festkörperphysik and DFG-Center for Functional Nanostructures (CFN), Karlsruhe Institute of Technology (KIT), 76128 Karlsruhe, Germany

The experimental realizations of quantum dots, e.g., in photonic crystal waveguides and cavities, motivate the incorporation of Hertzian point dipoles in computational methods such as the Fourier Modal Method (FMM) that are capable of dealing with periodic structures. Since periodicity is broken by a single source it is necessary to isolate the unit cell with perfectly matched layers (PMLs). Thus we present the results of an implementation that isolates sources with PMLs in the lateral plane of the three-dimensional computational domain. We optimized the parameters of the PMLs by comparing the analytical field distribution of a Hertzian point dipole with the simulations. In addition we investigated the influence of adaptive coordinates on the convergence behavior in such a setup.

HL 85.4 Thu 18:00 P4

Few-photon transport in low-dimensional waveguides with a quantum-impurity — •Christoph Martens, Jean-Christophe Blancon, Paolo Longo, and Kurt Busch — Institut für Theoretische Festkörperphysik and DFG-Center for Functional Nanostructures (CFN), Karlsruhe Institute of Technology (KIT), 76128 Karlsruhe, Germany

We present our recent results on the dynamics of few-photon quantum transport in waveguiding systems in the presence of a quantum impurity. Based on a multimode Jaynes-Cummings model, recent studies show interesting transport properties [1,2,3,4], for instance, effective photon-photon interactions [1,3] and interaction-induced radiation trapping [3]. By monitoring the time evolution of few-photon pulses we investigate the transmission characteristics and the conditions under which atom-photon bound states can be excited. Furthermore, we analyze functional elements which are important for possible experimental realizations.

[1] J. T. Shen and S. Fan, Phys. Rev. Lett. 98, 153003 (2007)
[2] P. Longo et al., J. Opt. A: Pure Appl. Opt. 11, 114009 (2009)
[3] P. Longo et al., Phys. Rev. Lett. 104, 023602 (2010)
[4] D. Witthaut et al., New Journal of Physics 12, 043052 (2010)

HL 85.5 Thu 18:00 P4

New features about angle-resolved fluorescence microscopy in Photonic Crystals — •Lars Heerklotz, Rebecca Wagner, and Frank Cichos — University of Leipzig, Leipzig, Germany

Periodical spatial variations of a materials properties lead, via the Bloch condition, to the formation of bands, causing partial and total band gaps. That holds for electrons in a semiconductor, where the core potential is periodic, as well as for photons in a Photonic Crystal (PC), where the dielectric constant is periodic. In the photonic case

this means, that light can not propagate in the band gap regions. To observe these features we produced face-centered cubic (fcc) PCs by evaporation from a solution of fluorescent dye beads and polystyrene beads, which form the PC. In the past conventional wide field or confocal setups have been used intensively to study the behavior of light sent from many dyes in three dimensional PCs. We are using our home-build novel confocal setup to investigate the behavior of light emitted from single dye beads inside the PC. Advantage, compared to former setups, is the acquisition of spectra for several angles in one measurement. This method, angle resolved fluorescence microscopy, is applied to measure the fractional local density of states for different depths of dyes inside the crystal and to observe the threefold structure in the first Brillouin-zone of the fcc-lattice.

HL 85.6 Thu 18:00 P4

Coupling of Quantum Dots to Strongly Interacting Photonic Resonator Systems — •Stefan Declair, Torsten Meier, and Jens Förstner — University of Paderborn, Department of Physics and CeOPP, Warburger Str. 100, D-33098 Paderborn, Germany

We numerically investigate the coupling between semiconductor heterostructures like quantum dots and strongly interacting photonic resonators like coupled photonic crystal cavities or microdisks using a Finite-Difference Time-Domain method. The light-matter Hamiltonian is used to calculate the macroscopic polarisation via dynamic equations for the interband coherence of the semiconductor heterostructure [1].

For photonic systems of multiple coupled one-dimensional cavities and quantum dots, clear anticrossing behavior is observed when the quantum dot gap frequency is tuned through the resonances of the coupled cavity system. Also, strong coupling is shown for a system of two coupled two-dimensional high-Q nanocavities [2] with an embedded quantum dot.

[1] C. Dineen et al., Electromagnetic field structure and normal mode splitting in photonic crystal nanocavities, Optics Express 13, 4980 (2005).

[2] Y. Akahane et al., High-Q photonic nanocavity in a twodimensional photonic crystal, Nature 425, 944 (2003).

HL 85.7 Thu 18:00 P4

Crossed Photonic Crystal Waveguides for Quantum Dots Signal Detection — •Xiaohong Song, Torsten Meier, and Jens Förstner — Department Physik and Center for Optoelectronics and Photonics Paderborn (CeOPP), Universität Paderborn, Warburger Str. 100, D-33098 Paderborn, Germany

Separation of typically very weak quantum dot signals from the exciting laser light is important for the investigation of the excitation dynamics of quantum dots. Using a combined Maxwell-Bloch approach[1], we theoretically investigate a crossed perpendicular photonic crystal waveguide structure to achieve this aim[2]. The waveguides are designed so that the light can only propagate along one direction and is forbidden in the other directions. When the quantum dots are embedded in this structure, the nearly pure quantum dot signal can be detected in the transverse direction.

[1] C. Dineen, J. Förstner, A.R. Zakharian, J.V. Moloney, S.W. KochOptics Express 13, 4980 (2005).

[2] S. G. Johnson, C. Manolatou, S. Fan, P. R. Villeneuve, J. D. Joannopoulos, H. A. Haus, Opt. Lett. 23, 1855 (1998).

HL 85.8 Thu 18:00 P4

Tunable Transmission in Rolled-Up Three Dimensional Metamaterials — •Aune Koitmäe, Stephan Schwaiger, Matthias Klingbeil, Markus Broell, Jochen Kerbst, Ricardo Costa, Andrea Stemmann, Yuliya Stark, Detlef Heitmann, and Stefan Mendach — Institut für Angewandte Physik, Universität Hamburg, Hamburg, Deutschland

Metamaterials are artificial materials with tuneable permittivity and permeability. Alternating layers of metal/dielectric films are rolled up with multiple rotations into three-dimensional microtubes. The walls of these tubes represent three dimensional metamaterials with a well defined lattice constant and a tuneable anisotropic permittivity [1]. By integrating quantum wells as optical amplifiers into the walls of the microtube we can modify the transmission through the tube walls. Transmission measurements are performed using a tapered optical fibre which illuminates the tube from the inside. A microscope objective collects the light transmitted through the tube walls. The same objective is used to focus a pumping laser on the tube. By comparing measurements with and without laser pumping we obtain a characteristic modification of the transmission through the tube walls.

We gratefully acknowledge support by the DFG through GrK 1286.

[1] S. Schwaiger et al., Phys. Rev. Lett. 102, 163903 (2009)

HL 85.9 Thu 18:00 P4

Numerical Simulation of Exciton Dynamics at Ultra Low Temperature — •Sunipa Som[1] and Heinrich Stolz[2] — [1]Institut für Physik, Universität Rostock, Rostock, Germany — [2]Institut für Physik, Universität Rostock, Rostock, Germany

The possibility of Bose-Einstein condensation of excitons in cuprous oxide has been actively pursued for many years, because in the low density limit excitons are bosons, and therefore obey Bose-Einstein statistics. Cuprous oxide is of high interest due to its long exciton lifetime. We have studied theoretically the relaxation behaviour of excitons at ultra low temperatures below 1K, by solving the Boltzmann equation [1,2], while the excitons are confined within a parabolic potential trap. We have included deformation potential phonon scattering but not collision of excitons.

The Boltzmann equation has been solved by finite difference method and the method of lines using MATLAB. Using initial condition representative for actual experimental studies, we are getting the exciton occupation numbers as a function of momentum, space and time. From these we have calculated the effective temperature and studied how it is changing with time. For temperatures above 1K, the effective temperature is coming down to bath temperature within ten nanoseconds. This is different for temperatures below 1K, where the effective temperature is coming down to bath temperature very slowly within hundreds of nanoseconds only.

[1] Ashcroft and Mermin, Solid State Physics (Harcourt Brace, Fortworth, 1976). [2] A. L. Ivanov et al., Phys. Rev. E 55, 6363 (1997)

HL 85.10 Thu 18:00 P4

Magneto-Optical Ellipsometry of Ferromagnetic Thin Films — •Tobias Herzig, Tammo Böntgen, Rüdiger Schmidt-Grund, Michael Lorenz, and Marius Grundmann — Universtät Leipzig, Institut für Experimentelle Physik II, Linnéstr. 5

We have investigated the optical properties of ferromagnetic thin films by means of spectroscopic ellipsometry. From the Müller Matrix (MM) obtained through these measurements one can derive the optical constants as well as the magneto-optical properties of the sample. The diagonal MM elements are a measure for the optical constants (refraction index, absorption). They were modeled using tabulated reference for the refractive index and absorption from the literature. The off-diagonal MM elements on the other hand contain information about the energy conversion between polarization modes. Thus modeling these elements gives inside into the magneto-optical properties of the sample. We determined these properties for Cobalt and magnetite thin films as model systems. The method proved to be a reliable tool to measure important optical properties and magneto-optical effects simultaneously.

HL 85.11 Thu 18:00 P4

Optical properties of crystalline and amorphous TiO2 modifications — •Marc Landmann[1], Thomas Köhler[2], Eva Rauls[1], Thomas Frauenheim[2], and Wolf Gero Schmidt[1] — [1]Lehrstuhl für Theoretische Physik, Universität Paderborn, Germany — [2]Bremen Center for Computational Materials Science, Germany

In its crystalline form TiO2, is traditionally used as a pigment in industrial applications. Moreover, TiO2 surfaces are among the most studied substrates in catalysis and used as a template for crystalline organic film growth for both light-emitting diodes and field-effect transistor applications [1]. TiO2 also offers the possibility of low cost dye-sensitized solar cells based on optically transparent films of nanocrystalline TiO2. To fully exploit the technological potential of TiO2, a detailed understanding of the bulk and surface optical properties is required. Here, we have calculated the optical response of ordered rutile, anatase and brookite bulk material as well as of the the rutile (110)(1x1) surface. The calculations have been done on the density-functional theory (RPA), quasiparticle (GW) and Bethe-Salpeter equation (BSE) level of theory [2]. The results are interpreted in terms of self-energy and excitonic contributions to the optical spectra and compared with the available experimental data and previous calculations [3]. We find characteristic differences between the various bulk phases as well as between the crystalline and amorphous material.

[1] G. Koller et al. Adv. Mater. 16, 2159 (2004).

[2] W. G. Schmidt et al. Phys. Rev. B 67, 085307 (2003).

[3] H. Sano et al. Phys. Rev. B 70, 125411 (2004)

HL 85.12 Thu 18:00 P4

Investigation of the effect of plasmonic metal nanostructures on nanocrystalline TiO_2:Eu^{3+} nanoparticles — CAHIT BENEL[1], •BARAT KURBANJAN[1], ULRICH HERR[1], MANUEL GONCALVES[2], OTHMAR MARTI[2], JOHANNES BONEBERG[3], and PAUL LEIDERER[3] — [1]Inst. of Micro and Nanomaterials, University of Ulm, Germany — [2]Inst. of Experimental Physics, University of Ulm, Germany — [3]Dept. of Physics, University of Konstanz, Germany

Rare-earth-doped materials are used in a variety of photonic applications such as phosphors, X-ray imaging, scintillators, display panels and photonic band gap materials. In this work, Eu^{3+} doped TiO_2 nanoparticles have been produced via chemical vapor synthesis (CVS). Samples with different Eu^{3+} ion concentration ranging from 0.05 at% to 1.51 at% were prepared. XRD results show that the samples primarily consist of the anatase phase. However, with increasing dopant level, an increasing amount of the rutile phase is found. Luminescence lifetime measurements monitoring $^5D_0$-$^7F_2$ transition of Eu^{3+} ions were performed at different excitation wavelengths for both as-prepared and annealed samples. We find two different lifetime components, which are attributed to contributions from surfaces and possibly other defects. The nanoparticles have been deposited on Ag nanostructures, which were prepared by nanosphere lithography on glass substrates. Different sizes of spheres have been used. The samples have been characterized by laser scanning confocal microscopy. Local photoluminescence spectra are used to search for possible luminescence enhancements due to plasmonic effects.

HL 85.13 Thu 18:00 P4

Statistical properties of photon modes in random arrays of ZnO nano-needles — •CHRISTOPH MINZ, DAVID LEIPOLD, and ERICH RUNGE — Technische Universität Ilmenau, 98693 Ilmenau, Germany

Localization of electromagnetic waves in random media received renewed interest in the last years. Recent ultrafast optical experiments [1] indicate the existence of highly localized photon modes in a system of homogeneous, randomly distributed, vertically aligned ZnO nanoneedles. In particular, hot spots in the spatial distribution of the second harmonic generation (SHG) were found.

In this work, we discuss the optical near field, which we obtain from full 3D solutions of Maxwell's equations of a model system in time domain. The spatial distribution of the electric near-field and the squared electric near-field intensity are investigated with statistical methods. The results are compared to the experimental findings.

[1] We thank Manfred Maschek, Slawa Schmidt, Martin Silies and Christoph Lienau from the Carl von Ossietzky Universität Oldenburg as well as Takashi Yatsui, Kokoro Kitamura and Motoichi Ohtsu from the University of Tokyo for sharing their experimental data with us prior to publication.

HL 85.14 Thu 18:00 P4

Heavy *n*-doping: Wannier-Mott and Mahan excitons in ZnO — •ANDRÉ SCHLEIFE, CLAUDIA RÖDL, KARSTEN HANNEWALD, and FRIEDHELM BECHSTEDT — Institut für Festkörpertheorie und -optik and European Theoretical Spectroscopy Facility, Friedrich-Schiller-Universität Jena, 07743 Jena, Germany

Transparent conductive oxides such as ZnO are highly interesting within the modern field of optoelectronics since they have large fundamental band gaps while intentional as well as unintentional *n*-doping renders them conductive. However, the free electrons in the material form a degenerate electron gas which occupies the lowest conduction-band states and whose effect on the optical properties is unknown.

In addition to the Pauli blocking of the lowest optical transitions, the degenerate electron gas significantly influences the screening of the electron-hole interaction. We generalize the solution of the Bethe-Salpeter equation for the polarization function to investigate both of these aspects as well as their interplay with the excitonic effects for *n*-ZnO. We introduce **k**-dependent occupation numbers to account for the Pauli blocking. The additional screening due to the free electrons is taken into account by means of a Thomas-Fermi approach.

Our approach essentially captures the involved physics, hence, we observe a Mahan exciton at the absorption edge – in perfect agreement with a measured result. We show that due to the strong decrease of the binding energy and the oscillator strength with an increasing free-electron concentration in the material an excitonic Mott transition is barely observable.

HL 85.15 Thu 18:00 P4

Optical properties of as-grown and ion implanted Cu2O thin films — •CHRISTIAN MÜLLER[1], SEBASTIAN GEBURT[1], ANDREAS LAUFER[2], BRUNO K. MEYER[2], and CARSTEN RONNING[1] — [1]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — [2]I. Physikalisches Institut, Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, 35392 Gießen, Germany

Copper(I) oxide is a promising material for future photovoltaic applications, especially due to its environmental friendly and cheap preparation process. The properties of copper(I) oxide are still a hot topic of research and especially n-doping is difficult. But similar problems could be solved in the past at materials like CIS, CGS and CIGS [1].

Copper(I) oxide thin filmes on glas substrates were prepared by reactive oxygen sputtering. The crystal quality and band edge properties were examined using UV-VIS transmission and reflectivity measurements combined with XRD. The layers were annealed in different atmospheres to investigate the effects on the quality of the films in term of phase transformation and the influence on the energy gap. Temperature and power dependent cathodo- and photoluminescence measurements on intrinsic samples were performed to investigate the emission properties with regard to excitonic effects and donator/acceptor behavior. Ion implanted samples were examined to discover extrinsic donor- and acceptor species and optical active impurities.

[1] Biccari F.: Defects and Doping in Cu2O. University of Rome, Diss., 2009

HL 85.16 Thu 18:00 P4

UV photoluminescence spectroscopy of AlGaN alloys with different Al-contents — •CHRISTOPH REICH, JESSICA SCHLEGEL, JOACHIM STELLMACH, PATRICK VOGT, and MICHAEL KNEISSL — Technische Universität Berlin, Institut für Festkörperphysik, Hardenbergstr. 36, 10623 Berlin, Germany

AlGaN alloys are very promissing materials for ultraviolet (UV) light emitting diodes and lasers in the spectral range between 360 nm and 200 nm. However, for high efficiency devices further improvement of material quality and better understanding of the optical properties is needed. In order to investigate the influence of the composition and defect density on the emission characteristics we have characterized AlGaN layers with different Al-content using temperature dependent and excitation power dependent UV photoluminescence (PL) spectroscopy. The samples were grown by metalorganic vapor phase epitaxy either on (0001) GaN/sapphire or on (0001) AlN/sapphire to minimize lattice mismatch within the entire composition range. We observe a decrease in the PL intensity and an increase in the full width at half maximum with higher Al-content, which can be attributed to a reduction of the crystal quality as well as an increase in composition fluctuation. The emission characteristics and the temperature dependence of the bandgap energy for different AlGaN compositions will be discussed.

HL 85.17 Thu 18:00 P4

Disorder Effects in Ga(AsBi) — •CHRISTIAN WAGNER[1], SEBASTIAN IMHOF[1], ALEXEJ CHERNIKOV[2], MARTIN KOCH[2], NICO S. KÖSTER[2], KOLJA KOLATA[2], SANGAM CHATTERJEE[2], STEFAN W. KOCH[2], XIANFENG LU[3], SHANE R. JOHNSON[3], DANIEL A. BEATON[4], THOMAS TIEDJE[5], OLEG RUBEL[6,7], and ANGELA THRÄNHARDT[1] — [1]Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz, Germany — [2]Fachbereich Physik, Philipps-Universität Marburg, 35032 Marburg, Germany — [3]Department of Electrical Engineering, Arizona State University, Tempe, Arizona 85287-6206, USA — [4]Department of Physics and Astronomy, University of British Columbia, Vancouver, British Columbia V6T 1Z4, Canada — [5]Department of Electrical and Computer Engineering, University of Victoria, Victoria, British Columbia V8W 3P6, Canada — [6]Thunder Bay Regional Research Institute, Thunder Bay, Ontario P7A 7T1, Canada — [7]Department of Physics, Lakehead University, Thunder Bay, Ontario P7B 5E1, Canada

In recent years, Ga(AsBi) has been shown to be an interesting material for laser applications since its band gap can be varied over wide frequency range. The growth process, however, is still challenging and carrier dynamics remains governed by hopping processes. We show that emission spectra are well described by a two-scale disorder model (S.Imhof et al., Appl.Phys.Lett. 96, 131115 (2010)) and discuss time-dependent simulations and measurements. Theory and experiment show a good agreement in all cases.

HL 85.18 Thu 18:00 P4

Photoluminescence of Ga(AsBi) — •NILS ROSEMANN[1], ALEXEJ

Chernikov[1], Verena Bornwasser[1], Niko S. Köster[1], Martin Koch[1], Kolja Kolata[1], Sangam Chetterjee[1], Stephan W. Koch[1], Sebastian Imhof[2], Christian Wagner[2], Angela Tränhardt[2], Xianfeng Lu[3], Shane R. Johnson[3], Dan A. Beaton[4], Thomas Tiedje[5], and Oleg Rubel[6,7] — [1]Fachbereich Physik, Philipps-Universität Marburg, 35032 Marburg, Germany — [2]Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz, Germany — [3]Department of Electrical Engineering, Arizona State University, Tempe, Arizona 85287-6206, USA — [4]Department of Physics and Astronomy, University of British Columbia, Vancouver, British Columbia V6T 1Z4, Canada — [5]Department of Electrical and Computer Engineering, University of Victoria, Victoria, British Columbia V8W 3P6, Canada — [6]Thunder Bay Regional Research Institute, Thunder Bay, Ontario P7A 7T1, Canada — [7]Department of Physics, Lakehead University, Thunder Bay, Ontario P7B 5E1, Canada

Ga(AsBi) is a promising candidate for GaAs-based near-infrared emitters at telecommunication wavelength. To evaluate the potential of this material system we study the photoluminescence from such a bulk sample as function of pump power and lattice temperature. Strong disorder-related features are observed. To better quantify the experiments we analyze the data using a Monte Carlo approach. A two-scale model is introduced to account for both cluster localization and alloy disorder.

HL 85.19 Thu 18:00 P4

Optical properties of positioned InAs-based nanowire arrays — •Andreas Brenneis, Simon Hertenberger, Sonja Matich, Gerhard Abstreiter, Alexander Holleitner, and Gregor Koblmüller — Walter Schottky Institut and Physik Department, TUM Garching, Germany

Small bandgap semiconducting nanowires allow fabricating nanoscale light-sensitive devices like broadband solar cells or mid-infrared (mir) photodetectors. We discuss the optical properties of positioned InAs-based nanowires. To this end, p-Si(111) substrates with a top layer of SiO_2 are structured via e-beam lithography by holes with a diameter of approximately 80 nm. The nanowires are then grown vertically on the substrates by solid-source molecular beam epitaxy. The optical properties of the nanowires are characterized by FTIR transmission and angle dependent reflection measurements. To fabricate optoelectronic devices, we subsequently embed the nanowires in an insulator (SiO_2 by PECVD and PVD; SOG). After an etch back step, the nanowires are then contacted by depositing a thin conducting layer on top. The p-Si substrate provides the second electronic contact of the optoelectronic two-terminal devices.

HL 85.20 Thu 18:00 P4

Optical investigation on a monolithic planar microcavity containing InP quantum dots as active medium — •Marcus Müller[1], Alexander Franke[1], Thomas Hempel[1], Jürgen Christen[1], Wolfgang-Michael Schulz[2], Marcus Eichfelder[2], Robert Rossbach[2], Michael Jetter[2], and Peter Michler[2] — [1]Otto-von-Guericke-University Magdeburg, Institut of Experimental Physics, Germany — [2]Universität Stuttgart, Institut Für Halbleiteroptik und Funktionelle Grenzflächen, Germany

The change of the spontaneous emission properties by the resonator of a planar VCSEL structure was analyzed using spatially resolved photoluminescence (PL). The samples consists of a λ GaInP cavity embedding InP quantum dots (QDs) as active medium grown on top of an 45 layer AlAs/$Al_{0.5}$GaAs bottom distributed Bragg reflector (DBR). For comparison samples without, 10 AlAs/$Al_{0.5}$GaAs and 34 $Al_{0.5}$GaAs/$Al_{0.95}$GaAs layer pairs were grown. Integral PL spectra taken at each sample show a dominant QD emission in the red spectral range at 1.84 eV.

To achieve a stronger carrier confinement the InP-QDs were embedded inside an AlGaInP cavity, too. PL spectra taken at the structure without top DBR show again QD emission at 1.84 eV. In addition a second emission line at 1.63 eV arises from the formation of different type of QDs.

The optical and structural behavior of both QD species was investigated using excitation and temperature dependent PL as well as scanning electron and atomic force microscopy.

HL 85.21 Thu 18:00 P4

Polariton lasing from a GaAs microcavity: a temperature dependent analysis in the spectral and temporal domain — •Jean-Sebastian Tempel[1], Franziska Veit[1], Marc Assmann[1], Lars Erik Kreilkamp[1], Manfred Bayer[1], Arash Rahimi-Iman[2], Andreas Löffler[2], Sven Höfling[2], Stephan Reitzenstein[2], Lukas Worschech[2], and Alfred Forchel[2] — [1]Experimentelle Physik 2, Technische Universität Dortmund, D-44221 Dortmund, Germany — [2]Technische Physik, Physikalisches Institut, Wilhelm Conrad Röntgen Research Center for Complex Material Systems, Universität Würzburg, D-97074 Würzburg, Germany

We present a spectral and temporal analysis of the emission from a strongly coupled GaAs/GaAlAs microcavity in the temperature range 10-110K. Two distinct transitions in the ground state emission from the lower polariton branch are observed up to 70K; thereby, we evidence polariton lasing in the pump power regime between the thresholds. In particular, we show that the two transitions are clearly evidenced in the emission pulse duration and in the photon statistics based on the second-order correlation function. With further increasing temperature up to 110K changes in the spectral as well as in the temporal domain are observed.

HL 85.22 Thu 18:00 P4

Solitary pulse propagation through quantum dot media — •Matthias-René Dachner, Maria Schuld, Harald Engel, and Andreas Knorr — Institut für Theoretische Physik, Technische Universität Berlin, Germany

The propagation of optical pulses through quantum dot media is investigated. We concentrate on solitary solutions in the conservative and the gradual transition to the dissipative regime. The influence of dissipation and pumping on the solutions is taken into account microscopically, by means of phonon assisted quantum dot–wetting layer interaction. We present numerical studies which are carried out by solving the Maxwell-Bloch equations using the finite difference time domain (FDTD) approach and compare the results to solutions of a microscopically derived Ginzburg-Landau equation.

HL 85.23 Thu 18:00 P4

Ultrafast X-Ray Diffraction on Photoexcited Superlattices: Simulation and Experiment — •Marc Herzog[1], Daniel Schick[1], Ionela Vrejoiu[2], and Matias Bargheer[1,3] — [1]Institut für Physik und Astronomie, Universität Potsdam, Potsdam, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany — [3]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany

Ultrafast x-ray diffraction (XRD) is a well-suited method to monitor and hence understand the details of atomic motions in a solid-state material on its intrinsic timescales. However, the interpretation is not always straightforward. This presentation focuses on time-resolved XRD on superlattices (SL) in which photoexcited coherent acoustic phonons modulate the x-ray structure factor of various SL Bragg reflections [1]. The resulting time-dependent strain field manifests itself in transient changes of diffraction efficiencies and shifts of the Bragg angles. From the observation of transient rocking curves we can deduce the structural dynamics initiated by an optical pump pulse and thereby gain knowledge of material properties as well as excitation and coupling mechanisms. We analyze a linear-chain model to simulate the strain field and use dynamical x-ray diffraction theory to calculate the corresponding rocking curves. We identify general features of the transient x-ray reflections of such optically excited SLs and compare the predictions to experimental results. We find almost perfect agreements for a large range of linear and non-linear phenomena and different samples.

[1] Herzog et al., Appl. Phys. Lett. 96, 161906 (2010).

HL 85.24 Thu 18:00 P4

Ultrafast X-Ray Diffraction on a STO/SRO Superlattice — •Daniel Schick[1], Marc Herzog[1], Clemens von Korff Schmising[2], Peter Gaal[1], and Matias Bargheer[1] — [1]Institut für Physik und Astronomie, Universität Potsdam, Karl-Liebknecht-Str. 24-25, 14476 Potsdam, Germany — [2]Atomic Physics Division, Department of Physics, Lund University, P.O. Box 118, SE-221 00 Lund, Sweden

Ultrafast x-ray diffraction is capable of probing atomic motions on the fs-timescale. With the new laser-driven table-top plasma x-ray source at the University of Potsdam we are able to generate $\approx$ 100 fs pulses of Cu K_α radiation with a repetition rate of 1 kHz and a total flux of 5×10^5 ph/s on the sample.

Here we compare ultrafast optical reflectivity changes and ultrafast x-ray diffraction data of a $SrTiO_3$/$SrRuO_3$ superlattice (SL) in order to highlight the relative phase of oscillations in all-optical pump-probe data to the phase of the atomic motion. For high pump fluences we

observed for the first time that on longer time scales (15 ps) the Bragg-peaks not only shift due to the lattice expansion but rather split into two separate Bragg-peaks, which can accurately be predicted by simulations of the phonon dynamics in a linear chain model and dynamical x-ray diffraction theory.

HL 85.25 Thu 18:00 P4

Ultrafast optical spectroscopy of layered hole-doped manganites — •Lena Maerten, Marc Herzog, and Matias Bargheer — Institut für Physik und Astronomie, Universität Potsdam

Sr-doped perovskite oxide $LaMnO_3$ is widely studied for its ferromagnet to paramagnet and concomitant metal to insulator phase transition. Inserting a monolayer of SrO following each n unit cells of $(LaSr)MnO_3$ (Ruddlesden-Popper Series) introduces an intrinsic superlattice structure with strongly anisotropic properties such as a reduced dimensionality of the electron gas. Alternatively, artificial superlattices with dielectric oxides as interlayers can be prepared. Ultrafast optical spectroscopy reveals on which timescales the coupled electronic, lattice and spin degrees of freedom interact. Using IR pump / white-light probe and NOPA-based pump-probe techniques we measure transient reflectivity curves of bulk ($n \to \infty$) and layered ($n = 2$, $n = 3$) $SrO(La_{0.65}Sr_{0.35}MnO_3)_n$ for temperatures above and below the ferromagnetic transition. Fast electronic heating, consecutive electron-phonon coupling and a slow transfer of energy into the magnetic system can be observed. We discuss transient spectral changes and the build-up of zone-folded coherent acoustic phonons in the layered samples.

HL 85.26 Thu 18:00 P4

Pump-Probe Spectroscopy on Superlattices: Experiment and Simulation — •Andre Bojahr, Marc Herzog, Lena Maerten und Matias Bargheer — Institut für Physik und Astronomie, Universität Potsdam, Potsdam, Germany

We present an experimental setup for highly-sensitive pump-probe measurements using a mode-locked Ti:Sa oscillator at 80 MHz in the weak excitation regime ($20\,\mu J/cm^2$). To reach a sensitivity on the order of $\Delta R/R_0 = 10^{-9}$, we rapidly scan the delay line. This setup enables us to conduct high-precision optical experiments with a time-resolution of about 100 fs. In particular, we show transient reflectivity measurements on weakly excited oxide superlattices which exhibit modulations due to the generation of coherent acoustic phonons resulting in standing and propagating strain waves. The results are compared to strong-excitation experiments with kHz amplifier systems in which the observed reflectivity oscillations are phase-shifted. In order to gain understanding, we propose a model that allows the calculation of the transient reflectivity from the modulation of optical properties by the time-dependent strain field within the sample.

HL 85.27 Thu 18:00 P4

Photocurrents in Semiconductor Carbon Nanotubes with Spin-Orbit Interaction — Hong Liu[1,2], Huynh Thanh Duc[1], Stefan Schumacher[1], and •Torsten Meier[1] — [1]Department Physik and CeOPP, Universität Paderborn, D-33098 Paderborn, Germany — [2]Physics Department, Nanjing Normal University, Nanjing 210046, China

In recent years, single-walled carbon nanotubes (SWCNTs) have received widespread attention due to their perfect quasi-one-dimensional structure and unique physical properties, as well as their potential for applications. In the present work, we calculate the band structure of SWCNTs using an atomistic tight-binding model including spin-orbit interaction[1]. We combine this approach with a many-particle calculation of the nonlinear optical response using multi-band semiconductor Bloch equations[2]. We show that, for SWCNTs lacking inversion symmetry, the intrinsic spin-orbit interaction can give rise to single-color photoinduced charge and spin currents. In particular, we study the influence of excitonic effects on these photoinduced currents and draw the analogy to recent investigations on single-color injection of photocurrents in semiconductor quantum wells[2].

[1]Hong Liu, Physica B **406**, 104-107 (2011)

[2]Huynh Thanh Duc, Jens Förstner, and Torsten Meier, Phys. Rev. B **82**, 115316 (2010).

HL 85.28 Thu 18:00 P4

Analysis of Multidimensional Fourier Transform Spectroscopy for Semiconductors with a Phenomenological Level Model — •Christian Wiebeler, Matthias Reichelt, and Torsten Meier — Department of Physics and CeOPP, University of Paderborn, Warburger Str. 100, D-33098 Paderborn, Germany

Optical two-dimensional Fourier transform spectroscopy has been used to study the properties of semiconductor nanostructures in four-wave-mixing like experiments. [1] Applying a phenomenological level model, we numerically and analytically analyze the main features of excitonic and biexcitonic contributions [2] in a semiconductor quantum well by solving the optical Bloch equations. The method is extended to three-dimensional Fourier transform spectroscopy [3] to investigate a recent experiment. [4].

[1] K. W. Stone et al. Science **324**, 1169 - 1173 (2009).
[2] T. Zhang et al. Proc. Nat. Acad. Sci. **104**, 14227 (2007).
[3] C. Wiebeler, *Modellrechnungen zur mehrdimensionalen Spektroskopie exzitonischer Resonanzen in Halbleiter-Nanostrukturen*, Bachelor Thesis, University of Paderborn (2010).
[4] S. Cundiff, private communication.

HL 85.29 Thu 18:00 P4

Numerical analysis of strong coupling in an absorber-cavity system with two-dimensional Fourier-transform spectroscopy — •Peter Kölling, Matthias Reichelt, and Torsten Meier — Universität Paderborn, Warburger Str. 100, 33098 Paderborn

Strongly coupled absorber-cavity systems have become an important research topic in optics and solid state physics[1]. In this work, we present different simulations of a Four-Wave-Mixing experiment on the basis of a self-consistent Finite-Difference-Time-Domain method in combination with two-dimensional Fourier-transform spectroscopy[2].

[1] Reithmaier et al., Nature 432, 197 (2004)
[2] T. Zhang et al., Proceedings of the National Academy of Sciences of the USA 104, 14227-14232 (2007)

HL 85.30 Thu 18:00 P4

Anisotropic and spin polarization dependent spin dephasing in a 110-grown high-mobility AlGaAs/GaAs quantum well measured by resonant spin amplification technique — •M. Griesbeck[1], V. Lechner[1], I. Caspers[1], M. Glazov[3], T. Korn[1], D. Schuh[1], W. Wegscheider[1,2], and C. Schüller[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, 93040 Regensburg, Germany — [2]present adress: ETH Zürich, 8093 Zürich, Switzerland — [3]A.F. Ioffe Physical-Technical Institute, 194021 St. Petersburg, Russia

The spin dynamics in zincblende-based two-dimensional electron systems (2DESs) are dominated in many cases by the D'yakonov-Perel spin dephasing mechanism and the underlying spin orbit (SO) fields. One exception can be found in symmetrically grown and doped AlGaAs/GaAs quantum wells with the growth axis along the 110-direction, where the Rashba contribution is neglectable and the effective Dresselhaus type SO field is perpendicular to the sample plane. In such a system, consisting of a 30 nm-wide double-sided δ-doped single quantum well with a very high mobility of about 3 million cm^2/Vs, we observed the expected strongly anisotropic spin lifetimes for in- and out-of-plane spin orientations by resonant spin amplification (RSA) measurements. In our experiments, the ratio of in-plane and out-of-plane spin lifetimes is strongly dependent on the sample temperature, the excitation density and also the initial spin polarization of the 2DES. The shape of the RSA traces is modeled using an analytical expression, from which the SDTs are extracted.

HL 85.31 Thu 18:00 P4

Spin dephasing anisotropy in two-dimensional electron systems: dependence on temperature and quantum well width — •Michael Griesbeck[1], Dominik Waller[1], Gerd Plechinger[1], Elisabeth Leierseder[1], Tobias Korn[1], Dieter Schuh[1], Werner Wegscheider[1,2], and Christian Schüller[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, 93040 Regensburg, Germany — [2]present adress: Laboratorium für Festkörperphysik, ETH Zürich, 8093 Zürich, Switzerland

The spin dynamics in most AlGaAs/GaAs-based two-dimensional electron systems are governed by the D'yakonov-Perel spin dephasing mechanism, which results from the underlying spin-orbit (SO) fields. In samples with an asymmetric growth profile, there are contributions to the effective internal SO fields mainly due to the lack of inversion symmetry of the crystal structure, as well as the built-in electric field caused by the asymmetric band profile. The different symmetries of the

Dresselhaus and Rashba SO fields lead to the well-known spin dephasing anisotropy (SDA), where the spin dephasing time strongly depends on the spin orientation. In this study we have investigated the temperature dependence of the SDA in samples with different quantum well width, ranging from 10 nm to 25 nm. By means of time-resolved Kerr rotation technique we were able to determine the relative strengths of Dresselhaus and Rashba SO fields from liquid Helium temperature up to 130 K, including the interesting case, where the two contributions have the same strength. Such a system could be a working base of the proposed non-ballistic spin-FET.

HL 85.32 Thu 18:00 P4

Generation of coherent and incoherent LO phonons by optical excitation of electrically biased quantum wells — •Thomas Papenkort[1], Tilmann Kuhn[1], and Vollrath Martin Axt[2] — [1]Institut für Festkörpertheorie, Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany — [2]Institut für Theoretische Physik III, Universität Bayreuth, 95440 Bayreuth, Germany

Coherent phonons in solids can be generated by optical excitation in a number of different ways, which depend on the material, its structure and the excitation conditions. Although it is the electronic subsystem which the light field predominantly couples to, its detailed characteristics and dynamics can often be left out when explaining the mechanism of phonon generation. In this contribution we will focus on the opposite case where the dynamics of the electronic subsystem plays a vital role to the generation of coherent phonons. An example is the resonant generation of coherent phonons in quantum wells as observed in recent experiments by Mizoguchi et al. [Appl. Phys. Lett. 94, 171105 (2009)], in which a strong coherent phonon amplitude has been achieved by tuning an electronic quantum beat to the LO phonon frequency. We show quantum kinetic calculations of the electronic and phononic dynamics in an optically driven quantum well. We find that the resonant mechanism is very efficient in generating coherent phonons when compared to other mechanisms, but still most of the energy goes into incoherent phonons. Our model also reproduces the limiting cases of phonon generation in which an effective direct coupling of phonons and light field can be assumed.

HL 85.33 Thu 18:00 P4

Squeezing of lattice displacement due to anharmonic decay of phonons in a semiconductor quantum dot — •Jonas Daniels[1], Tilmann Kuhn[1], and Vollrath Martin Axt[2] — [1]Institut für Festkörpertheorie, Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster — [2]Institut für Theoretische Physik III, Universität Bayreuth, 95440 Bayreuth

Squeezed states of light have attracted large interest due to a possible reduction in the noise limit of quantum measurements. A standard tool for the generation of squeezed light is parametric down conversion. In many semiconductor materials similar processes exist for phonons, e.g., the anharmonic decay of a longitudinal optic (LO) phonon into a pair of longitudinal acoustic (LA) phonons. Here we study theoretically the fluctuation properties of the lattice displacement and the lattice momentum connected to the LA phonons generated by this decay process. We consider the impulsive creation of an exciton in a semiconductor quantum dot structure. This is accompanied by the generation of LO phonons, which then may decay into entangled pairs of LA phonons. We perform quantum kinetic calculations to analyze the lattice fluctuations related to these LA phonons. We find that a squeezing of the lattice fluctuations occurs, which is confined within the dot area, although LA phonon wave packets travel out of the dot. The strength and the localization of the squeezing effect can be manipulated by an external electric field which strongly affects the coupling of the exciton to the LO phonons and thus the generation process of the LO phonons.

HL 85.34 Thu 18:00 P4

Output control by quantum focusing in multiterminal billiards — •Christian Morfonios[1], Daniel Buchholz[2], and Peter Schmelcher[1] — [1]Zentrum für Optische Quantentechnologien, Universität Hamburg, Germany — [2]Theoretische Chemie, Physikalisch-Chemisches Institut, Universität Heidelberg, Germany

By exploring the four-terminal transmission of a half-elliptic open quantum billiard in dependence of its geometry and an applied magnetic field, the possibility to construct a controllable quantum cross-junction between its terminals is demonstrated. Depending on the eccentricity of the half-ellipse and the width and placement of the leads, high transmittivity at zero magnetic field is reached through states guided along the curved boundary or focused onto the straight boundary of the billiard. For small eccentricity, attachment of leads at the ellipse foci can yield optimized corresponding transmission, while depart from this condition demonstrates the inapplicability of purely classical considerations in the deep quantum regime. The geometrically achieved high transmittivity is altered by the phase-modulating and deflecting effect of the magnetic field, which switches the pairs of efficiently connected leads. At higher field strengths edge states form and the multiterminal transmission coefficients are determined by the topology of the system. The combination of magnetotransport with geometrically controlled transmission leads to an efficient control of pathways for a charged particle through the multiterminal structure, which is of advantage in designing transport through nanoelectronic devices.

HL 85.35 Thu 18:00 P4

Linear and non-linear properties of ballistic electron-focusing devices — •Arkadius Ganczarczyk[1], Martin Geller[1], Axel Lorke[1], Dirk Reuter[2], and Andreas D. Wieck[2] — [1]Experimental Physics and CeNIDE, Universität Duisburg-Essen — [2]Chair of Applied Solid State Physics, Ruhr-Universität Bochum

Ballistic electron focusing in nanostructured, two-dimensional electron gases was first demonstrated more than 20 years ago [1]. While the linear transport characteristics of such devices were examined in detail, possible nonlinear effects of the device were investigated to a lesser extent so far. However, non-linear transport may be of great interest for possible functional devices such as ballistic rectifiers and transistors. In this work detailed studies of non-linear (and linear) transport properties of ballistic electron focusing devices are presented. For increasing negative injection bias (emission of electrons above the Fermi energy E_F), we observe an increase in the resonant magnetic field in agreement with the increased velocity of the injected electrons. For small positive bias, a similar electron focusing pattern is observed as for negative bias, which can be understood in the framework of electron-hole-symmetry. For increasing positive bias, however, the resonances are shifted towards smaller magnetic fields, indicating that the transport can also be probed for (missing) carriers below E_F [2].

[1] C.W.J. Beenakker *et al.*, Europhys. Lett. **7**, 359 (1988).
[2] J.G. Williamson *et al.*, Phys. Rev. B **41**, 1207 (1990); Surf. Sci. **229**, 303 (1990).

HL 85.36 Thu 18:00 P4

Boltzmann equation approach to rectification at a potential step — •Stephan Rojek, Daniel Urban, Fred Hucht, and Jürgen König — Theoretische Physik, Universität Duisburg-Essen and CeNIDE, 47048 Duisburg, Germany

Ref. [1, 2] shows an experimental analysis of a two-dimensional electron gas with two regions separated by a potential step. The difference in the potential originates from two parallel gates on top of the two-dimensional electron gas.

A bias voltage parallel to the potential step leads to a transverse voltage proportional to the square of the applied bias voltage. This effect can be exploited for rectification, since the transverse voltage does not depend on the bias polarity.

We model the system by means of the Boltzmann equation in the relaxation time approximation. We allow the scattering times to be energy dependent and consider different relaxation times for scattering processes with energy transfer larger and lower than k_BT. In order to study the rectification effects, the distribution function has to be calculated to second order in the applied electric field. We discuss the relevance of the determined transverse voltage for the measurements in Ref. [1, 2].

[1] A. Ganczarczyk *et al.*, arXiv:0804.0689v3 (2009).
[2] A. Ganczarczyk *et al.*, AIP Conf. Proc. **1199**, 143 (2009).

HL 85.37 Thu 18:00 P4

Transport properties of ferromagnet-semiconductor hybrids — •Lakshmy Ravindran[1], Rasmus Ballmer[1], Sven Buchholz[1], Saskia F. Fischer[2], Ulrich Kunze[1], Arne Ludwig[3], Dirk Reuter[3], and Andreas Wieck[3] — [1]Werkstoffe und Nanoelektronik, Ruhr-Universität Bochum, D-44780 Bochum, Germany — [2]Neue Materialien, Humboldt Universität zu Berlin, D-12489 Berlin, Germany — [3]Angewandte Festkörperphysik, Ruhr-Universität Bochum, D-44780 Bochum, Germany

Ferromagnet-semiconductor hybrid devices integrate nanoscale magnets with semiconductor nanostructures leading to magnetoelectronic devices with high storage density and reduced energy dissipation. In

a ferromagnet-semiconductor hybrid device the resistivity of the semiconductor could be controlled by the ferromagnetic element [1]. Our devices consist of GaAS/AlGaAs heterostructure field effect transistor(HFET) with a ferromagnetic Permalloy(Py) nanogate only 35 nm apart from the GaAs channel. The nanostructuring is done with electron beam lithography and the GaAs channel is patterned by shallow wet etching. The 20 nm thick Py gate is fabricated by electron beam lithography, metal evaporation and lift-off process. The angle-dependent magnetoresistance measurements in external low magnetic fields of the order of 150 mT are done with lock-in technology. The measurements infer a positive magnetoresistance for an external magnetic field applied in the longitudinal direction which is due to the magnetic fringing fields emanating from the Py gate.

[1] J.P.Bird, et al., IEEE Trans, Magn, 44, 4707(2008)

HL 85.38 Thu 18:00 P4

Concept of a ballistic transfer device in a GaAs/AlGaAs 4-terminal structure using electron refraction — •Michael Szelong[1], Daniel Salloch[1], Ulrich Kunze[1], Dirk Reuter[2], and Andreas Wieck[2] — [1]Lehrstuhl für Werkstoffe und Nanoelektronik, Ruhr-Universität Bochum — [2]Lehrstuhl für angewandte Festkörperphysik, Ruhr-Universität Bochum

We present a concept of a ballistic four-terminal device based on electron trajectory refraction, resembling a directional coupler. The device structure consists of a straight stem (1 μm wide and 2 μm long) while two branches merge at each end of the stem under an angle of 45° (27°) with the stem's longer axis of symmetry. Devices with different angles and injector widths are processed on a high-mobility GaAs/AlGaAs heterostructure with a two-dimensional electron density and mobility of $n_{2D} = 2 \cdot 10^{11}\text{cm}^{-2}$ and $\mu = 2.4 \cdot 10^6\text{cm}^2/\text{Vs}$, respectively, resulting in a mean free path of 18 μm at $T = 4.2$ K. A mix-and-match process is used which combines the advantages of nano-scale electron beam lithography with time-saving UV-lithography. The resist pattern is transferred into the heterostructure by wet etching in a citric acid solution. After contact alloying a local Schottky-gate is deposited onto the stem. Electron trajectories, starting at one branch, will be refracted at the boundary of the gate-controlled region according to Snell's law of electron refraction [1]. Depending on the direction of refraction electrons will be reflected more or less often at the stem's boundaries and finally hit one of the opposite branches.

[1] Spector *et al.*, Appl. Phys. Lett. **56**, 2433 (1990)

HL 85.39 Thu 18:00 P4

Preparation of quantum transport in GaAs/AlGaAs core/shell nanowires — •Pascal Heintzmann, Stephan Wirths, Christian Blömers, Karl Weis, Kamil Sladek, Andreas Penz, Hilde Hardtdegen, Stefan Trellenkamp, Thomas Schäpers, and Detlef Grützmacher — Institut für Bio- und Nanosysteme (IBN-1), Forschungszentrum Jülich, 52425 Jülich, Germany

One of the key advantages of the growth of self assembled nanowires is the possibility to fabricate axial and radial heterostructures in a single growth step. Here we focus on GaAs/AlGaAs core/shell structures in order to achieve one-dimensional electron confinement in the GaAs core. These core/shell heterostructure nanowires are promising for improved electron mobility due to reduced surface impurity scattering.

The GaAs/AlGaAs nanowires used for our investigations were grown by selective area metal organic vapor phase epitaxy on a GaAs (111) substrate. Our wires consist of a GaAs core surrounded by an intrinsic AlGaAs layer, an n-doped AlGaAs layer, an intrinsic AlGaAs layer and finally a thin GaAs cap layer. For electrical characterization the wires were removed mechanically from the original substrate and subsequently placed on a prepattered SiO_2-covered Si (100) substrate. Each wire was contacted individually with Ni/AuGe/Ni/Au electrodes using electron beam lithography. In order to optimize the contact resistance the nanowires were annealed in a rapid thermal processing furnace for different times and temperatures. By performing 2-terminal and 4-terminal transport measurements information on the contact resistance and nanowire conductivity is obtained.

HL 85.40 Thu 18:00 P4

Effect of the interface structure on the cross-plane thermoelectric transport in laterally microstructured ZnO-based stripe structures — •Steve Petznick, Gerd Homm, Martin Eickhoff, Bruno K. Meyer, and Peter J. Klar — 1. Physikalisches Institut, Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, 35392 Gießen, Deutschland

As a starting material MBE-grown ZnO was used, into which stripe structures perpendicular to the direction of the heat gradient or external electric field, and thus the current, were microstructured using photolithography, followed by wet-chemical etching. After the etching ZnO:Ga was sputtered into the grooves between the host material.

As the current must flow through the interfaces, all interface parameters will effect the transport behavior significantly. The shape of the interfaces of different samples is varied systematically to simulate different surface roughnesses. Temperature dependent measurements of the Seebeck coefficient and the electric conductivity will be performed in the temperature range from 80 K to 300 K. The results will be compared with a theoretical simulation based on a network model and other measurement series.

HL 85.41 Thu 18:00 P4

Electrical transport properties of TiO_2 single nanotube — •Tuhin Subhra Maity[1], José Quiquia[1], Winfried Böhlmann[1], Pablo Esquinazi[1], Tobias Ruff[2], and Patrik Schmuki[2] — [1]Division of Superconductivity and Magnetism, Institute for Experimental Physics II,University of Leipzig — [2]Department of Materials Science and Engineering, University of Erlangen Nüremberg

In the present work we investigate the electrical conductivity of single TiO_2 nanotubes. TiO_2 nanotubes were synthesized by anodization of Ti in fluoride containing electrolytes. For the characterization of the sample morphology scanning electron microscope and EDX-detector was used. The structural property was determined by XRD. Electron lithography method was used to make the gold contact on the nanotubes. The electrical properties of single nanotubes were measured at different temperatures and magnetic fields. Resistivity values at room temperature were found of the order of $\sim 10^{-2}$ Ωcm. Furthermore, we explored the effects of atmospheric conditions and light irradiation on conductivity of single TiO_2 nanotubes.

HL 85.42 Thu 18:00 P4

Temperature dependent transport measurements in quasi-freestanding graphene on SiC(0001) — •Epaminondas Karaissaridis[1], Sonja Weingart[1], Claudia Bock[1], Ulrich Kunze[1], Florian Speck[2], and Thomas Seyller[2] — [1]Werkstoffe und Nanoelektronik, Ruhr-Universität Bochum — [2]Technische Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg

We report on magneto- and ballistic transport measurements in 2D Hall bars and 1D orthogonal cross junctions fabricated from quasi-freestanding monolayer graphene on SiC(0001).

The investigated films are produced by conversion of the $(6\sqrt{3} \times 6\sqrt{3})\text{R}30°$ reconstruction into graphene via hydrogen intercalation [1]. The hole concentration of $6 \cdot 10^{12}\,\text{cm}^{-2}$ and a mobility of $1900\,\text{cm}^2(\text{Vs})^{-1}$ are derived from Hall effect measurements at 2D structures. These values are constant in a temperature range of $1.4\,\text{K} \leq T \leq 300\,\text{K}$ and correspond to a constant mean free path of $l_e \approx 50\,\text{nm}$. At $T = 1.4\,\text{K}$ the bend resistance characteristic of the 1D orthogonal cross junctions ($w = 50\,\text{nm}$) shows magnetic field dependent negative peaks indicating ballistic transport. As temperature is increased to $T = 50\,\text{K}$ a transition from the ballistic into the diffusive transport regime is observed. These results demonstrate that additional scattering in 1D systems plays an important role.

[1] F. Speck, *et al.*, Mat. Sci. Forum **645-648**, 629 (2010).

HL 85.43 Thu 18:00 P4

Transport Measurements on Bilayer Graphene Systems — •Alexander W. Heine, Hennrik Schmidt, Patrick Barthold, Thomas Lüdtke, and Rolf J. Haug — Institut für Festkörperphysik, Leibniz Universität Hannover, D-30167 Hannover, Germany

We analyse electronic transport properties of coupled bilayer graphene sheets. Similar to monolayer graphene, bilayer graphene samples show a strong field effect but exhibit a different Berry's phase in Shubnikov-de Haas oscillations. Our samples are prepared by micromechanical exfoliation and placed on top of a silicon wafer with a 330 nm thick layer of silicon dioxide. After that they are contacted using electron beam lithography and structured by plasma etching. Low temperature measurements were performed at temperatures down to 1.5 K in a liquid helium cryostat. The conductivity of the samples shows a strong dependence to an applied backgate voltage. By applying a magnetic field up to 13 T we observed Shubnikov-de Haas oscillations. As expected, the bilayer samples show a Berry's phase different to the one of monolayer graphene. In the vertical resistance plateaus according to the minima of the oscillations are observed with a double step around filling factor zero which is typical for graphene bilayer systems.

HL 85.44 Thu 18:00 P4

Terahertz-Photoleitungsmessungen an Graphen-basierten Strukturen — •Markus Golla[1], Majdi Salman[1,2], Fathi Gouider[1], Yuri.B Vasilyev[3], Hennrik Schmidt[2,4], Rolf. J. Haug[2,4] und Georg Nachtwei[1,2] — [1]Institut für Angewandte Physik, Technische Universität Braunschweig, D-38106 Braunschweig, Germany — [2]Niedersächsische Technische Hochschule, D-38106 Braunschweig, D-38678 Clausthal-Zellerfeld, D-30167 Hannover, Germany — [3]A.F. Ioffe Physical Technical Institute, RUS-194021 St. Petersburg, Russia — [4]Institut für Festkörperphysik, Abt. Nanostrukturen, Leibniz Universität Hannover, D-30167 Hannover, Germany

Wir haben die Photoleitung im THz-Spektralbereich an Graphen-basierten Strukturen gemessen. Um die hier untersuchten Graphen-Proben zu charakterisieren, wurden Messungen des Shubnikov-de Haas-Effekts bei einer Temperatur von $T \approx 4$K und im Bereich der Magnetfelder von $0 \leq B \leq 10$T durchgeführt. Aus diesen Messungen lässt sich die Elektronendichte im Graphen bestimmen. Bei der anschließenden Messung der Photoleitung an den verwendeten Graphenproben wurde zur Erzeugung der THz-Wellen ein p-Ge-Laser verwendet. Dieser ist im Wellenlängenbereich von $120\mu\text{m} \leq \lambda \leq 180\mu\text{m}$ kontinuierlich durchstimmbar. Die monochromatische THz-Strahlung wurde durch einen Wellenleiter, der in flüssigem Helium eingetaucht war, auf unsere Graphen-Probe übertragen.

HL 85.45 Thu 18:00 P4

Thermally activated Transport in Quantum Hall Systems — •Martina Flöser[1], Serge Florens[1], and Thierry Champel[2] — [1]Institut Néel, CNRS-Université Joseph Fourier, Grenoble — [2]LPMMC, CNRS-Université Joseph Fourier, Grenoble

We study the thermally activated charge transport in the regime of the quantum Hall effect, where temperature is smaller than the Landau level spacing, but large compared to the onset of quantum tunneling. We show, using diagrammatic methods within a local conductivity model, that smooth disorder leads to slow fluctuations in the Hall components, and provides a small dissipative conductance. Our results demonstrate a microscopic connection between the macroscopic longitudinal and transverse resistance and the disorder distribution, which can be tested experimentally by simultaneous transport and local spectroscopy measurements.

HL 85.46 Thu 18:00 P4

Transport properties of InAs spin-filter cascades in magnetic fields of different directions and strengths — •Hauke Lehmann, Till Benter, Alexander Buhr, and Jan Jacob — Institut für Angewandte Physik und Zentrum für Mikrostrukturforschung, Universität Hamburg, Jungiusstraße 11, 20355 Hamburg

We present a three-terminal all-semiconductor nanostructure fabricated from an InAs heterostructure, which separates an unpolarized current into two oppositely spin-polarized currents of equal magnitude by the intrinsic spin Hall effect. If this device is fed with an already spin-polarized current, the conductances of its two outputs are different enabling all-electrical detection of the spin polarization in two-stage spin-filter cascades [1]. The transport measurements are conducted at millikelvin temperatures in a DC-biased lock-in technique. Magnetic fields perpendicular to the two-dimensional electron system introduce a Lorenz force that allows inference on the strength of the intrinsic spin Hall effect. In-plane fields normal to the direction of the electrons' motion change the spin-orbit coupling. If the field is applied normal to the center wire that connects the two filter stages, the spin precession length is changed leading to oscillations in the conductance fractions of the second filter's outputs [2]. By applying the field normal to the input wire the separation of spin-up and spin-down electrons in this wire can be tuned.

[1] J. Jacob, G. Meier, S. Peters, T. Matsuyama, U. Merkt, A. Cummings, R. Akis, and D. Ferry. J. Appl. Phys. **105**, 093714 (2009).

[2] P. Brusheim and H. Q. Xu, arXiv: 0810.2186v2 (2009).

HL 85.47 Thu 18:00 P4

Room-temperature nanosecond spin-lifetimes in bulk cubic GaN — Jan Heye Buss[1], Jörg Rudolph[1], •Jeanette Gorewoda[1], Thorsten Schupp[2], Donat As[2], and Daniel Hägele[1] — [1]AG Spektroskopie der kondensierten Materie, Ruhr-Universität Bochum, Germany — [2]Universität Paderborn, Department Physik, Warburger Str. 100, 33095 Paderborn, Germany

The metastable zincblende phase of GaN is a highly interesting material system for semiconductor spintronics due to its small spin-orbit coupling. Systematic investigations of the electron spin dynamics are, however, missing so far. We present time-resolved Kerr-rotation measurements of the temperature and magnetic field dependence of electron spin relaxation in moderately n-doped cubic GaN samples and compare the results with the electron spin dynamics in wurtzite GaN. The higher cubic symmetry of the zincblende phase is shown to lead to significantly slower spin relaxation than in the wurtzite phase with hexagonal symmetry. The room-temperature spin-lifetimes of > 2 ns exceed all values reported for III-V bulk materials so far.

HL 85.48 Thu 18:00 P4

Basic design of a three-terminal semiconductor structure for electrical spin-storage and read-out — •Johannes Zeller, Rouven Diehm, Pablo Asshoff, Andreas Merz, Heinz Kalt, and Michael Hetterich — Karlsruhe Institute of Technology (KIT)

In recent years, spin light-emitting diodes have become well-established devices in the spintronics community. In this contribution, we discuss a novel structure design allowing for spin-injection, prolonged spin-storage and spin-readout with all of these processes controlled individually and all-electrically. This structure consists of a diluted magnetic semiconductor as spin-injector and quantum dots which are selectively loaded with either electrons or holes.

HL 85.49 Thu 18:00 P4

Silicon pin solar cells investigated by multi-frequency EDMR — •Christoph Meier[1], Christian Teutloff[1], Jan Behrends[1], Matthias Fehr[2], Alexander Schnegg[2], Klaus Lips[2], and Robert Bittl[1] — [1]Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Institut für Silizium-Photovoltaik, Helmholtz-Zentrum Berlin für Materialien und Energie, Kekuléstr. 5, 12489 Berlin, Germany

Electrically detected magnetic resonance (EDMR) can be used to investigate paramagnetic centres influencing charge transport in semiconductors even at concentrations well below the sensitivity threshold of conventional electron paramagnetic resonance (EPR). This technique measures conductivity changes in the sample that occur when spin transitions cause an enhancement or a quenching of currents. EDMR was e.g. successfully employed to microcrystalline Si pin solar cells in X-band (9.7 GHz). We present the application of EDMR to Si pin solar cells at Q-band frequency (34 GHz). We could demonstrate a gain of spectral resolution. With multi-frequency EDMR we distinguished between field-dependent and field-independent interactions. Further, we realized EDMR in a non-resonant setup at 94 GHz (W-band) and will show first results.

HL 85.50 Thu 18:00 P4

Low-temperature processed Schottky-gated field-effect transistors based on amorphous oxide channel material — •Michael Lorenz[1], Alexander Lajn[1], Heiko Frenzel[1], Holger von Wenckstern[1], Marius Grundmann[1], Pedro Barquinha[2], Elvira Fortunato[2], and Rodrigo Martins[2] — [1]Universität Leipzig, Fakultät für Physik und Geowissenschaften, Institut für Experimentelle Physik II, Linnéstr. 5, 04103 Leipzig — [2]CENIMAT/I3N, Departamento de Ciência dos Materiais, Faculdade de Ciências e Tecnologia, FCT, Universidade Nova de Lisboa and CEMOP-UNINOVA, 2829-516 Caparica, Portugal

We demonstrate metal-semiconductor field-effect transistors based on room temperature deposited indium-zinc-oxide and gallium-indium-zinc-oxide channel material on Corning 1737 glass substrates by radio-frequency magnetron sputtering. The devices were processed by standard photolithography using lift-off technique and metalization of the electrodes was accomplished by dc-magnetron sputtering. The best devices exhibit a subthreshold swing of S = 69 mV/decade and gate sweep voltages of 1.6 V, reach field-effect mobilities up to 15 cm^2/Vs and on-off-current ratios over 8 orders of magnitude [1]. The influence of a low temperature annealing step ($T = 150°\text{C}$) for the thin-films is furthermore investigated.

[1] M. Lorenz et al., Appl. Phys. Lett., *in press* (2010)

HL 85.51 Thu 18:00 P4

First Principles Investigation of La incorporation in high-κ Dielectric Film of the Field Effect Transistors — •Ebrahim Nadimi[1], Rolf Öttking[2], Philipp Plänitz[2], Martin Trentzsch[3], Torben Kelwing[3], Rick Carter[3], Christian Radehaus[2], and Michael Schreiber[1] — [1]Institut für Physik, Technische Universität Chemnitz — [2]GWT TU Dresden GmbH, Geschäftsstelle Chemnitz — [3]Global Foundries, Dresden

The introduction of high-k dielectric and metal gate in silicon field effect transistors (FETs) has involved many challenges. The key requirements are threshold voltage adjustment, reliability of the gate dielectric, low leakage and high channel mobility. Incorporation of metals such as La, Sr, Nb and Mg into thin HfO2 film has been shown to improve the device in terms of threshold voltage, reliability and leakage current. In this work La doping into the HfO2 were investigated on microscopic level using first principles method. Our calculations show that the doped La atoms are energetically favorable when they replace Hf atoms in the first neighboring lattice site of an oxygen vacancy. Furthermore, their interaction with oxygen vacancy leads to the passivation of O-vacancy defect states. Further calculations in multilayer system (Si/SiO2/HfO2) reveal that La atoms tend to migrate into the SiO2/HfO2 interface. This leads to an induced dipole at the interface, which is responsible for the desirable shift in the band alignment. This work was supported by the German ministry of education and research BMBF under SIMKON project Grant No. 01M3138A. The authors are responsible for the content of this paper.

HL 85.52 Thu 18:00 P4

Transverse thermoelectric devices — •Christina Reitmaier and Hans Lengfellner — University of Regensburg, 93053 Regensburg, Germany

Multilayer structures A−B−A... consisting of alternating layers of a metal A and a semiconductor B can show large anisotropy in their transport properties, depending on the properties of the constituents. Multilayer stacks, prepared of alternating layers of Pb and n-type Bi_2Te_3, were obtained by a heating procedure. Depending on thickness ratio $p = d_{BiTe}/d_{Pb}$, where d_{BiTe} and d_{Pb} are the thicknesses of Bi_2Te_3 and Pb layers, respectively, a large thermoelectric anisotropy up to $\Delta S \approx 200\mu V/K$ was observed. In tilted multilayer structures, where layer planes and sample surface include a nonzero tilt angle, non-vanishing off-diagonal elements in the sample's transport tensors lead to transverse Seebeck- and Peltier effects. Achievable temperature differences and figures of merit for transverse Peltier cooling are discussed and compared with experiments, coefficients of performance for transverse power generation are calculated.

HL 85.53 Thu 18:00 P4

Cascading enables ultrafast gain recovery dynamics of quantum dot semiconductor optical amplifiers — •Niels Majer, Kathy Lüdge, and Eckehard Schöll — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin

Optoelectronic devices based on semiconductor quantum dots are promising candidates for future high speed telecom applications with low operation currents, high temperature stability, low chirp and ultrafast gain recovery dynamics and hence pattern effect free amplification at high bit rates. In this work [1] the ultrafast gain recovery dynamics of a quantum dot semiconductor optical amplifier is investigated on the basis of semiconductor Bloch equations including microscopically calculated carrier-carrier scattering rates between the 2D carrier reservoir and the confined quantum dot ground and first excited state. By analyzing the different scattering contributions we show that the cascading process makes a major contribution to the ultrafast recovery dynamics.

[1] N. Majer, K. Lüdge, and E. Schöll, Phys. Rev. B **82** (2010), in print.

HL 85.54 Thu 18:00 P4

Influence of interface roughness on relaxation rates and optical gain in a quantum cascade laser — •Milan Žeželj[1], Vitomir Milanović[2], Jelena Radovanović[2], and Igor Stanković[1] — [1]Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia — [2]Faculty of Electrical Engineering, University of Belgrade, Bul. kralja Aleksandara 73, 11020 Belgrade, Serbia

We present a model for calculating the optical gain in a midinfrared GaAs/AlGaAs quantum cascade laser in a magnetic field, based on solving the set of rate equations that describe the carrier density in each level, accounting for the optical-phonon and interface roughness scattering processes. The confinement caused by the magnetic field strongly modifies the lifetimes of electrons in the excited state and results in pronounced oscillations of the optical gain as a function of the field. Numerical results are presented for the structure designed to emit at 11.4μm, with the magnetic field varying in the range of 10-60T, mean height of roughness is 0.15nm and correlation length 6nm. The effects of band nonparabolicity are also included. The conclusion of presented work is that influence of interface roughness scattering is not negligible and it gives a very important contribution in calculating optical gain of quantum cascade laser.

HL 85.55 Thu 18:00 P4

Optical Characteristics of an InP/AlGaInP quantum dot laser emitting at 660 nm — •Jan Wagner, Wolfgang-Michael Schulz, Marcus Eichfelder, Robert Rossbach, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen, Universität Stuttgart, Allmandring 3, 70569 Stuttgart, Germany

Semiconductor quantum dot (QD) laser diodes have gained much interest in recent years due to their superiority in many properties over regular quantum well (QW) lasers. Especially in the visible red spectral range (630-710 nm) QD laser would enhance applications like data storage, medical applications e.g. photodynamic therapy (PDT), pumping solid state lasers or display applications e.g. laser projection. Theory predicts better properties compared to standard quantum well (QW) lasers due to the zero-dimensional character of the structure. For example lower threshold current density, higher differential gain, and higher temperature stability are expected. We characterized electrically pulsed InP/AlGaInP quantum dot lasers with different length at different operating parameters, which are pulse width, frequency and temperature. We achieved lasing operation at room temperature with a relatively low threshold current density of 792 A/cm^2 and a lasing wavelength of 660 nm with an optical output power of more than 41 mW per facet.

HL 85.56 Thu 18:00 P4

1550 nm quantum dot lasers with high modal gain — Christian Gilfert, •Vitalii Ivanov, and Johann Peter Reithmaier — Technische Physik, Institute of Nanostructure Technologies and Analytics, University of Kassel, Heinrich-Plett Str. 40, D-34132 Kassel, Germany

In the last years a strong effort was made in the development of InP based quantum dot (QD) structures to obtain high performance 1550 nm lasers. However, most of the work is related to QDash active materials. In this work the conditions for the formation of InAs QDs and QDashes on the quaternary InAlGaAs surfaces, lattice-matched to n-type InP (100) were investigated. It could be shown that the supply of different types of As molecules allow to switch between QDs and QDashes growth modes. A formation of rather round-shaped dots was observed under As2 atmosphere. These new type of QD layers exhibited a significantly reduced height distribution, which reduces the inhomogeneous linewidth to about 23 meV (see APL 96, 191903 (2010)). Based on these QD structures diode lasers with an SCH design were realized. The laser structure consists of 6 QD layers embedded in an InGaAlAs core waveguide and 1700 nm InP top cladding layer. The QD lasers exhibit a low internal absorption of 8 cm-1 and a rather high modal gain of about 60 cm-1, which is nearly a factor of two higher than for any other reported comparable InP based QD laser. We attribute this strong improvement to a much higher spectral gain, which is consistent with the observed very narrow photoluminescence linewidth.

HL 85.57 Thu 18:00 P4

Gain and reflectance measurements of a 1050nm VECSEL chip — •Sebastian Haupt[1,2], Michael Furitsch[1], Hans Lindberg[1], Ines Pietzonka[1], Uwe Strauss[1], and Gerd Bacher[2] — [1]Osram Opto Semiconductors GmbH , Leibnitzstrasse 4, 93055 Regensburg — [2]WET Universität Duisburg-Essen , 47057 Duisburg

Optically pumped Vertical External Cavity Surface Emitting Lasers (VECSELs) have a wide range of applications due to a combination of output power, high efficiency and a good beam quality in the infrared spectral range. Furthermore the visible spectrum is accessible with intra cavity frequency-doubling.

We will present a method to measure the gain of a 1050 nm VECSEL chip based on a resonant periodic gain (RPG) structure with a reflectance measurement. In the case of a VECSEL the reflectance is determined by the Bragg mirror reflectance and the quantum wells. The reflectance is less than one for carrier densities below transparency and more than one above transparency. In this latter we have an amplification of the light and hence a net gain.

This method has enabled us to measure the gain for a wide spectral, pumping power and temperature range. Additionally we study the influence of different VECSEL Chip anti reflection coatings. The measured gain curves are to be found in good agreement with experiments

in laser operation.

HL 85.58 Thu 18:00 P4

Biofunctionalization of ZnO nanowires for DNA sensory applications — Ulrich Christian Schröder[1], •Martin Gnauck[1], Robert Möller[2], Bettina Rudolph[2], Wolfgang Fritzsche[2], and Carsten Ronning[1] — [1]Institute of Solid State Physics, University of Jena, Max-Wien-Platz 1, D-07743 Jena — [2]Institut für Photonische Technologien e.V., Albert-Einstein-Straße 9, D-07745 Jena

In recent years, DNA detecting systems have received a growing interest due to promising fields of application like DNA diagnostics, gene analysis, virus detection or forensic applications[1]. Nanowire-based DNA biosensor allows both miniaturization and easy continuous monitoring of a detection signal by electrical means. The label free detection scheme based on electrochemical changes of the surface potential during immobilization of specific DNA probes was heretofore mainly studied for silicon [2]. In this work a surface decoration process with bifunctional molecules known as silanization was applied to VLS-grown ZnO nanowires which both feature a large sensitivity for surface modification, are biocompatible and easy to synthesize as well. Successfully bound DNA was proved by fluorescence microscopy. Dielectrophoresis (DEP) was chosen and optimized for quickly contacting the ZnO nanowires. Furthermore, electrical signal characterization was performed in preparation for DNA sensory applications.

[1] Sassolas, A.; Leca-Bouvier, B. D. & Blum, L. J., Chemical Reviews, Amer Chemical Soc, 2008, 108, 109-139; [2] Corso, C. D.; Dickherber, A. & Hunt, W. D., Elsevier Advanced Technology, 2008, 24, 805-811

HL 85.59 Thu 18:00 P4

Preparation and immobilization of noble metal nanoparticles for plasmonic solar cells — •Ruoli Wang[1,2], Martin Pitzer[1,2], DongZhi Hu[1,2], Daniel M. Schaadt[1,2], and Ljiljana Fruk[2] — [1]Institut für Angewandte Physik,Karlsruhe Institut für Technologie (KIT),76131 Karlsruhe — [2]DFG Centrum für Funktionelle Nanostrukturen (CFN), KIT

Thin-film solar cells are of high interest due to good electrical properties and low material consumption. Traditional thin-film cells, however, have considerable transmission losses because of the reduced absorption volume. A promising way to enhance absorption in the active layer is the light-trapping by plasmonic nanostructures. Metallic nanoparticles have in particular shown large enhancement of the photocurrent in thin-film devices. In this poster, we present preparation of Au,Ag and Pt nanoparticles by polyol method and seed mediated methods for use in plasmonic solar cells. Polyol method typically uses ethylene glycol as the solvent and reducing agent,and in seed-mediated synthesis small nanoparticle seeds are first prepared and then used to promote the growth of different shapes of nanoparticles. We particulary focus on the use of nanocubes and nanospheres for solar cell design. Following the nanoparticle preparation, a new method to immobilize particles on GaAs surfaces via covalent chemical bonds has been developed which prevents agglomerations and allows control of the surface density. Photocurrent spectra of GaAs pin solar cells with and without particles have been recorded. These measurements show the dependence of the photocurrent enhancement on particle material, shape and density.

HL 85.60 Thu 18:00 P4

Semiconductor-Insulator-Semiconductor solar cells on wet-chemically etched silicon nanowire carpets using different tunnel barrier materials — •Martin Schreivogel[1], Björn Hoffmann[1], Gerald Brönstrup[1], Vladimir Sivakov[1], and Silke Christiansen[1,2] — [1]Institut für Photonische Technologien, Jena — [2]Max-Planck-Institut für die Physik des Lichts, Erlangen

Nanostructured semiconductor substrates are an intensively investigated possibility to improve solar cell performance. For this purpose we prepare chemically etched silicon nanowire carpets with adjustable geometrical structure. The etching process is cheap and easily scalable, is performed at room temperature and uses no photolithography-step. The produced nanowire carpets show high absorption over a broad spectral range. The nanowires are used as substrate for semiconductor-insulator-semiconductor (SIS) solar cells. Therefore we generate a very thin layer of an insulating oxide on the nanowires and deposit a transparent conductive oxide (TCO) as top electrode. The insulating tunnel barrier is prepared either by chemically oxidizing the substrate material receiving silicon oxide or by depositing aluminium oxide by atomic layer deposition (ALD). Sputtered or ALD-Aluminum-doped zinc oxide (AZO) is used as TCO. We characterize the solar cells by I-V-curve measurements and calculation of the pseudo efficiency, which is reproducibly more than 8%. The structure of the produced devices is investigated by SEM and FIB. To prove the electrical contribution of the nanowires we performed electron beam induced current (EBIC) measurements on solar cell cross sections.

HL 85.61 Thu 18:00 P4

Crystallographic structure and grain size of polycrystalline Cu_2ZnSnS_4 nanoparticles and thin films studied with XRD and SEM — •Folker Zutz, Christine Chory, Ingo Riedel, and Jürgen Parisi — Thin Film Photovoltaics, Energy and Semiconductor Research Laboratory, University of Oldenburg, D-26111 Oldenburg

Cu_2ZnSnS_4 (CZTS) is a compound semiconductor with an absorption coefficient of $>10^4 cm^{-1}$ and energy gap of about 1.5 eV. Because CZTS is comprised of abundant and non-toxic precursor elements the semiconductor represents an attractive material for low-cost thin film solar cells. CZTS nanoparticles (NP) were prepared in a low-temperature colloidal synthesis yielding high amounts per synthesis cycle. For thin film deposition the NPs were converted to an ink which can be processed to thin films via printing techniques. Finally, the thin films were annealed in argon atmosphere at different temperatures in order to control the growth of microcrystallites. The photoelectrical quality of the semiconductor sensitively depends on the relative concentrations of the precursor elements (band gap, crystallographic phases) and the average grain size (charge transport). We report on structural investigations (X-ray diffraction, electron microscopy) of CZTS dried powders and thin films processed from inks with varying chemical compositions. Further, the evolution of the grain size was studied as function of the annealing temperature.

HL 85.62 Thu 18:00 P4

Spatially resolved photoluminescence and AFM measurements on Cu(In,Ga)Se_2-based thin film absorbers prepared with different throughput speeds — •Max Meessen[1], Oliver Neumann[1], Stephan J. Heise[1], Rudolf Brüggemann[1], Wolfram Witte[2], Dimitrios Hariskos[2], and Gottfried H. Bauer[1] — [1]Institut für Physik, Carl von Ossietzky Universität Oldenburg, Germany — [2]Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg (ZSW), Stuttgart, Germany

We study the behavior and interdependence of quantities such as photoluminescence (PL) yield, quasi-Fermi level splitting and AFM-determined surface roughness on CIGS thin-film absorbers with different thicknesses between 0.25 and 3 μm achieved by varying the throughput speed in an in-line physical vapor deposition (PVD) process. These quantities are studied on the macroscopic as well as on the microscopic scale with a resolution of approximately 1 μm. It is shown that the structural sizes of the inhomogeneities of the absorber layer itself and its lateral photoluminescence properties decrease with decreasing absorber thickness. These results are compared to those on samples thinned by bromine-methanol etching.

Furthermore, we show that varying the thickness of the CdS buffer layer on top of the absorber influences surface recombination and thereby PL yield and quasi-Fermi level splitting. A decrease in surface recombination at higher buffer thicknesses has to be weighed against the increase in absorption in the buffer layer, which in turn decreases carrier generation in the absorber layer.

HL 85.63 Thu 18:00 P4

Variation of sulfur content in Cu(In,Ga)(S,Se)2 thin film solar cells — •Martin Knipper, Robin Knecht, Ingo Riedel, and Jürgen Parisi — Energy and Semiconductor Research Laboratory, Department of Physics, University of Oldenburg, 26111 Oldenburg, Germany

Chalcopyrite thin film solar cells made of the compound semiconductor Cu(In,Ga)$(S,Se)_2$ (CIGSSe) have a strong potential for achieving high efficiencies at low production costs. Volume production of CIGSSe-modules has already started to exploit their favorable attributes such as low cost processing and reasonable module efficiency. In this study we studied industrially produced CIGSSe modules obtained from rapid thermal processing (RTP) for sulfurization. In detail, we investigated the effect of sulfur offer and RTP temperature (500°C to 580°C) on the photoelectric characteristics of small-area solar cells cut from the modules. Current-voltage profiling under standard test conditions revealed a strong influence of the particular process recipe on the open circuit voltage whereas significant variations of the maximum quantum efficiency can be observed. X-ray diffraction was employed to relate

these effects to the crystallographic structure of the actual CIGSSe films. Lock-in thermographic imaging was employed to link apparent film inhomogeneities and disruptions to the specific process recipe.

HL 85.64 Thu 18:00 P4

Series resistance mapping of Cu(In,Ga)Se_2 solar cells by voltage dependent electroluminescence — •Felix Daume[1,2], Christian Scheit[1], Stefan Puttnins[1,2], Andreas Rahm[1], and Marius Grundmann[2] — [1]Solarion AG, Ostende 5, 04288 Leipzig, Germany — [2]Institut für Experimentelle Physik II, Universität Leipzig, Linnéstr. 5, 04103 Leipzig, Germany

Cu(In,Ga)Se_2 (CIGSe) thin film solar cells deposited on flexible polyimide foil promising innovative applications and a fabrication in continuous roll-to-roll processes currently reach efficiencies up to 17.6 %.

The optimization of the solar cell efficiency requires the reduction of inherent losses in the cell. In order to achieve this goal preferably spatially resolved access to parameters characterizing ohmic losses like series and shunt resistances are indispensable.

We will apply an interpretation method for electroluminescence (EL) images taken at different voltages which is known for solar cells made of crystalline silicon from literature to solar cells made of polycrystalline CIGSe. The theory of this method to obtain a mapping of the series resistance and the EL imaging process as well as the data interpretation will be reviewed and demonstrated on an example. Furthermore, the benefit of this method for the characterization of solar cells under accelerated aging conditions (damp heat) which is important for the estimation of the long-term stability will be shown.

HL 85.65 Thu 18:00 P4

A theoretical investigation on the Cd doping of $CuIn_5Se_8$ — •Janos Kiss, Thomas Gruhn, and Claudia Felser — Institut für Anorganische Chemie und Analytische Chemie, Johannes Gutenberg-Universität, D-55099 Mainz, Germany

Due to its attractive optical, electrical, and chemical properties the ternary $CuInSe_2$ (CIS) chalcopyrite-type semiconductor is widely employed as absorber layer in thin film photovoltaic devices. In the industrial fabrication of thin film solar cells on top of the CIS layer a CdS films is deposited as buffer layer. Despite the exhaustive experimental and theoretical research, the atomic and electronic structure of the CIS–CdS interface is not well understood due to its complex nature. In the contemporary literature it is well accepted that the CIS surface regions are Cu-depleted and doped with Cd through the diffusion of Cd atoms from the buffer layer. Still, the concentration of the Cd dopant atoms and their arrangement in the Cu-depleted CIS is not yet unambiguously determined. To gain new insights on the doping of Cu-depleted CIS phases, we have investigated the Cd doping of bulk $CuIn_5Se_8$ via performing density functional theory (DFT) calculations on large supercells. We found that bulk $CuIn_5Se_8$ can be doped with Cd up to a Cd concentration of about 0.6–0.8%. Moreover, our calculations show that energetically it is favorable for Cd dopant atoms to occupy Cu antisites in $CuIn_5Se_8$.

HL 85.66 Thu 18:00 P4

Preparation and characterization of Bi_2S_3 thin films grown with the hot-wall deposition method — •Sebastian ten Haaf and Gerhard Jakob — Institut für Physik, Johannes Gutenberg Universität Mainz, 55099 Mainz, Germany

As a first step in the search for new absorbing materials in inorganic thin film photovoltaics with the benefit of reduced costs in comparison to currently used CIGS, polycrystalline Bi_2S_3 was deposited in vacuum and examined for its suitability for solar cells.

The bismuth sulfide thin films were grown in a recently designed ultra high vacuum chamber with the hot-wall deposition method under conditions close to thermodynamic equilibrium on ITO coated glass substrates with variation of substrate, wall and source temperature.

For further structural characterization, Bi_2S_3 was additionally deposited on epitaxial $LaAlO_3$ and $SrTiO_3$ substrates in order to enhance directional growth of the thin films.

HL 85.67 Thu 18:00 P4

Optical and Electrical Characterization of InP-based Low Bandgap Multijunction Solar Cells — •Anja Dobrich, Nadine Szabó, Klaus Schwarzburg, and Thomas Hannappel — Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

At present, III-V triple junction (3J) solar cells are achieving the highest conversion efficiencies (η=41.6%) worldwide. The current record multi junction solar cell grown on germanium, having Ge, Ga(In)As and GaInP as subcells, but still considerably higher efficiencies can be achieved with a four junction (4J) configuration, which has optimized band gaps around 1.9, 1.4, 1.0 and 0.7 eV. This can be realized with a mechanically stacked GaAs-based GaInP/GaAs tandem and an InP based InGaAsP/InGaAs tandem cell. For this purpose, we have grown InGaAsP/InGaAs tandem solar cells lattice-matched to InP by MOVPE.

The lifetime of minority charge carriers affects strongly the performance of solar cells, hence it is one of the most important properties of photovoltaic absorbers. Results of minority carrier lifetime measurements for the IR-bandgap compounds InGaAsP (1.03 eV) / InGaAs (0.73 eV) are presented. This technique is sensitive for both, the quality of the bulk material within the double hetero structure (DHS) as well as the interface preparation between barrier and bulk. Furthermore, by scanning the sample, spatial inhomogeneities in the lifetime can be detected. We show the effect of different interface preparation routines on the minority charge carrier lifetime.

HL 85.68 Thu 18:00 P4

Herstellung, Kontaktierung und Charakterisierung von GaAs Mikro-Photovoltaikzellen — •Michael Kwiatek, Arne Ludwig, Rüdiger Schott und Andreas D. Wieck — Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum

In den letzten Jahren hat die Bedeutung von alternativen und regenerativen Energiequellen für den zentralen Energiebedarf immer weiter zugenommen. Doch besonders auch für dezentrale Energieversorgungslösungen eignet sich die Photovoltaikzelle als möglicher Weg.

In der Informationstechnologie werden derzeit die Weichen zur stärkeren Einbindung optischer Übertragungswege gestellt. So können größere Distanzen mit höherer Bandbreite zurückgelegt werden. Ein Problem stellt sich hier jedoch in der Energieversorgung der angeschlossenen Endgeräte.

Dieser Beitrag zeigt die ersten Ergebnisse der hergestellten Mikro-Photovoltaikzellen auf GaAs Basis. Im Speziellen wird auch die Möglichkeit erörtert, kleinere Chipsysteme, wie Flashspeicher, über eine optische Faser mit genügend Energie zu versorgen um ihre Funktionalität unabhängig von stark längenbeschränkten Kupferzuleitungen zu gewährleisten. Außerdem ergibt sich durch die vollständige galvanische Trennung von Sender und optisch angesteuertem Endgerät eine höhere Unanfälligkeit beziehungsweise Unempfindlichkeit gegenüber Störungen und Potentialschwankungen.

HL 85.69 Thu 18:00 P4

Electroluminescence of Thin Film Silicon Solar Cells — •Viola Mönkemöller[1], Matthias Niederkrüger[2], Helmut Stiebig[2], and Ulrich Heinzmann[1] — [1]Molecular and Surface Physics, Bielefeld University — [2]Malibu GmbH & Co. KG, Bielefeld

Electroluminescence (EL) and Dark-Lock-In-Thermography (DLIT) are commonly used methods to characterize crystalline silicon solar modules.

We have applied these methods to analyze thin-film silicon-PV-minimodules based on amorphous silicon (a-Si) and microcrystalline silicon (μc-Si).

DLIT shows the heat dissipation of the solar cell which originates mainly from the ohmic losses in the Transparent Conductive Oxide (TCO). Defects e.g. electrical short cuts of the cell (shunts) provide a large DLIT signal, due to the high temperature caused by the increased current. In contrast EL shows effects of the semiconductor material. Shunts caused by dust particles in the thin film appear as dark lateral spots since less luminescent recombination takes place.

Furthermore EL allows the distinguishing between a-Si and μc-Si. The different semiconductor band gaps lead to different emission spectra ($\lambda_{\mu c-Si} > \lambda_{a-Si}$). Using adequate filters this behavior leads to the analysis of the individual diodes of tandem modules.

In general EL and DLIT show a similar image of a systematic signal distribution. This effect results from the inhomogeneous voltage and current distribution across the cells in the semiconductor and TCO which is caused by the integrated series connection.

HL 85.70 Thu 18:00 P4

Metal-assisted Chemical Etching of Multicrystalline Silicon Wafers for Solar Cell Application — •Xiaopeng Li[1,2], Stefan L. Schweizer[2], and Ralf B. Wehrspohn[2,3] — [1]Max-Planck Institute of Microstructure Physics — [2]Martin-Luther-Universität Halle-Wittenberg — [3]Fraunhofer Institute for Mechanics of Materials

Metal-assisted Chemical Etching (MaCE) has been proved as a cost-effective route to create semiconductor nanostructures. In this study, MaCE was employed to texturize different kinds of multicrystalline silicon (mc-Si). Noble nanoparticles were firstly deposited on the non-polished mc-Si by a galvanic displacement reaction, and then further acted as catalysts for silicon etching in a solution containing HF and DI water. By using different metal nanoparticles (Ag, Au, Pt and Pd), we obtained various nano/micro structures on the mc-Si surface, including nanoporous layer, nanowire, and cone-shaped microstructures. These silicon structures are formed independent of crystal orientation and uniform in the wafer size, which exhibited strong light-trap capabilities. This has the potential to allow three dimensional p-n junction to achieve more efficient mc-Si solar cell.

HL 85.71 Thu 18:00 P4

Semi-coherent optical modelling of thin film silicon solar cells — •Cordula Walder, Jürgen Lacombe, Karsten von Maydell, and Carsten Agert — NEXT ENERGY, EWE-Forschungszentrum für Energietechnologie e.V., Carl-von-Ossietzky-Straße 15, 26129 Oldenburg, Germany

At NEXT ENERGY the experimental investigation of thin film silicon solar cells is combined with numerical simulations using the software Sentaurus TCAD from Synopsys. We present the results of optical modelling with Sentaurus TCAD based on the one-dimensional semi-coherent optical model by Janez Krč [1]. The idea of this model is that after interacting with a rough interface the incident light is split into a direct coherent part treated as electromagnetic waves and in a diffuse incoherent part treated as light beams. The proportion of either direct or diffuse part is determined by the haze parameter which can be obtained from spectrometer data. In order to describe the scattering effects at rough interfaces the intensities of the diffuse light are scaled with angular distribution functions. These functions are obtained from angle resolved scattering measurements.

The optical model will be verified by experimental data and compared to the Raytracer and the Transfer Matrix Model. Furthermore the influence of different angles of incidence and of the spectral dependency on the solar cell performance will be investigated.

[1] J. Krč, F. Smole, M. Topič. One-dimensional semi-coherent optical model for thin-film solar cells with rough interfaces. Informacije MIDEM 2002; 32(1): 6-13.

HL 85.72 Thu 18:00 P4

Texturing transparent conductive oxide (TCO) and use of antireflective (AR) coating to optimize light-trapping in amorphous silicon thin film solar cells (a-Si:H) for high stabilized efficiencies: A simulative Approach — •Kambulakwao Chakanga — NEXT ENERGY, EWE-Forschungszentrum für Energietechnologie e.V.

The advantages of the a-Si:H technology range from low material consumption, less manufacturing energy required, possibility of efficient rapid mass production to the abundance of the raw material silicon. One major drawback of the a-Si:H pin structure is the light induced degradation (Staebler-Wronski effect) which causes a reduction in the efficiency. The effect is profound in cells with thick intrinsic layers. Thus thinner layers are desirable which however constraints the short-circuit current density. The required light-trapping can be achieved by implementing AR, textured TCO and back contact (BC).

This study aims to reduce the intrinsic layer by implementing an effective light coupling using a simulative approach. The software Sentaurus TCAD is used to model the optical behavior of the a-Si:H pin cell consisting of AR/glass/TCO/pin/BC using numerical models. Successful simulation can illustrate the behavior of fictitious structures and permit a better understanding of the physical processes. Hence it would be possible to predict the ideal system that would provide an effective light trapping for a given absorber thickness. Emphasis is put on light scattering effect of various TCO surface structures and AR on the performance of the cell.

HL 85.73 Thu 18:00 P4

Epitaktische Kristallisation von Silicium mit einem Diodenlaser — •Thomas Schmidt, Gudrun Andrä und Fritz Falk — Institut für Photonische Technologien e.V., Jena, Deutschland

Dünnschichtsolarzellen aus kristallinem Silicium sind eine günstige Alternative zu Waferzellen. Multikristalline Dünnschichtzellen aus Silicium auf einem Substrat aus Borosilikat–Glas können mit Hilfe eines laserinduzierten Epitaxieprozesses hergestellt werden.

Es werden Ergebnisse präsentiert, bei denen durch Diodenlaserbestrahlung von amorphem Silicium sowohl auf einkristallinen Substraten als auch auf polykristallinen Schichten (Korngrößen $> 100\,\mu$m) epitaktisches Wachstum erreicht werden konnte. Die Epitaxie fand dabei durch Erstarren der geschmolzenen Phase oder durch direkte Festphasenumwandlung des amorphen Materials im ms– bis s–Bereich statt. Durch Messung der Reflektivität während der Bestrahlung zusammen mit numerischen Simulationen konnte dabei der Kristallisationsvorgang zeitaufgelöst verfolgt werden.

HL 85.74 Thu 18:00 P4

Epitaxie auf kristallinem Silizium durch Excimer-Laser Bestrahlung — •Ingo Sill, Gudrun Andrä und Fritz Falk — Institut für Photonische Technologien e.V., Jena

Dünnschichtsolarzellen aus kristallinem Silizium sind eine günstige Alternative zu Waferzellen. Multikristalline Dünnschichtzellen aus Silizium auf einem Substrat aus Borosilicat-Glas können mit Hilfe des LLC Prozesses (Layered Laser Crystallization) hergestellt werden. In diesem Prozess wird eine hoch Bor-dotierte a-Si Schicht durch einen cw-Diodenlaser kristallisiert, sodass Kristallite in der Größenordnung von 100 μm entstehen. Diese Keimschicht wird anschließend epitaktisch verdickt, indem darauf Bor-dotiertes a-Si durch Elektronenstrahlverdampfen abgeschieden und gleichzeitig das a-Si durch wiederholtes Bestrahlen mit dem Puls eines Excimer-Lasers epitaktisch kristallisiert wird. Um den Prozess hinsichtlich der Abscheidung großer a-Si Schichtdicken zwischen den einzelnen Laserpulsen und geringer Substrattemperatur optimieren zu können, wurde ein einzelner Kristallisationsschritt untersucht. Dabei wurde die Keimschichtdicke, die a-Si Dicke, die Substrattemperatur und die Fluenz des Excimer-Lasers variiert, um die Abhängigkeit des Epitaxieintervalls von diesen Parametern zu messen und zu verstehen. Experimentelle Ergebnisse werden mit Simulationsrechnungen verglichen.

HL 85.75 Thu 18:00 P4

Thickening of polycrystalline silicon layers by solid phase epitaxy — •Ingmar Höger, Annett Gawlik, and Fritz Falk — Institut für Photonische Technologien, Albert-Einstein-Str. 9, D-07745 Jena, Germany

Crystalline silicon solar cells on glass substrates are considered to be an alternative to well established wafer-based concepts due to their potentials for cost reduction. This work deals with a seed-layer approach to obtain thin silicon films. First of all an amorphous silicon layer is deposited on bare glass substrates. Diode-laser crystallization by means of continuous-wave irradiation results in grain diameters of 100 μm. Next, the absorber gets deposited by high rate electron beam evaporation which needs to be crystallized via solid phase epitaxy in a tube furnace at temperatures around 600 °C. In this way the crystallographic information of the seed-layer can be transferred to absorbers up to 1,5 μm in thickness. The maximum thickness is limited by the onset of nucleation in the amorphous material beginning after a certain retardation time and leading to crystallites several micrometers in seize. The kinetics of the solid phase epitaxy strongly depends on crystallographic orientation, doping concentrations and the a-Si preparation conditions. In order to prevent the formation of defects the interface between seed and absorber layer needs to be clean as well.

HL 85.76 Thu 18:00 P4

Time-resolved photoluminescence imaging of silicon wafers using a CCD camera — •David Kiliani, Gabriel Micard, Bernd Raabe, and Giso Hahn — Abteilung Photovoltaik, Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany

A method to record and evaluate time-resolved photoluminescence images of crystalline silicon wafers using a standard silicon-CCD camera was developed. The use of a fast rotating shutter wheel decouples the obtained temporal resolution from the camera exposure time, making it possible to record the decay curve of free minority charge carriers. The transient curve for each pixel is determined from a set of photoluminescence images, making the method calibration-free and much faster than measurements of microwave-detected photoconductance. Lifetime maps for different injection levels can be calculated and show good agreement with steady-state photoluminescence images and quasi-steady-state photoconductance measurements. Compared with dynamic methods using a CMOS camera, a high spatial resolution at much lower equipment cost can be obtained.

HL 85.77 Thu 18:00 P4

Transmission Electron Microscopy for thin film solar cells — •Nies Reininghaus[1], Vitalij Schmidt[1], Wiebke Hachmann[1],

Stefan Gruss[2], Helmut Stiebig[2], and Ulrich Heinzmann[1] — [1]Molecular and Surface Physics, Bielefeld University — [2]Malibu GmbH & Co. KG, Bielefeld

Thin-film amorphous and microcrystalline silicon are promising materials for photovoltaics as they have the potential to reduce the solar cell costs. In case of microcrystalline silicon the crystalline volume fraction is related to the efficiency factor of solar cells because it provides information about the microstructure of the material and the defect density. With Transmission Electron Microscopy of cross-sections it is possible to show the microstructure of the cells. However to determine the structure of the bulk it is necessary to analyse the diffraction of the electron beam. For the purpose of imaging diffraction patterns and displaying dark fields a new camera system has been installed in the Phillips CM200. With much higher sensitivity and a larger photoactive area it is possible to take images of the low-intensity diffraction and the dark field patterns.

HL 85.78 Thu 18:00 P4

Lasing in ZnO and CdS Nanowires — •Andreas Thielmann, Sebastian Geburt, Michael Kozlik, Julian Kühnel, Christian Borschel, and Carsten Ronning — Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena

The development of nanoscaled semiconductor lasers could be the key resolution to the still persistent size mismatch between integrated microelectronic devices and semiconductor optoelectronic devices[1]. Semiconductor nanowires offer an elegant path to the development of nanoscaled lasers as their geometry with two planar end facets naturally combines a fiber-like waveguide with an optical resonator. The possible stimulation of the material's emission processes enables lasing of resonant optical modes[2].

ZnO and CdS nanowires of different aspect ratios have been synthesized via the VLS mechanism and were characterized by SEM, EDX and ensemble PL measurements. Power dependent PL measurements on single nanowires excited with pulsed laser light at 355 nm have been performed between 10 K and room temperature and were set in correlation to the nanowires' respective morpholgy. Sharp emission lines which show characteristics of Fabry-Pérot modes could be observed above a power threshold. The measured power dependencies reveal amplified stimulated emission and lasing at high excitation densities.

[1] Ning, C. Z. (2010), physica status solidi (b), 247: 774-788.
[2] M. A. Zimmler et al (2010), Semicond. Sci. Technol., 25: 024001

HL 85.79 Thu 18:00 P4

Atomic and electronic structure of non-planar Si/SiO_2 interfaces — •Kaori Seino[1], Friedhelm Bechstedt[1], and Peter Kroll[2] — [1]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Jena, Germany — [2]Department of Chemistry and Biochemistry, University of Texas at Arlington, Arlington, TX, USA

Silicon (Si) nanocrystals (NCs) are promising objects for quantum and photovoltaic devices. However, there are open questions concerning the influence of the embedding amorphous SiO_2 matrix and the NC-matrix interface. In contrast to the planar Si/SiO_2 interfaces with defined crystallographic orientation in layered heterostructures, the NCs are surrounded by almost spherical interfaces with various facets. Here we study the interfacial electronic and bonding properties of Si NCs embedded in SiO_2 by large-scale first-principles calculations. They are based on the density functional theory (DFT) implemented in the VASP code. In our simulations Si NCs with nominal diameters up to 1.6 nm, i.e. systems with more than 1000 atoms, are treated. The atomic geometries are optimized within full quantum-mechanical calculations. The fundamental gap of the NC depends significantly on the matrix. The Si−Si bonds in the NC core are stretched while in the interface regions both types of bonds, stretched and compressed ones, occur. We compute the spatial variation of the electronic structure. The local band edge profiles exhibit different band gaps in the Si NCs and in the matrix region. Significant differences are found comparing embedded Si NCs and planar Si/SiO_2 interfaces.

HL 85.80 Thu 18:00 P4

Dopant-induced morphology evolution of silicon via wet chemical etching — •Guodong Yuan[1,2] and Saskia F. Fischer[1,2] — [1]Institute of physics, Humboldt-Universität zu Berlin, D-12489 Berlin, Germany — [2]Werkstoffe und Nanoelektronik, Ruhr-Universität Bochum, D-44780 Bochum, Germany

Silicon nanowires (SiNWs), as promising building blocks for future nanoelectronic devices, have been the intensive research focus in past decade due to their unique 1-D morphology and related properties. A lot of methods have been developed to fabricate SiNWs, for example, vapour-liquid-solid (VLS), reactive ion etching and electroless etching [1-2]. Among all these methods, the electroless etching approach for SiNWs is rather fascinating with respect to the traditional chemical vapour deposition (CVD) method, which always needs high temperature, hazardous precursors, long duration, expensive source materials and complex vacuum furnace systems. We found that the doping level of silicon wafer can influence morphology of the final etched structures. In low doped silicon wafer, the etching process produced the solid SiNWs, while in the case of highly doped silicon wafer, the wet chemical etching resulted in porous SiNWs or porous silicon due to the interaction between the dopants and aqueous chemical. The morphology evolution with the dopants is discussed in this work.

[1] K. Q. Peng, Y. Wu, H. Fang, X. Y. Zhang, Y. Xu, J. Zhu, Angew. Chem., Int. Ed. 2005, 44, 2737. [2] G. D. Yuan, Y. B. Zhou, C. S. Guo, W. J. Zhang, Y. B. Tang, Y. Q. Li, et al, ACS Nano, 2010, 4, 3045.

HL 85.81 Thu 18:00 P4

Low temperature Coulomb anomaly in CMOS compatible silicon quantum dots — •Stefan Jauerneck[1], Matthias Ruoff[1], Dharmraj Kotekar-Patil[1], David Wharam[1], Dieter Kern[1], Marc Sanquer[2], and Maud Vinet[3] — [1]Eberhard Karls Universität, Tübingen — [2]CEA INAC, Grenoble, France — [3]CEA LETI, Grenoble, France

Due to the ever decreasing sizes in CMOS technology, it has become possible to investigate transport in small geometries, where both Coulomb charging and quantum-mechanical effects play an important role. Furthermore fluctuations in the number of dopants in the active region of transistors are important and such dopants may act as an ultimate quantum dot with huge charging energies as compared to artificial silicon islands and lead to high temperature operation.

We report on transport measurements of nanoscale enhancement mode nanowire SOI-FETs, which clearly show Coulomb blockade behaviour. The size of the Coulomb diamonds is modulated in source-drain direction with an enveloping diamond structure, which may be explained by Coulomb charging effects due to a dopant in or near the barrier. Additionally the measurements feature regularly spaced lines with a slope $dV_{sd}/dV_g > 1$. We have investigated these features with respect to the symmetry of the measurement setup and show that they become independent of source-drain bias when the dot is symmetrically biased. Alternative explanations for this behaviour are considered.

HL 85.82 Thu 18:00 P4

Ivestigation of an InGaN - GaN nanowire heterstructure — •Friederich Limbach[1], Tobias Gotschke[1], Toma Stoica[1], Raffaella Calarco[1], Eli Sutter[2], Jim Ciston[2], Ramon Cusco[3], Luis Artus[3], Stefan Kremling[4], Sven Höfling[4], Lukas Worschech[4], and Detlev Grützmacher[1] — [1]Institute of Bio- and Nanosystems (IBN-1), Research Center Jülich GmbH, D-52425 Jülich, Germany, and JARA-Fundamentals of Future Information Technology — [2]Center for Functional Nanomaterials, Brookhaven National Laboratory, Upton, New York 11973, USA — [3]Institut Jaume Almera, Consell Superior d'Investigacions Científiques (CSIC), 08028 Barcelona, Catalonia, Spain — [4]University Wurzburg, Wilhelm Conrad Rontgen Research Centre Complex Matter Systems, D-97070 Wurzburg, Germany

InGaN/GaN nanowire (NW) heterostructures grown by molecular beam epitaxy were studied in comparison to their GaN and InGaN counterparts. The InGaN/GaN heterostructure NWs are composed of a GaN NW, a thin InGaN shell, and a multi-faceted InGaN cap wrapping the top part of the GaN NW. Transmission electron microscopy images taken from different parts of a InGaN/GaN nanowire show a wurtzite structure of the GaN core and the epitaxial InGaN shell around it. Photoluminescence spectra of these heterostructure NW ensembles show an emission peak at 2.1 eV. However, μ-PL spectra measured on single nanowires reveal much sharper luminescence peaks. A Raman analysis reveals a variation of the In content between 20 % and 30 %, in agreement with PL and TEM investigations.

HL 85.83 Thu 18:00 P4

Influence of the nanowire interdistance on growth conditions and crystal structure of self-catalyzed GaAs nanowires grown via MBE — Joachim Hubmann[1], •Benedikt Bauer[1], Andreas Rudolph[1], Anna Fontcuberta i Morral[2], Dieter Schuh[1], Do-

minique Bougeard[1], Josef Zweck[1], and Elisabeth Reiger[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Germany — [2]Laboratoire des Matériaux Semiconducteurs, EPFL Lausanne, Switzerland

Nanowires grown in bottom-up processes are considered as possible building blocks for future electronic devices. For this use it is necessary to gain control over the growth position of single nanowires. By nanopatterning the SiO_2/GaAs substrate with e-beam lithography we could restrict nanowire growth to predefined sites using the self-catalyzed, Ga-assisted growth technique[1]. We found that there is a correlation between the interdistance of the predefined growth sites and the probability of nanowire growth. This indicates that the effective growth conditions that are seen by a single nanowire are influenced by its local surrounding, in particular by the distance to its neighbours. We attribute the difference of the effective growth conditions to be caused by different diffusion lengths for Ga and As atoms on the SiO_2 surface. As the nanowire crystal structure can be tuned via the growth parameters we further examine how the change of the effective growth conditions affects the crystal structure of the grown nanowires.

[1]Bauer *et al.*, Nanotechnology 21 (2010), 435601.

HL 85.84 Thu 18:00 P4

Voltage-dependent excited state spectroscopy of single lateral InGaAs quantum dot molecules — •Meike Seible[1], Matthias Heldmaier[1], Jie Peng[2], Gabriel Bester[2], Lijuan Wang[2], Armando Rastelli[3], Oliver G. Schmidt[3], and Peter Michler[1] — [1]Institut für Halbleiteroptik und Funktionelle Grenzflächen, Allmandring 3, 70569 Stuttgart, Germany — [2]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany — [3]Institut für Integrative Nanowissenschaften IFW Dresden, Helmholtzstraße 20, 01069 Dresden, Germany

We investigate single laterally coupled quantum dot molecules (QDMs) which are grown using a combination of molecular beam epitaxy and in situ atomic-layer precise etching. Each QDM consists of two individual quantum dots (QDs) which are coupled along the [1-10] crystal direction via electron tunneling, while the holes are strongly localized in either of the QDs. The electronic coupling can be influenced by applying an electric field along the molecular coupling axis. This leads to a shift between the intensities of the excitonic emission lines of the respective dots. For the investigation of the behaviour of the excited states in this system under different coupling conditions, detailed photoluminescence excitation (PLE) spectroscopy measurements have been carried out, using a wideband tunable Ti:Sapphire laser source under systematic variation of the applied lateral electric field. We compare these results with theoretical calculations of absorption spectra, using an empirical many-body pseudo-potential approach with random composition of the QDMs.

HL 85.85 Thu 18:00 P4

Time-dependent measurements of single In(Ga)As quantum dots embedded in GaAs reversed pyramid cavities — •Christoph Reinheimer, Daniel Rülke, Daniel Schaadt, Heinz Kalt, and Michael Hetterich — Institut für Angewandte Physik and DFG Center for Functional Nanostructures (CFN), Karlsruhe Institute of Technology (KIT), Wolfgang-Gaede-Str. 1, 76131 Karlsruhe, Germany

We have investigated the exciton decay in single In(Ga)As quantum dots (QD) embedded in GaAs reversed micropyramids by means of time-correlated single photon counting (TCSPC). Pyramids with square and octagonal shape are manufactured by a wet-chemical etching process utilizing an AlAs sacrificial layer. The slope angle can be tailored by the composition of the etching solution. A layer of In(Ga)As QDs is situated close to the pyramid tip (25 nm distance). This ensures an extremely low number of dots in the cavity which is important for potential applications like single photon sources. Since light emitted by the QDs is mainly radiated through the top of the reversed pyramid due to reflection at the facets, this type of cavity is useful to efficiently detect the emission of single QDs. To investigate the exciton lifetime, we have studied the emission of single QDs under pulsed laser excitation. Furthermore, we have studied the temporal auto-correlation of subsequent photons emitted by the excitonic decay of a single QD using a Hanbury-Brown and Twiss setup in order to investigate the suitability of this approach as single photon emitter.

HL 85.86 Thu 18:00 P4

Optical properties of terbium doped ZnS nanowires — •Franziska Riedel, Sebastian Geburt, and Carsten Ronning — Friedrich-Schiller-Universität Jena, Institut für Festkörperphysik, Jena

Semiconductor nanowires have the potential for fundamental future application in optoelectronic devices to act as nanoscaled light emitters (LED), waveguides or nanolasers. Doping of the nanowires with optical active elements (e.g. rare earth) could offer new optical properties, as it combines the features from well known material with the quasi-1D-structure. Terbium doped ZnS is a promising candidate as it shows strong green emission in thin-film electroluminescence devices, but there are no investigations on 1-D Tb doped ZnS nanostructures yet.

ZnS nanowires were synthesized via the VLS mechanism with diameters between 150-400 nm and lengths of about 60 μm. The doping with Tb was realized using ion beam implantation and annealing for the recovery of the implantation damage. The structural and morphological properties were analyzed using SEM and TEM. The optical properties were investigated using spatial resolved cathodoluminescence. The Tb doped ZnS nanowires show a strong intra-4f-luminescence. Several transitions could be identified and the luminescence properties of samples with Tb concentrations between $2 \cdot 10^{-3}$ and 2 at.% were examined at different temperatures and excitation powers.

HL 85.87 Thu 18:00 P4

Optical Spectroscopy on Single Charge-Tunable InGaAs/GaAs Quantum Dots — •Jan Kettler[1], Sven M. Ulrich[1], Matthias Heldmaier[1], Daniel Richter[1], Wolfgang-Michael Schulz[1], Robert Rossbach[1], Michael Jetter[1], Lijuan Wang[2], Armando Rastelli[2], Oliver G. Schmidt[2], and Peter Michler[1] — [1]Institut für Halbleiteroptik und Funktionelle Grenzflächen, Allmandring 3, 70569 Stuttgart, Germany — [2]Institut für Integrative Nanowissenschaften IFW Dresden, Helmholtzstraße 20, 01069 Dresden, Germany

We investigate the optical properties of self-assembled InGaAs/GaAs quantum dots (QDs) embedded into a n-i-Schottky diode structure which is placed on top of a distributed Bragg reflector in order to increase the photoluminescence (PL) extraction efficiency. The application of a bias voltage enables to control the charge state of the QDs. The ability to deterministically prepare a negative trion and its excited states is a preliminary requirement for future optical spin pumping experiments. Two similar sample structures are spectroscopically analyzed, one with QDs grown in molecular beam epitaxy and a second with QDs grown in metal organic vapor phase epitaxy. Micro-PL measurements in combination with photon cross-correlation measurements demonstrate the preparation of a negative trion ground state (X^-). Polarization resolved micro-photoluminescence excitation spectroscopy is applied to reveal the excited negative trion states (X^{-*}).

HL 85.88 Thu 18:00 P4

Influence of the inhomogeneous broadening of quantum dots in microcavity lasers — •Alexander Foerster and Jan Wiersig — Institut für Theoretische Physik, Universität Magdeburg

Microcavity lasers have recently attracted a considerable interest in semiconductor physics. Previous models [1] ignored the inhomogeneous broadening of quantum dots, i.e. they used the assumptions of identical quantum dots in resonance with the laser mode. Here we present a microscopic theory, which accounts for the energetic detuning of the different quantum dots. We use a four level laser model based on the cluster expansion method.

The impact of inhomogeneous broadened quantum dots on various properties of the laser is studied. The contribution of each quantum dot in the system is analysed. With increasing detuning a shift in the Input-Output characteristics becomes visible.

[1] C. Gies, J. Wiersig, M. Lorke, and F. Jahnke, Phys. Rev. A 75, 013803 (2007)

HL 85.89 Thu 18:00 P4

Optical properties of GaAs quantum dots fabricated by filling of self-assembled nanoholes — •Andreas Graf[1], David Sonnenberg[1], Christian Heyn[1], Andrei Schliwa[2], and Wolfgang Hansen[1] — [1]Institut für Angewandte Physik, Universität Hamburg, 20355 Hamburg, Germany — [2]Institut für Festkörperphysik, Technische Universität Berlin, 10623 Berlin, Germany

Local droplet etching (LDE) is a technique to fabricate self-assembled patterning of semiconductor surfaces. Using LDE, we drill nanoholes (depth ≥ 7 nm) with Al droplets on the AlGaAs substrate and partially fill these with GaAs. This results in strain-free GaAs quantum dots

(QDs) [1]. By control of the filling level a very narrow size distribution is achieved within the QD ensemble. We study photoluminescence spectra of QD ensembles as well as of single QDs and discuss the observations in view of QD size dependence, the shell structure, and the excited states in the QDs. In particular, the fine-structure splitting of neutral exciton and biexciton peaks of single QDs is studied. Furthermore, a model using the eight-band k·p theory and configuration interaction [2] is used to interpret the experimental results.

[1] Heyn et al., Appl. Phys. Let. **94**, 183113 (2009)
[2] Schliwa et al., Phys. Rev. B **80**, 161307 (2009)

HL 85.90 Thu 18:00 P4

Towards site controlled growth of InAs quantum dots on patterned GaAs by microsphere photolithography — •Ulrich Rengstl, Elisabeth Koroknay, Robert Rossbach, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen, Universität Stuttgart, Allmandring 3, 70569 Stuttgart, Germany

To use quantum dots (QDs) in single photon applications, like quantum information processing, we are working on separate addressable, site controlled QDs. For this, we generate surface potential modulations by patterning the GaAs surface before the overgrowth in a metal-organic vapor-phase epitaxy system (MOVPE). Conventional patterning techniques, such as electron beam lithography or site controlled surface oxidation using scanning tunneling microscopy, have the disadvantage of high time consumption. A faster method for prepatterning a large surface uses microsphere photolithography [1]. For partial exposure of UV-sensitive photoresist, we use a hexagonal close-packed microsphere monolayer as an array of microlenses to focus UV-light. We obtained structures with controllable diameters of 300 to 700 nm in the photoresist, which can be used as an etching mask for wet chemical etching to generate holes in the GaAs surface. After this, various steps of post etch cleaning and oxide removal are necessary to obtain a GaAs buffer with low defect density and high optical quality after the following overgrowth. The prepatterning also leads to an increased accumulation of deposited InAs inside the holes, which supports island growth.

[1] W. Wu et al, Nanotechnology 18, 485302 (2007)

HL 85.91 Thu 18:00 P4

Transport spectroscopy of many-particle hole states in InAs quantum dots coupled to a two-dimensional hole gas — •Andreas Beckel[1], Bastian Marquardt[1], Martin Geller[1], Axel Lorke[1], Tobias Nowozin[2], Andreas Marent[2], and Dieter Bimberg[2] — [1]Faculty of Physics, University of Duisburg-Essen, Lotharstraße 1, 47057 Duisburg, Germany — [2]Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany

Interactions between self-organized InAs quantum dots (QD) and a two-dimensional hole gas (2DHG) can be used to probe the charge state in future memory applications [1]. We demonstrate that the conductance of the 2DHG is a very sensitive tool, also for time-resolved measurements. This enables us to measure the tunneling dynamics between the 2DHG and the QDs [2] for very weakly coupled QDs exhibiting tunneling times in the order of several seconds. The time-resolved spectroscopy makes it possible to measure the density of states in the QD ensemble with single charge resolution up to 75 K. These results demonstrate the feasibility of high temperature read-out of the quantum states in self-assembled QDs using a 2DHG.

[1] A. Marent et al., Appl. Phys. Lett. **95**, 242114 (2009).
[2] B. Marquardt et al., Appl. Phys. Lett. **95**, 22113, (2009).

HL 85.92 Thu 18:00 P4

Mobility and carrier density in nanoporous indium tin oxide films — •Jaqueline Weissbon[1], Andreas Gondorf[1], Martin Geller[1], Axel Lorke[1], Martina Inhester[2], Anna Prodi-Schwab[2], and Dieter Adam[2] — [1]Fakultät für Physik and CeNIDE, Universität Duisburg-Essen, D-47048 Duisburg — [2]Evonik Degussa GmbH, D-45772 Marl, Germany

Indium tin oxide (ITO) has become an indispensable material for a range of electronic devices. It is transparent in the entire visible range and electrically conducting, hence, a well suited material for transpar- ent electrodes. An interesting possibility to realize transparent, con- ducting films without the use of vacuum techniques is the printing of dispersions containing ITO nanoparticles[1]. We study here the charge carrier concentration and mobility of various nanoporous in- dium tin oxide (ITO) films, using Hall measurements and optical spectroscopy[2]. For the carrier density inside the particles ($2 - 4 \cdot 10^{20}\mathrm{cm}^{-3}$), the results of these complementary measurement techniques are in good agreement with each other and suggest that even in highly porous materials the common equations for the Hall resistance can be applied. However, for the mobilities in these layers the results differ very strongly: from 50 $\frac{\mathrm{cm}^2}{\mathrm{Vs}}$ in optical spectroscopy (which is comparable to bulk ITO) to 0.4 $\frac{\mathrm{cm}^2}{\mathrm{Vs}}$ in Hall measurements.This suggests that the mobility for electrical transport in nanoporous ITO films is strongly suppressed by scattering at interparticle boundaries.

[1] Ederth et al. Phys. Rev. B **68**, 155410 (2003).
[2] Gondorf et al. Phys. Rev. B., submitted (2010).

HL 85.93 Thu 18:00 P4

Electronic properties of GaN nanowires with different doping concentrations — •Markus Schaefer[1], Pascal Hille[1], Florian Furtmayr[1,2], and Martin Eickhoff[1] — [1]I. Physikalisches Institut, Justus-Liebig-Universitaet Giessen, Heinrich-Buff-Ring 16, D-35392 Giessen, Germany — [2]Walter Schottky Institut, Technische Universitaet Muenchen, Am Coulombwall 3, D-85748 Garching, Germany

Semiconductor nanowires (NWs) are promising candidates for future generations of electronic and optoelectronic devices with a high density of integration. For this purpose it is interesting to combine available top-down approaches with bottom-up growth of NWs.

We report on electronic properties of detached GaN NWs with a typical length of about 500 nm placed on a pre-structured substrate. The NWs were grown in a self-assembled process by plasma assisted molecular beam epitaxy, substrate patterning was achieved by optical and electron beam lithography. The NWs were aligned by dielectrophoretic manipulation, which allows us a parallel deposition of several NWs from the fluid to the pre-patterned electrodes. The influence of different doping concentrations and illumination during measurements to the electronic properties of the NWs is reported.

HL 85.94 Thu 18:00 P4

Atomistic tight binding models of semiconductor quantum dots — •Elias Goldmann and Frank Jahnke — Institut für Theoretische Physik, Universität Bremen, 28359 Bremen

In recent years, semiconductor nanostructures such as quantum dots have been the subject of intense theoretical and experimental research due to their large potential for next generation device applications.

We present results of an atomistic empirical tight-binding model (ETB) for the calculation of electronic properties of semiconductor nanostructures. We choose a sp^3s^* basis set localized at each atomic site to correctly reproduce the electronic band structure in the relevant part of the Brillouin-zone and include next-neighbour-interaction as well as spin-orbit-coupling.

A Jacobi-Davidson algorithm in connection with the folded spectrum method is used to compute the eigenstates and eigenenergies of the resulting TB-Hamiltonian of the supercell that contains about $4 \cdot 10^5$ atoms.

Within this ETB model we investigate the electron and hole wavefunctions and confinement energies of semiconductor nanostructures such as spherical- and pyramidal-shaped self-assembled InAs quantum dots in a $In_xGa_{1-x}As$ quantum well, embedded in a GaAs matrix, which are known as dots-in-a-well (DWELL) structures [1,2]. The influences of dot size, shape and Indium-concentration on the confined states are presented.

[1] S. Krishna, J. Phys. D: Appl.Phys.**38** 2142 (2005)
[2] A. Amtout *et al.*, J. Appl. Phys. **96** 3782 (2004)

HL 85.95 Thu 18:00 P4

X-ray characterization of Au-free grown GaAs nanowires on Si — •Andreas Biermanns[1], Steffen Breuer[2], Anton Davydok[1], Lutz Geelhaar[2], and Ullrich Pietsch[1] — [1]Universität Siegen, Festkörperphysik, Germany — [2]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany

Semiconductor nanowires (NW) are of particular interest due to the ability to synthesize single-crystalline 1D epitaxial structures and heterostructures in the nanometer range. However, many details of the growth mechanism are not well understood. In this contribution we present a x-ray diffraction study of the early stage of Au-free GaAs nanowire growth on Si(111)-substrates with native oxide using the nano-focus setup available at the ID1 beamline of ESRF. The GaAs NWs were grown by molecular beam epitaxy (MBE), and their formation was induced by Ga droplets. Using a nanometer-sized x-ray beam, size and lattice parameters of individual wires were measured sepa-

rately. Using asymmetric x-ray diffraction on particular zinc-blende (ZB) and wurtzite (W) sensitive reflections, we show that under the used conditions the NW growth starts with predominantly WZ phases and continues mainly in ZB phase. In addition we can show that the WZ segments of the NWs exhibit a different vertical lattice parameter compared to the zinc-blende segments. A combination of x-ray diffraction from single wires and grazing incidence diffraction shows that the base of the NW is compressively strained along the inplane direction. This strain is released within 20nm from the substrate-interface.

HL 85.96 Thu 18:00 P4

Coupled Quantum Dots for Thermopower Measurements — •Holger Thierschmann, Luis Maier, Johannes Knorr, Mathias Mühlbauer, Hartmut Buhmann, and Laurens W. Molenkamp — Physikalisches Institut (EP3), Universität Würzburg, Germany

A detailed knowledge of the physics of quantum dots is of fundamental importance in modern solid state physics. For this purpose thermoelectric transport measurements are a powerful method since they are known to be more sensitive to details of the electronic structure than conventional conductance measurements. In recent years, thermoelectric transport measurements have revealed additional insight in a number of single quantum dot phenomena [1,2]. However, there are only few experiments that investigate the thermoelectric properties of two coupled quantum dots. To fill this gap, we have designed samples that enable us to perform conductance measurements as well as thermoelectric measurements on two parallel quantum dots. We use gate electrodes on top of a GaAs/AlGaAs interface 2DEG to define lateral quantum dots and to tune their size and coupling strength to their surrounding. The dots are situated adjacent to a heating channel through which a current is passed so that a temperature gradient across the dot can be provided. Detailed potential simulations were run on a number of different gate designs. The designs were realized using optical and e-beam lithography and the performance of the structures was analyzed in a dilution refrigerator at electron temperatures below 100 mK.

[1] R. Scheibner et al,. Phys. Rev. B 75, 041301 (2007)
[2] R. Scheibner et al., Phys. Rev. Lett. 95, 176602, (2005)

HL 85.97 Thu 18:00 P4

Electroluminescence from silicon nanoparticles — •Jens Theis[1], Martin Geller[1], Axel Lorke[1], Hartmut Wiggers[2], and Cedrik Meier[3] — [1]Fakultät für Physik and CeNIDE, Universität Duisburg-Essen — [2]Institut für Verbrennung und Gasdynamik and CeNIDE, Universität Duisburg-Essen — [3]Nanophotonics & Nanomaterials Group, University Paderborn

Si nanoparticles are tuneable light emitters and therefore a promising material for optoelectronic applications. We have fabricated an electroluminescence device based on silicon nanoparticles on a micropatterned semiconductor heterostructure. The Si nanoparticles have been synthesized from the gas phase in a low-pressure microwave plasma using SiH_4 as a precursor. The nanoparticles were dispersed from an aqueous solution onto the patterned substrate. For carrier injection, the particle layer was sandwiched between a transparent ITO layer and a Si-doped GaAs back contact. A strong EL emission from the Si nanoparticles is observed with the unaided eye[1]. The EL spectra of the devices were investigated in a μ-photoluminescence setup, confirming that the EL in the visible range is indeed caused by the Si nanoparticles. Additionally, we study the influence of the waveform, frequency and amplitude of the driving AC voltage on the electroluminescence.

[1] Theis et al. *Nanotechnology* **21**, 455201 (2009)

HL 85.98 Thu 18:00 P4

Engineering self-assembled SiGe islands for robust electron confinement in Si — •Roman O. Rezaev[1,2], Suwit Kiravittaya[1], Vladimir M. Fomin[1], Armando Rastelli[1], and Oliver G. Schmidt[1] — [1]Institute for Integrative Nanosciences, IFW-Dresden, D-01069 Dresden, Germany — [2]Laboratory of Mathematical Physics, Tomsk Polytechnic University, 634050 Tomsk, Russia

The confinement potential and the energy of localized electron states in the Si matrix surrounding self-assembled SiGe/Si(001) islands are evaluated with realistic structural parameters. For homogeneously alloyed islands overgrown with Si at low substrate temperatures, a non-monotonic dependence of the energy levels on size and composition is obtained and conditions to achieve the deepest confinement potential are derived within the framework of the available parameters. Shape changes occurring during Si capping at high substrate temperatures are shown to lead to a substantial reduction in the confinement potential. This work was supported by DAAD, DFG SPP 1386, Grant of President of the Russian Federation SS-871.2008.2, Russian Science and Innovations Federal Agency Contract 02.740.11.0238, and Russian Federal program Kadry Grant P691.

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Analysis of squeezed LO phonon states in a QD with the help of the Wigner function — •Daniel Wigger[1], Doris Reiter[1], Tilmann Kuhn[1], and Vollrath Martin Axt[2] — [1]Institut für Festkörpertheorie, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster — [2]Theoretische Physik III, Universität Bayreuth, 95440 Bayreuth

We study the fluctuation properties of non-classical phonon states within the model of an optically excited semiconductor quantum dot (QD). The QD is modeled in the strong confinement limit as a two level system. An ultrashort laser pulse creates an exciton in the QD which can be manipulated by further pulses. The exciton is coupled to the longitudinal optical (LO) phonons and, thus, lattice vibrations are created by the optical manipulation of the QD. For two pulses with a certain time delay and relative phase we find that the lattice fluctuations are squeezed, i.e., the fluctuations fall below the fluctuations of the phonon vacuum. [Sauer et al. PRL 105, 157401 (2010)] The quantum mechanical characteristics of the phonon states are studied using the Wigner function which allows an instructive interpretation of the phononic system. With the Wigner function we analytically calculate the fluctuation properties of the lattice displacement and momentum caused by the LO phonons and explain the mechanisms leading to squeezing.

HL 85.100 Thu 18:00 P4

Effects of phonon-induced dephasing on Rabi oscillations in GaAs quantum dots — •Sebastian Lüker[1], Doris Reiter[1], Vollrath Martin Axt[2], and Tilmann Kuhn[1] — [1]Institut für Festkörpertheorie, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster — [2]Theoretische Physik III, Universität Bayreuth, 95440 Bayreuth

We discuss the laser-induced Rabi oscillation of the exciton occupation in a GaAs quantum dot (QD). Considering the strong confinement limit we model the QD as a two level system. In principle arbitrary superpositions of these two states can be prepared by using light-induced Rabi oscillations. However, the control of the quantum state is limited by dephasing caused by electron-phonon interaction which reduces the coherence of the system and leads to a damping of the Rabi oscillations. Due to the energy structure only phonon-induced pure dephasing is taken into account. We study the impact of the dephasing on the coherence in the density matrix formalism. The many body nature of the problem leads to an infinite hierarchy of equations of motion which we truncate by a correlation expansion. The resulting closed set of equations is solved numerically. The influence of the different orders of this hierarchy is discussed. Recent experiments on Rabi oscillations in semiconductor QDs have been performed showing damped Rabi oscillations in the occupation of the QD exciton state [Ramsey et al., PRL **105**, 177402 (2010)]. We compare our model with the experimental data and find a very good qualitative and quantitative agreement.

HL 85.101 Thu 18:00 P4

Growth of GaAs-Nanowires on GaAs (111)B substrates induced by focused ion beam — •Rüdiger Schott, Dirk Reuter, and Andreas D. Wieck — Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum

Semiconductor nanowires are a promising system for applications in the areas of electronics and photonics and also for exploring phenomena at the nanoscale. There are several approaches to grow nanowires at arbitrary sites on the wafer. We report about growing GaAs-nanowires on GaAs (111)B substrates via the vapour-liquid-solid (VLS) mechanism in an ultra-high-vacuum (UHV)-cluster of a molecular beam epitaxy (MBE) and a focused ion beam (FIB) system. Our idea is to implant metal seeds (especially Au) for the nanowire growth by in situ patterning using FIB. Due to the UHV transfer between the FIB and the MBE chamber, no further cleaning step of the substrate surface is necessary. Formations of organized GaAs-nanowires and high aspect ratios are observed.

HL 85.102 Thu 18:00 P4

Geometry effects on Coulomb charging in CMOS-compatible SOI-SETs — •Matthias Ruoff[1], Dharmraj Kotekar-Patil[1], Stefan Jauerneck[1], David Wharam[1], Dieter Kern[1], Marc

Sanquer[2], and Maud Vinet[3] — [1]Eberhard Karls Universität, Tübingen — [2]CEA INAC, Grenoble, France — [3]CEA LETI, Grenoble, France

The charging energy of a single electron transistor (SET) and therefore its suitability for high-temperature operation is determined by the effective size of the Coulomb island. Nanowire SOI-FETs with nominally undoped channels of different widths and thicknesses and various gate lengths, fabricated in the FP7 project AFSID with a CMOS compatible process, have been investigated. In this case the Coulomb island may be formed by a small body of undoped silicon, a single stray dopant from source/drain implantation, or one or more dopant atoms in the access regions of the channel. The investigated devices show clear Coulomb blockade oscillations. From their period the gate capacitance can be directly obtained. Gate efficiency and total capacitance can be extracted by fitting theoretical models to conductance peak shapes and from charge stability diagrams. Capacitances resulting from different geometrical models are compared with those obtained from the transport measurements.

HL 85.103 Thu 18:00 P4

Kondo effect in double quantum dots with magnetic field-tuned coupling — Daniel Tutuc[1,3], Rolf Haug[1,3], •Brendan Coughlan[2,3], Lars Musiol[2,3], Sabine Tornow[2,3], and Gertrud Zwicknagl[2,3] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, D-30167 Hannover — [2]Institut für Mathematische Physik, Technische Universität Braunschweig, D-38106 Braunschweig — [3]NTH School for Contacts in Nano Systems, Braunschweig-Clausthal-Hannover

We study the variation with magnetic field of the Kondo effect in a double quantum dot system coupled via an open conducting region. The transport measurements [1] indicate a competiton between Kondo singlet formation and magnetic alignment via the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction which has been in the focus of interest in heavy electron systems during the past year. Tuning the coupling by a magnetic field provides insight into the relative importance of the different interactions (excluded volume, RKKY, etc) between Kondo impurities. Novel features originate from the chirality of the coupling in finite magnetic fields. Theoretically we model the double quantum dot system by two Anderson impurities which are both coupled to individual fermionic baths representing the leads as well as to a central fermionic reservoir representing the common source. We calculate equilibrium and transport properties of this model using a variational ansatz for the ground state and discuss the validity of simplified effective coupling models.

[1] Daniel Tutuc et al., arXiv:1010.5692

HL 85.104 Thu 18:00 P4

X-ray characterization Si-doped InAs nanowires grown on GaAs — •Muhammad Saqib[1], Andreas Biermanns[1], Thomas Grap[2], Mihail Lepsa[2], and Ullrich Pietsch[1] — [1]Universität Siegen, Festkörperphysik, Germany — [2]Forschungszentrum Jülich, Institut für Bio- und Nanosysteme (IBN-1),Germany

Semiconductor nanowires (NW) are of particular interest due to the ability to synthesize single-crystalline 1D epitaxial structures and heterostructures in the nanometer range. However, many details of the growth mechanism are not well understood. In particular, understanding and control of doping mechanisms during NW growth are important issues for technological applications. In this contribution we present a x-ray diffraction study of the influence of Si-doping in InAs NWs grown on GaAs (111) substrates using In-assisted MBE growth. With the help of coplanar and asymmetric x-ray diffraction, we monitor the evolution of the lattice constants and structure of the InAs NWs as function of doping concentration. We observe that increasing the nominal doping concentration leads to the appearance of additional diffraction maxima corresponding to material whose vertical lattice parameter is 1% smaller than that of the undoped nanowires. Those lattice parameters can be attributed with alloy formation in the form of island like crystallites.

HL 85.105 Thu 18:00 P4

Electronic transport properties of InAs nanowires — •Önder Gül, Christian Blömers, Hilde Hardtdegen, Mihail Ion Lepsa, Kamil Sladek, Andreas Penz, Thomas Grap, Detlev Grützmacher, and Thomas Schäpers — Institute of Bio- and Nanosystems (IBN-1) and JARA - Fundamentals of Future Information Technology, Forschungszentrum Jülich GmbH, D-52425 Jülich, Germany

III-V nanowires have recently attracted a lot of interest, because they are promising building blocks for future nanoscale applications, such as high density field effect transistors, high performance solar cells or sensing devices. In this context, InAs is especially interesting because of its low effective electron mass, its high predicted electron mobility, and its low direct band gap. Additionally ohmic contacts are easy to prepare because of the intrinsic surface electron accumulation. We investigated the transport properties of InAs nanowires, grown by means of molecular beam epitaxy and metal organic vapor phase epitaxy. In a temperature range from 300K down to 4K we determined basic transport parameters such as contact resistance, resistivity, mobility, and carrier concentration. At low temperatures, magnetotransport measurements were carried out in order to observe electron interference effects.

HL 85.106 Thu 18:00 P4

Spin noise spectroscopy of single semiconductor quantum dots — •Ramin Dahbashi[1], Michael Schmidt[1], Klaus Pierz[2], Hans Werner Schuhmacher[2], Jens Hübner[1], and Michael Oestreich[1] — [1]Institute for Solid State Physics, Leibniz Universität Hannover, Appelstr. 2, D-30167 Hannover, Germany — [2]Physikalisch-Technische Bundesanstalt, Bundesallee 100, D-38116 Braunschweig, Germany

We demonstrate spin noise spectroscopy [1] as a technique for the nearly perturbation free measurement of the electron spin dynamics in single semiconductor quantum dots charged with one electron or one hole. The investigated sample are InAs quantum dots with a density gradient enclosed in a Bragg mirror cavity. The charge status is determined via the spectral and polarization dependence of the photoluminescence. We present preparatory photoluminescence measurements to ensure that we can detect single quantum dot photoluminescence. The measurements are set up in a self-designed sample rod for ordinary helium bottles to realise an intrinsically stable, low temperature measurement system with direct optical access.

[1] G. M. Müller, M. Oestreich, M. Römer, and J. Hübner, Semiconductor spin noise spectroscopy: Fundamentals, accomplishments, and challenges, Physica E 43, 569 (2010).

HL 85.107 Thu 18:00 P4

Magnetotransport on ferromagnetiv (Ga,Mn)As/GaAs core-shell nanowires — •Christian Butschkow[1], Stefan Geissler[1], Andreas Rudolph[1], Marcello Soda[1], Elisabeth Reiger[1], Dieter Schuh[1], Werner Wegscheider[2], and Dieter Weiss[1] — [1]Institute for Experimental and Applied Physics, Universität Regensburg, Universitätsstraße 31, 93053 Regensburg — [2]Solid State Physics Laboratory, ETH Zurich, 8093 Zurich, Switzerland

We performed magnetotransport measurements on individually contacted GaAs/(Ga,Mn)As nanowires at low temperatures. The core nanowires were grown by MBE using gold as catalyst at a temperature of 530°C. For the (Ga,Mn)As shell growth, the substrate temperature was decreased to 205°C. A Curie-Temperature of 17K to 20K was observed by SQUID measurements on an ensemble of 10^8 nanowires as well as by transport measurements. Investigating the magnetoresistance effects for various field directions we can determine the magnetic anisotropy to be strongly uniaxial with a magnetic easy axis pointing along the nanowire axis. The observed effects are very pronounced when compared to (Ga,Mn)As bulk material with a similar manganese concentration. Also the anisotropy field and coercive fields are significantly larger than for (Ga,Mn)As bulk material.

HL 85.108 Thu 18:00 P4

Triple dot structures from CMOS-compatible SOI-FETs — •Dharmraj Kotekar-Patil[1], Matthias Ruoff[1], Stefan Jauerneck[1], Dieter Kern[1], David Wharam[1], Marc Sanquer[2] und Maud Vinet[3] — [1]Eberhard Karls Universität, Tübingen — [2]CEA INAC, Grenoble, France — [3]CEA LETI, Grenoble, France

We report on electronic transport in triple quantum dots in series created by three closely spaced top gates on the same SOI-nanowire. Each quantum dot is individually characterised as a single electron transistor(SET) exhibiting clear Coulomb blockade oscillations. We also study the electrostatic coupling between 2 dots at a time with the third dot kept at a fixed bias. From charge stability measurements for each combination of gates, interdot capacitances and cross capacitances between dots and gates are extracted and correlated with geometrical models. Device fabrication is compatible with advanced CMOS processes so the devices may serve as building blocks for charge based quantum

computes or quantum cellular automata (QCA).

HL 85.109 Thu 18:00 P4

Droplet epitaxy of InGaAs quantum dots on (100) GaAs substrate — •Verena Zuerbig, Aleksandar Gushterov, Mohamed Benyoucef, and Johann Peter Reithmaier — Technische Physik, Institute of Nanostructure Technologies and Analytics, University of Kassel, Heinrich-Plett-Strasse 40, 34132 Kassel, Germany

In 1991 N. Koguchi et al. has proposed an alternative growth technique named droplet epitaxy (DE) for fabrication of self-organized nanostructures. DE offers the fabrication of nanostructures with reduced or without wetting layer on both lattice matched and lattice-mismatched substrates in comparison to the widely used Stranski-Krastanov (SK) growth mode, which is extremely attractive for the growth of lattice-mismatched substrates. Many groups use low temperature QD DE growth to prevent material redistribution. But the low temperature results in poor crystal quality of the QD structures, which needs additional annealing steps at high temperatures. We report on the structural (atomic force microscope) and optical (macro- and micro-photoluminescence) properties of InGaAs QDs grown by DE on undoped (100) GaAs substrates at elevated growth temperatures in the range from 410 °C to 500 °C to preserve the crystal quality of QDs. By using different growth conditions such as substrate temperature, amount and deposition rate of In, As flux and the opening time of the As valve, QDs with small sizes (height: 2-6 nm) and narrow photoluminescence linewidth (30 meV) are fabricated. Sharp and intense luminescence lines obtained by micro-photoluminescence spectroscopy showed good quality of QDs formed by DE.

HL 85.110 Thu 18:00 P4

Optical properties of ZnO/ZnMgO nanowire heterostructures — •Nils Neubauer[1], Bingqiang Cao[2], Marius Grundmann[2], and Frank Cichos[1] — [1]Molecular Nanophotonics Group, University of Leipzig, Linnéstraße 5, 04103 Leipzig — [2]Semiconductor Physics Group, University of Leipzig, Linnéstraße 5, 04103 Leipzig

ZnO nanowires are promising candidates for the fabrication of nanoscaled light emitting devices. Due to the large energy bandgap and exciton binding energy of ZnO, it offers the possibility for nanoscale light emitters in the UV spectral region working at room temperature. Pulsed laser deposition (PLD) enables the growth of defined nanowire shapes and nano-heterostructures to modify their optical properties. Due to quantum confinement effects in such heterostructures even single-photon emission is possible, a key requirement for future communication technologies like quantum cryptography. We have investigated ZnO nanowires with a radial and axial ZnO/ZnMgO quantum well heterostructure. These core/shell nanostructures were grown by a two step PLD process, which leads to a low area-density of the nanowires to provide homogeneous growth of the quantum well heterostructures. Optical studies were carried out in a photoluminescence setup. Excitation is done with a frequency quadrupled Nd:YVO_4 laser in a TIRF (Total Internal Reflection Fluorescence) configuration. The emitted light is collected confocally and is detected in a Hanbury Brown-Twiss setup to study photon correlations.

HL 85.111 Thu 18:00 P4

Control of the carrier density of an inverted GaAs/$Al_xGa_{1-x}As$ high electron mobility transistor (HEMT) heterostructure with embedded quantum dots via a backgate — •Sascha René Valentin, Arne Ludwig, Dirk Reuter, and Andreas D. Wieck — Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, Universitätsstrasse 150, D-44780 Bochum

InAs quantumdots coupled to a two-dimensional electron gas (2DEG) are already widely studied but the tuning of the charge of the quantum dots is always accompanied by a change of the carrier density of the 2DES. In this contribution we show a structure with a backgate which is capable of charging the quantum dots independently of the density of the carriers in the 2DEG. Different approaches for such a backgated structure will be discussed.

HL 85.112 Thu 18:00 P4

Asymmetric optical nuclear spin pumping in a single uncharged quantum dot — •Heike Schwager[1], Florian Klotz[2], Vase Jovanov[2], Johannes Kierig[2], Emily C. Clark[2], Gerhard Abstreiter[2], Martin Brandt[2], Geza Giedke[1], and Jonathan Finley[2] — [1]Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Straße 1, 85748 Garching — [2]Walter Schottky Institut, Technische Universität München, Am Coulombwall 3, 85748 Garching

Highly asymmetric dynamic nuclear spin pumping is observed in a single self-assembled InGaAs quantum dot subject to resonant optical excitation of the neutral exciton transition. A large maximum polarization of 54% is observed and the effect is found to be much stronger upon pumping of the higher energy Zeeman level. Time-resolved measurements allow us to directly monitor the buildup of the nulcear spin polarization in real time and to quantitatively study the dynamics of the process. A strong dependence of the observed dynamic nuclear polarization on the applied magnetic field is found, with resonances in the pumping efficiency observed for particular magnetic fields. We develop a model that accounts for the observed behaviour, where the pumping of the nuclear spin system is due to hyperfine-mediated spin flip transitions between the states of the neutral exciton manifold.

HL 85.113 Thu 18:00 P4

Investigation of the local electronic structure of Cu-doped GaN by XANES and XLD — •Ralf Schuber[1], Philipp R. Ganz[1], Fabrice Wilhelm[2], Andrei Rogalev[2], and Daniel M. Schaadt[1] — [1]Institute of Applied Physics/DFG-Center for Functional Nanostructures, Karlsruhe Institute of Technology, Germany — [2]European Synchrotron Radiation Facility (ESRF), Grenoble, France

Cu doped GaN has been reported to exhibit ferromagnetic behavior at room temperature, in implanted films, nanowires and in grown films. However, there are yet many unanswered questions concerning the mechanism of ferromagnetism in this system. Above all, a detailed understanding of the incorporation of Cu in the GaN host is desirable. The local electronic structure of Cu-doped GaN can suitably be probed by the element specific x-ray linear dichroism (XLD) as well as the x-ray absorption near edge structure (XANES) at the K-edges of Cu and Ga. This was done at the ESRF ID12 beamline on a series of GaN:Cu samples grown by plasma assisted MBE with nominal Cu concentrations between 0% and 2.3%. To clarify the role of the surface compounds on the samples and to evaluate the Cu site position in the GaN host, i.e. Cu on Ga sites, N sites or interstitial sites, we performed simulations of the GaN:Cu and the Cu9Ga4 crystals for the Cu and Ga K-edges at different doping levels using the FDMNES code [1]. A comparison with the experimental results shows that the Cu atoms predominantly occupy Ga and interstitial sites. [1] Y. Joly, Phys. Rev. B, 63, 125120 (2001).

HL 85.114 Thu 18:00 P4

Interpretation of photoluminescence decay at the limits of time-resolution — •Markus Göthlich, Torsten Langer, Uwe Rossow, and Andreas Hangleiter — Institut für Angewandte Physik, Technische Universität Braunschweig

Time-resolved photoluminescence spectroscopy using time-correlated single photon counting is a reliable way to measure carrier lifetimes that are long compared to the temporal resolution of the instruments. But problems arise, when carrier lifetimes become comparable or even shorter than that: A convolution of the real intensity decay $I_{\mathrm{true}}(t)$ and the response function of the instruments $h(t)$ leads to a significant broadening of the resulting experimental intensity transients $I_{\mathrm{exp.}}(t) = \int_{-\infty}^{t} h(t-\tau) I_{\mathrm{true}}(\tau) d\tau$. This not only affects the lifetime values obtained from the experiment. There is also an influence on the shape of the transients. In this contribution, we discuss different numerical methods of deconvolving $h(t)$ with the aim to reconstruct the "true" decay transients and to improve the over-all time-resolution of the experimental setup. A possible method is based on Fourier transforms, as deconvolution is simple in Fourier space. Other numerical methods solve a set of linear equations: $I_{\mathrm{exp.},j} = h_{ji} \cdot I_{\mathrm{true},i}$. Both ways are very sensitive to experimentally inevitable noise, making deconvolution a sophisticated task. We test different algorithms by applying them to simulated convolved transients where the true lifetime is known. Furthermore, we demonstrate the application on measured transients of GaInN/GaN quantum well structures.

HL 85.115 Thu 18:00 P4

Defekterzeugung durch hohe elektrische Stromdichten im III-V-Halbleiter Galliumnitrid — •Christian Karrasch, Thomas Geruschke, Bert Kann und Reiner Vianden — Universität Bonn, Helmholtz-Institut für Strahlen- und Kernphysik, Nußallee 14-16 D-53115 Bonn

Galliumnitrid (GaN) besitzt vielfältige technische Anwendungen in der Halbleiterindustrie, wie z.B. Hochleistungsdioden und -transistoren. Dennoch ist über Schädigungsmechanismen in GaN und die durch elek-

trischen Strom erzeugten Kristalldefekte noch wenig bekannt. Mit Hilfe der Methode der gestörten Winkelkorrelation (PAC) können Gitterdefekte untersucht und klassifiziert werden. Als PAC Sonde wird ^{111}In in undotiertes GaN implantiert. Die dabei entstehenden Implantationsschäden werden durch thermische Behandlung ausgeheilt. Da Indium isoelektronisch zu Gallium ist und in einer ternären Verbindung in blauen InGaN-LEDs Verwendung findet, eignet es sich sehr gut als Sondenatom zur PAC-Messung. Aufgrund der relativ kurzen Halbwertszeit von ^{111}In ($t_{1/2}$ = 2,83 d) muss die Belastung durch elektrischen Strom mit sehr hoher Stromdichte (über 10^4 A/cm^2) durchgeführt werden. Anschließend wird die Schädigung des GaN Gitters durch den elektrischen Stromfluss untersucht. Zur weiteren Charakterisierung werden Hall-Effekt Messungen durchgeführt.

HL 85.116 Thu 18:00 P4

Properties of quaternary (Al, Ga, In)N layers and MQWs — •Lars Groh, Christoph Hums, Armin Dadgar, Jürgen Bläsing, and Alois Krost — Institut für Experimentelle Physik, Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg

The achievement of efficient green LEDs is at present mostly prohibited by the Quantum Confined Stark-Effect (QCSE), which leads to a low quantum efficiency for longer wavelengths. Responsible for the QCSE are strong polarization fields in growth direction of c-axis oriented group-III-nitride heterostructures, especially within the quantum wells. To reduce or eliminate these polarization fields, mainly two approaches are followed. The first and most popular one is to change the growth direction to semi- or non-polar facets. Our approach is to change the barrier material in order to control the band gap and in particular the polarization field strength. By this the polarization of well and barrier can be nearly matched, with the benefit of the well established growth in c-axis direction which is, e. g., low in stacking fault density. We have grown by MOVPE GaInN/AlGaInN MQWs on silicon and sapphire substrates to investigate the effect of different growth conditions on the composition and luminescence of these structures. PL, (HR)XRD and FE-SEM measurements have been performed. The results from these measurements are compared to the predictions from theory.

HL 85.117 Thu 18:00 P4

Influence of crystal defects on the magnetic properties of Gd-doped GaN — •Stepan Shvarkov[1], Dirk Reuter[1], Andreas D. Wieck[1], Hans-Werner Becker[2], Yvon Cordier[3], Jens Herford[4], and Achim Trampert[4] — [1]Ruhr-Universität Bochum, Lehrstuhl für Angewandte Festkörperphysik, Universitätsstr. 150, 44780 Bochum, Germany — [2]Ruhr-Universität Bochum, RUBION, Universitätsstr. 150, 44780 Bochum, Germany — [3]CNRS-CRHEA, rue Bernard Grégory, 06560 Valbonne, France — [4]Paul Drude Institut für Festkörperelektronik, Hausvogteiplatz 5-7, 10117 Berlin, Germany

Investigations on the role of crystal defects for the magnetic properties of Gd-doped GaN are presented. GaN layers were grown by molecular beam epitaxy (MBE) with Gd atoms incorporated during the growth. Defects were intentionally introduced by performing N^+ implantation. The magnetization measured by a superconducting quantum interference device (SQUID) increased after the N^+ ions were implanted. In addition, the electrical transport properties of Gd-implanted $Al_xGa_{1-x}N$/GaN high electron mobility transistor (HEMT) structures have been studied. Gd was implanted in the MBE-grown $Al_xGa_{1-x}N$/GaN heterostructures by focused ion beams (FIB). Two sets of the samples were prepared: one set of samples was analyzed as implanted, while the other one was thermally annealed after the Gd implantation so that the number of defects was reduced. Anomalous Hall effect (AHE) was observed for both types of samples. However, AHE measured on the as-implanted samples was found to be much more pronounced than the one of the annealed samples.

HL 85.118 Thu 18:00 P4

Band-to-band Auger recombination in GaInN from first principle calculations — •Markus Heinemann and Christian Heiliger — I. Physikalisches Institut, Justus Liebig University Giessen, D-35392 Giessen, Germany

Recent theoretical work [1] implies that inter-band Auger recombination causes a resonance in the Auger coefficient in the blue to green spectrum and opened a discussion whether this effect may lead to a loss in quantum efficiency of nitrite based light emitters. We investigate the possibility of intra- and inter-band Auger recombination in wurtzite $Ga_{1-x}In_xN$ alloys. Using density functional theory and the local density approximation we compute Auger recombination rates for Indium concentrations x ranging from 0 to 100%.

[1] K. T. Delaney, P. Rinke, and C. G. Van de Walle, Appl. Phys. Lett. **94**, 191109 (2009)

HL 85.119 Thu 18:00 P4

Locally resolved imaging of internal electric fields in GaN/GaInN quantum wells by differential phase contrast microscopy — •Matthias Lohr[1], Johannes Thalmair[1], Michael Jetter[2], Ferdinand Scholz[3], and Josef Zweck[1] — [1]Fakultät für Physik, Universität Regensburg, D-93053 Regensburg — [2]Fakultät für Physik, Universität Stuttgart, D-70569 Stuttgart — [3]Institut für Optoelektronik, Universität Ulm, D-89081 Ulm

InGaN/GaN-based laser diodes emitting in the green spectral range are still difficult to achieve. The efficiency "droop" in the green spectral range is strongly believed to be a consequence of the quantum confined Stark effect (QCSE), due to inner piezoelectric fields in the material, caused by strain at the interfaces.

Attempts are made to reduce the piezoelectric (PE) fields by choosing semi- or non-polar crystal facets for the growth of quantum wells. It is necessary to measure the existing PE fields in order to determine whether the various approaches actually can reduce the QCSE and to foster more efficient light emission.

We present first results using differential phase contrast (DPC) in a (S)TEM, where we measure directly the beam deflection due to the inner PE fields. The specimens contain quantum wells grown on different facets. The DPC images display the PE fields in strong contrast and laterally highly resolved over a large field of view. We observe effects not only in the quantum wells but also adjacent to them in the substrate layer and around stacking faults.

This work is part of the PolarCoN project (DFG FOR 957).

HL 85.120 Thu 18:00 P4

GaN-ZnO-InGaN/GaN core shell nanorods — •Ingo Tischer[1], Mohamed Fikry[2], Manfred Madel[2], Ferdinand Scholz[2], and Klaus Thonke[1] — [1]Institut für Quantenmaterie, Gruppe Halbleiterphysik, Universität Ulm, 89069 Ulm — [2]Institut für Optoelektronik, Universität Ulm, 89069 Ulm

For sensing application it is desirable to have GaN nanorods with InGaN quantum wells which are standing upright in a well defined pattern. Our approach starts with ordered GaN pyramids on which in a first step ZnO nanopillars were grown. This structure was overgrown with GaN, and subsequently with a radial GaN/InGaN multi quantum well structure.

We report about the structural and optical properties of this nanostructured material which we investigated by spatially resolved cathodoluminescence, photoluminescence, energy dispersive X-ray spectroscopy, and X-ray diffraction.

HL 85.121 Thu 18:00 P4

Optical investigation on the valence band structure of AlGaN with low Al content — •Tobias Meisch[1], Frank Lipski[2], Kamran Forghani[2], Benjamin Neuschl[1], Martin Feneberg[3], Ferdinand Scholz[2], and Klaus Thonke[1] — [1]Institut of Quantum Matter, Ulm University, 89069 Ulm, Germany — [2]Institut of Optoelectronics, Ulm University, 89069 Ulm, Germany — [3]Institut für Experimentelle Physik, Abt. Materialphysik,Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg

For the binary semiconductors GaN and AlN, the crystal field splitting determining the valence band structure changes from $\approx$ +20 meV (GaN) to $\approx$ -200 meV (AlN), whereas the spin orbit splitting should remain constant at $\approx$ 20 meV. Therefore, for unstrained AlGaN ternary layers an interchange of the character of the topmost valence band from Γ_9 to Γ_7 is theoretically expected for an Al content in the range of 5-10%, manifesting itself mainly in a change of polarization of optical transitions. Strain in epitaxial layers alters the situation and shifts this crossing point. Literature reports experimental values ranging from 20% to 75% Al for the crossover. We present results of temperature dependent photoluminescence and reflectivity experiments on AlGaN layers with Al content ranging from 0 to 30%, and find different contributions from free and bound excitons. The Al content and strain were determined from multiple HRXRD reflections, and entered in a 6x6 k·p model calculation. We discuss our experimental spectra on the basis of this calculation.

HL 85.122 Thu 18:00 P4

Scanning near-field optical microscopy on UV emitting

GaN/AlGaN quantum well structures — •Peter Clodius, Holger Jönen, Uwe Rossow, and Andreas Hangleiter — Technische Universität Braunschweig, Institut für Angewandte Physik, Mendelssohnstr. 2, 30106 Braunschweig

The efficiency of GaN/AlGaN quantum well (QW) structures is quite low compared to GaInN/GaN structures emitting in the blue/violet spectral region which show very high efficiencies despite the high defect density that is commonly observed in such structures. Our explanation for the high efficiency of GaInN/GaN structures is based on the observation that every dislocation in highly efficient c-plane GaInN/GaN structures is decorated with a so-called V-pit, a hexagonal shaped inverted pyramid with $(10\bar{1}1)$ sidewalls. On these sidewalls, thinner quantum wells act as a barrier, suppressing nonradiative recombination at the defects. TEM measurements on high efficiency GaN/AlGaN UV structures have shown that pit formation around defects also takes place in those structures [1]. In this contribution, we will present scanning near-field optical microscope (SNOM) measurements of the luminescence of these high efficiency UV emitting GaN/AlGaN quantum well structures with a spatial resolution below 100 nm. Light emission with a wavelength shorter than that of the c-plane QW, originating from the sidewalls of the pits, which is visible in low temperature measurements, indicates that a similar mechanism is present in UV structures.

[1]D. Fuhrmann et. al. Phys. Rev. B **79**, 073303 (2009)

HL 85.123 Thu 18:00 P4

Internal quantum efficiency of high In content GaInN quantum well structures — •Fedor Alexej Ketzer, Holger Jönen, Heiko Bremers, Uwe Rossow, and Andreas Hangleiter — Institute of Applied Physics, TU Braunschweig, Germany

The internal quantum efficiency (IQE) of GaN based light emitters shows a strong reduction for emission wavelenghts beyond 500 nm. In order to get LEDs and LDs emitting in the green spectral region the indium content has to be increased. This leads to stronger piezoelectric fields in the quantum wells resulting in a reduced oscillator strength. In addition the low growth temperatures needed for high In contents and the larger strain may lead to an increased defect density and stronger nonradiative recombination. In this contribution we analyze the internal quantum efficiency of GaInN quantum well structures measured by temperature and excitation power dependent photoluminescence. The samples were grown by MOVPE on sapphire or bulk GaN substrates. We investigated single and multiple quantum well structures with indium contents between 18% and 32% and quantum well thickness between 0.8 nm and 2.0 nm. For structures emitting at similar wavelengths the IQE can be optimized using thin quantum wells and high indium contents. Furthermore we studied the influence of subsequent layers on the optical properties of the QWs. The thickness and the growth rate of the GaN barrier directly following the QW turned out to be key parameters for improving the efficiency of our structures.

HL 85.124 Thu 18:00 P4

Dielectric functions of wurtzite GaN at elevated temperatures — •Christian Möller[1], Sviatoslav Shokhovets[1], Gerhard Gobsch[1], Klaus Köhler[2], and Oliver Ambacher[2] — [1]Technische Universität Ilmenau, Weimarer Str. 32, 98693 Ilmenau, Germany — [2]Fraunhofer-Institut für Angewandte Festkörperphysik, Tullastraße 72, 79108, Freiburg, Germany

Wurtzite GaN is already widely used for production of blue-ultraviolet and white light-emitting devices. In addition, numerous applications in high-power and high-temperature electronics are also possible. The knowledge of optical constants and understanding of optical processes in the vicinity of the excitonic absorption edge at room temperature as well as at elevated temperatures is crucial for the design and optimization of GaN-based devices. We carried out spectroscopic ellipsometry (SE) measurements of undoped and Si-doped c-plane epitaxial films of wurtzite GaN in a temperature range 300-800 K. The determined temperature-dependent dielectric functions (DFs) are analyzed in terms of contributions from discrete exciton states, excitonic continuum, band-to-band transitions, and phonon-assisted optical transitions into exciton-phonon complexes. Effects of Si-doping are discussed and the temperature dependence of band-gap and exciton energies and broadening parameters is presented.

HL 85.125 Thu 18:00 P4

Characterization and simulation of coupled GaInN quantum wells — •Christopher Hein, Holger Jönen, Heiko Bremers, Uwe Rossow, and Andreas Hangleiter — Institute of Applied Physics, TU Braunschweig, Germany

Despite the tremendous progress in the field of Group-III-nitrides, new applications and research topics are still emerging. One point of interest is the tunneling transport in nitride heterostructures, which can be realized by coupled quantum wells. In this contribution we present photoluminescence studies of coupled GaInN/GaN multiple quantum wells and the simulation of such structures using Nextnano++. The samples were grown by metal organic vapor phase epitaxy on c-plane sapphire. The In content and the thickness of the GaInN quantum wells determined by X-ray diffraction measurements was 38% and 0.26nm, respectively. The barrier width was varied for each sample between 4.15nm, 3.04nm, 1.3nm and 1.0nm. With decreasing barrier thickness the peak energies observed in photoluminescence decreased from 3.28eV to 3.12eV. In addition the sample structure was simulated by a self-consistent solution of Schrödinger's equation using Nextnano++. The measured PL emission energy was then used to check the results of the simulation and adjust simulation parameters. The decrease of photon energies related to reduced barrier widths can be described by an exponential function in good agreement with theoretical considerations.

HL 85.126 Thu 18:00 P4

Polaritonic effects in wide-gap semiconductors as a function of temperature — •Marie-Elena Kleemann[1], Sviatoslav Shokhovets[1], Gerhard Gobsch[1], and Oliver Ambacher[2] — [1]Technische Universität Ilmenau, Ilmenau, Deutschland — [2]Frauenhofer-Institut für Angewandte Festkörperphysik, Freiburg, Deutschland

Polaritonic effects are regarded as the properties of an excitonic crystal with the spatial dispersion, which is related to the ability of the exciton to move through the lattice.The influence of an increasing temperature on the excitonic polaritons consists in the increasing damping (broadening of optical transitions). In the limiting case of a high damping, the polaritonic effects should become not observable.

In this work we measured polarized reflectance and photoreflectance for high-quality c-plane epitaxial films of wurzite GaN and ZnO as well as of a-and m-plane ZnO crystals in the range from liquid-helium temperatures up to room temperature. In order to reveal the presence of polaritonic effects and their temperature dependence, the data is analyzed using two different models of the dielectric function, which describe the experimental results. While in the first model spatial dispersion is implemented, it is disregarded in the second model.

HL 85.127 Thu 18:00 P4

Optoelectronical properties of InGaN quantum well light emitting diodes on semipolar GaN — •Jens Rass, Marcus Stascheit, Simon Ploch, Tim Wernicke, Patrick Vogt, and Michael Kneissl — Technische Universitaet Berlin, Institute of Solid State Physics, Secretariat EW6-1, Hardenbergstrasse 36, 10623 Berlin, Germany

The performance of GaN-based light emitting diodes (LEDs) is strongly affected by polarization fields along the c-axis of the crystal. Due to the resulting quantum-confined Stark effect the radiative transition rate is reduced and the emission wavelength is blue-shifted when carriers are injected. By growing the structures on semipolar or nonpolar planes the polarization fields can be significantly reduced or even eliminated. In this work, InGaN single quantum well LEDs have been grown by metal-organic vapor phase epitaxy on different semipolar surfaces such as the $(10\bar{1}1)$ and $(20\bar{2}1)$ plane. The optoelectronic properties such as the light output power, the emission wavelength and its shift with injection current as well as the operating voltage have been studied. By employing capacitance-voltage- and current-voltage measurements, the size of the depletion region, the build-in potential, the saturation current and the doping concentrations have been determined. LEDs with emission wavelengths ranging from the violet to the blue and green region are presented and their performance characteristics are compared to LEDs grown on the polar c-plane surface.

HL 85.128 Thu 18:00 P4

Performance characteristic of GaN, InGaN and AlGaN based UV photodetectors with Ti/Al/Mo/Au-contacts — •Bertram Jaeger[1], Jessica Schlegel[1], Patrick Vogt[1], Michael Kneissl[1,2], Sylvia Hagedorn[2], Veit Hoffmann[2], Sven Einfeldt[2], and Markus Weyers[2] — [1]Technische Universität Berlin, Institut für Festkörperphysik, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfre-

quenztechnik, Gustav-Kirchhoff-Str. 4, 12489 Berlin, Germany

We have investigated UV photodetectors with Ti/Al/Mo/Au-contacts on GaN, $Al_{0.2}Ga_{0.8}N$, $In_{0.07}Ga_{0.93}N$ and $In_{0.11}Ga_{0.89}N$ respectively by photocurrent spectroscopy, transmission spectroscopy and I-V measurements. The influence of the different absorber materials on contact properties and device performance will be discussed. The spectral response of each detector has a cut-off wavelength according to the bandgap energy of its absorber material between 317 nm and 416 nm. The AlGaN detector has very low dark current in pA-range for an applied bias up to 100 V indicating a Schottky-like character of the contacts (MSM detector). The GaN and InGaN based detectors however show the behavior of photoconductors with ohmic contacts resulting in dark currents in the mA-range for biases of a few volts. The photocurrent of those detectors is sublinear with incident optical power, which hints at the presence of an internal gain mechanism and may explain the observed high currents. The photocurrent of the AlGaN-based detector is below 1 nA up to 100 V bias and linear with optical power.

HL 85.129 Thu 18:00 P4

Influence of the interdigitated contact geometry on the performance of $Al_{0.2}Ga_{0.8}N$ based MSM photodetectors — •Alexander Wolf[1], Jessica Schlegel[1], Patrick Vogt[1], Sylvia Hagedorn[2], Sven Einfeldt[2], Markus Weyers[2], and Michael Kneissl[1,2] — [1]Technische Universität Berlin, Institut für Festkörperphysik, Hardenbergstr. 36, 10623 Berlin — [2]Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, Gustav-Kirchhoff-Str. 4, 12489 Berlin

The device properties of metal-semiconductor-metal (MSM) photodetectors strongly depend on the interdigitated finger contact geometry. In order to optimize these parameters for visible-blind UV detectors we have characterized $Al_{0.2}Ga_{0.8}N$ MSM structures with Ti/Al/Mo/Au Schottky-contacts in varying finger geometries. We have analyzed the device properties by photocurrent spectroscopy and I-V measurements. The detectors have a cut-off wavelength of 315 nm. All structures show dark currents below 3 pA for bias voltages up to 100 V and linearity with optical power. Photocurrents up to 0.9 nA at 310 nm and a maximum responsivity of 57 mA/W at 310 nm and a bias voltage of 100 V have been obtained. For fixed bias voltages a smaller finger spacing leads to a higher responsivity due to the higher electric fields and reduced carrier transit times. The finger width is a crucial parameter for the optimization of the external quantum efficiency due to shadowing of the underlying semiconductor absorber layer. The dependence of the device properties on geometrical parameters of the interdigitated finger contacts will be presented and compared.

HL 85.130 Thu 18:00 P4

Study of transport processes in AlGaInN-based light-emitting diodes — •Bastian Galler, Ansgar Laubsch, Andreas Wojcik, Hans-Jürgen Lugauer, Alvaro Gomez-Iglesias, Matthias Sabathil, and Berthold Hahn — OSRAM Opto Semiconductors GmbH, Leibnizstraße 4, 93055 Regensburg, Germany

Several experiments investigating the efficiency droop in AlGaInN-based light-emitting diodes (LEDs) point to a loss mechanism resulting from a too high carrier density in the active region causing the decreasing efficiency at high currents [1,2]. Therefore, it is desirable to spread carriers over a larger active volume to achieve good efficiency values at high current densities. As this is difficult to achieve in GaN-based LEDs, a detailed understanding of the transport processes governing the carrier distribution in GaN/InGaN multi-quantum-wells (MQWs) is crucial for further brightness improvements. We study colour-coded LEDs featuring one QW emitting at a longer wavelength to analyze the carrier distribution experimentally. Although the absolute emission from such a high-indium QW is increased due to its more favourable energetic level, valuable insight can be gained analyzing the fraction of the colour-coded emission as a function of temperature and current density.

[1] Y.C. Shen et al., Appl. Phys. Lett. 91, 141101 (2007). [2] A. Laubsch et al., IEEE Transactions on Electron Devices, 7, No. 1 (2010).

HL 86: Quantum Dots: Growth and Characterization

Time: Friday 10:15–13:15 Location: FOE Anorg

HL 86.1 Fri 10:15 FOE Anorg

Effects of *in-situ* annealing on site-selective InAs quantum dots grown on pre-structured GaAs substrates — •Mathieu Helfrich[1,2], Daniel Rülke[1,2], Joshua Hendrickson[3], Michael Gehl[4], Dongzhi Hu[1,2], Michael Hetterich[1,2], Stefan Linden[5], Martin Wegener[1,2], Galina Khitrova[4], Hyatt M. Gibbs[4], Heinz Kalt[1,2], and Daniel M. Schaadt[1,2] — [1]DFG-Center for Functional Nanostructures (CFN), Karlsruhe Institute of Technology (KIT), Wolfgang-Gaede-Str. 1a, 76131 Karlsruhe, Germany — [2]Institut für Angewandte Physik, Karlsruhe Institute of Technology (KIT), Wolfgang-Gaede-Str. 1, 76131 Karlsruhe, Germany — [3]State Scientific Corp., 27-2 Wright Road, Hollis, NH 03049, U. S. A. — [4]College of Optical Sciences, University of Arizona, 1630 E. University Bld., Tucson, AZ 85721, U. S. A. — [5]Physikalisches Institut, University of Bonn, Nußallee 12, 53115 Bonn, Germany

Spatial localization of quantum dots has been achieved reproducibly within a certain range. The aim has shifted to improving the optical properties, decreasing the quantum dot density and controlling the occupation number of quantum dots per site. We report on our investigations of *in-situ* annealing of site-selective InAs quantum dots which aim at understanding the influence of this technique on the aforementioned parameters. We observed a morphological transition of double dots merging into single dots during annealing, accompanied by a reduction of quantum dot densities. The quantum dots are analyzed by atomic force microscopy and photoluminescence spectroscopy.

HL 86.2 Fri 10:30 FOE Anorg

Tuning the emission of GaAs and InGaAs quantum dots — •Eugenio Zallo, Paola Atkinson, Rinaldo Trotta, Armando Rastelli, and Oliver G. Schmidt — Institute for Integrative Nanosciences, IFW Dresden, Helmholtzstrasse 20, 01059 Dresden, Germany

We report on a method to obtain unstrained GaAs/AlGaAs and InGaAs/AlGaAs quantum dots with low surface densities and widely tunable emission wavelength. We first prepare a template of self-assembled nanoholes on a GaAs(001) surface by a droplet etching step which consists of the alternate deposition of Ga and GaAs at a substrate temperature of 520 °C. The template is then overgrown with a 7-10 nm thick AlGaAs layer. The resulting nanoholes, with a depth of 6-10 nm are then filled with different amounts of GaAs or InGaAs, followed by deposition of the top AlGaAs barrier. By gradually increasing the amount of GaAs we can tune the emission wavelength in the spectral range 690-780 nm. By replacing the GaAs with InGaAs, long wavelength emission can be obtained with smaller dots. The high quality of the dots is demonstrated by single-dot photoluminescence spectra, which show excitonic emission linewidths down to 25 μeV (our resolution limit). Finally, we present preliminary results on the effect produced by external biaxial stress on the emission of single initially unstrained QDs.

HL 86.3 Fri 10:45 FOE Anorg

Atomic structure of submonolayer grown InAs/GaAs quantum dots — •Holger Eisele, Andrea Lenz, Jonas Becker, Lena Ivanova, Mario Dähne, Ernst Lenz, Franziska Luckert, Konstantin Pötschke, André Strittmatter, Udo W. Pohl, and Dieter Bimberg — Institut für Festkörperphysik, Technische Universität Berlin, 10623 Berlin

Submonolayer quantum dots are formed by a cycled deposition of the dot material with a thickness well below one monolayer and several monolayers of matrix material. Structural correlation, both vertically as in plane is coupled to strain originating from the dot material. Here, cross-sectional scanning tunneling microscopy (XSTM) is the most powerful tool to determine the spatial structure as well as the stoichiometry with atomic resolution. XSTM measurements demonstrate clearly that there is an island formation instead of a layer-like structure. The InAs is not assembled within a single atomic plane, but segregated along growth direction. The lateral separation between the islands is only about 2 nm, resulting in a very high dot density in the

10^12 cm-2 range. The height of the islands is about 4-5 ML, and the width is approximately 5 nm. The vertical segregation is determined in detail by the analysis of the lattice parameter. At each layer where 0.5 ML InAs was deposited, the measured InAs concentration jumps up to a lattice parameter corresponding to xIn = 15-20%, followed by an exponential decrease. For both structures with differently thick GaAs spacer layers a segregation coefficient of about 0.73 was determined.

HL 86.4 Fri 11:00 FOE Anorg

MBE growth of InAs quantum dots and dashes grown on (100) silicon substrates — •Tariq Al Zoubi, Muhammad Usman, Mohamed Benyoucef, and Johann Peter Reithmaier — Technische Physik, Institute of Nanostructure Technologies and Analytics, University of Kassel, D-34132 Kassel, Germany

Self assembled InAs quantum dots (QDs) are grown by solid source molecular beam epitaxy after deposition of a 50 nm silicon buffer layer on (100) Si substrates using Stranski-Krastanov (SK) growth mode. Reflection high energy electron diffraction (RHEED) streak patterns confirm that the combination of the atomic hydrogen at 500 °C followed by thermal desorption at 900 °C is an efficient surface cleaning method. The evolution of size, density and shape of the QDs are ex-situ characterized by atomic-force microscopy (AFM). Different growth parameters such as InAs coverage, growth temperature, In-growth rate and V/III ratio are examined on differently prepared silicon surfaces including ex- and in-situ cleaning procedures. Additional improvement for the cleaning and growth is achieved by exposing the Si surface with Ga at low fluxes. The Ga treatment at a temperature of 560 °C for two minutes results in a strong reduction of the lateral size of InAs QDs and a significant enhancement of the homogeneity of the dot size and distribution. The InAs QDs density is strongly increased from 10^8 to 10^11 cm^-2 for V/III ratios in the range of 15-35, respectively. InAs QD formations are not observed at temperatures as high as 500 °C. Moreover, InAs quantum dashes are observed at higher In-growth rate of 0.3 ML/s.

HL 86.5 Fri 11:15 FOE Anorg

Nanostructuring of silicon for the growth of site-controlled III/V quantum dots — •Muhammad Usman, Tariq Al Zoubi, Mohamed Benyoucef, and Johann Peter Reithmaier — Technische Physik, Institute of Nanostructure Technologies and Analytics, University of Kassel, Heinrich-Plett-Strasse 40, D-34132 Kassel, Germany

In order to localize the nucleation of III/V quantum dots during MBE growth, the silicon (100) substrate has been patterned with sub 100 nm holes. The processes involved in the nano-patterning of silicon, including electron beam lithography (EBL) and dry etching process, have been optimized. An anisotropic dry etching recipe based on SF6+CHF3 plasma has been used with optimal parameters in order to insure the precise transfer of holes defined on e-beam resist to the underlying silicon substrate. The control over the diameter of the patterned holes has been achieved through optimal EBL parameters including beam acceleration voltage, aperture size and exposure dose for single pixel dot. Arrays of holes with different periods from 1 μm down to 200 nm have been fabricated on silicon substrates. The diameter of the holes has been found to be unchanged for holes with periods of 1 μm, 750 nm and 500 nm, while a slight increase in the diameter for holes with period of 200 nm has been observed due to proximity effect. Preliminary results for the MBE growth of III/V quantum dots on nano-patterned silicon substrate have shown highly selective formation of quantum dots in the patterned holes with 1μm period.

HL 86.6 Fri 11:30 FOE Anorg

Growth of small-period Si/Ge quantum dot crystals by MBE — •Svetlana Borisova[1], Julian C. Gerharz[1], Yasin Ekinci[2], Gregor Mussler[1], and Detlev Grützmacher[1] — [1]Institute of Bio- and Nanosystems 1, Forschungszentrum Jülich, D-52425 Jülich, Germany — [2]Laboratory for Micro- and Nanotechnology, Paul Scherrer Institut, CH-5232 Villigen-PSI, Switzerland

We report on growth of arrays of Ge quantum dots (QDs) on Si substrates. The energy structure of small-period QDs arrays is predicted to be significantly modified by the artificial periodicity. High quality self-assembled Ge QDs can be grown by solid source molecular-beam epitaxy (MBE). The main drawbacks of self-assembled Ge QDs are arbitrary positions where the QDs nucleate as well as broad size dispersion. To solve this problem, prepatterned Si substrates were used to define the position and the size of the QDs. Check-patterns with different periods down to 35 nm and depth of 5-20 nm were realized by extreme ultraviolet interference lithography (XIL) and independently by electron beam lithography followed by reactive ion etching (RIE). Influence of both methods on MBE growth was studied from the point of view of final quality of the holes and simplicity of access, usage and precision of positioning on the substrate. The prepatterned Si substrates were overgrown by few single layers of Ge. The influence of substrate temperature and buffer layer thickness on homogeneity of Ge dots in order to optimize growth procedure was investigated by means of atomic force microscopy (AFM) and in-situ scanning tunnelling microscopy (STM).

15 min. break

HL 86.7 Fri 12:00 FOE Anorg

Ultraviolet photoluminescence of zinc oxide quantum dots sputtered at room-temperature — •Gillian Kiliani[1], Reinhard Schneider[2], Dimitri Litvinov[2], Dagmar Gerthsen[2], Mikhail Fonin[1], Ulrich Rüdiger[1], Alfred Leitenstorfer[1], and Rudolf Bratschitsch[1] — [1]Center for Applied Photonics, Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany — [2]Laboratorium für Elektronenmikroskopie, Karlsruher Institut für Technologie, 76128 Karlsruhe, Germany

Zinc oxide (ZnO) quantum dots showing room-temperature ultraviolet photoluminescence are prepared for the first time by radio-frequency magnetron sputtering without any annealing steps. The quantum dots are embedded in amorphous silicon dioxide and have a narrow size distribution of 3.5 ± 0.6 nm. Room-temperature photoluminescence shows emission in the ultraviolet. Optical transmittance and photoluminescence spectra both exhibit a blueshift of the quantum dot absorption and emission compared to bulk ZnO material which is attributed to quantum confinement. Carrying out the fabrication entirely at room-temperature prevents the degradation of nanooptical devices containing quantum dots which might occur during annealing steps.

HL 86.8 Fri 12:15 FOE Anorg

InGaN quantum dots growth by metalorganic vapour phase epitaxy for green light emitters — •Tilman Schwaner, Abdul Kadir, Christian Meissner, Markus Pristovsek, and Michael Kneissl — Technische Universität Berlin, Institut für Festkörperphysik, Hardenbergstr. 36, 10623 Berlin, Germany

High efficiency green InGaN light emitting diodes and projection displays are one of the most important challenges in solid state lighting technology. To improve the device performance, we studied InGaN/GaN quantum dots as active region. Self-organized InGaN quantum dots were grown on GaN (0001) in the Stranski-Krastanov growth mode in a horizontal metalorganic vapour phase epitaxy reactor. We varied the growth temperature between 600°C - 725°C and the growth times between 20 s and 300 s. The resulting indium content was between 10% and 32% as determined by X-ray diffraction measurements. We could clearly see a transition from 2D to 3D growth mode by atomic force microscopy. The wetting layer thicknesses were 4 nm at 675°C and 3 nm at 625°C, which implies that the wetting layer thickness decreases with increasing indium content. Capping and stacking of multi-InGaN layers are still under investigation. Preliminary photoluminescence and electroluminescence showed strong green emission around 530 nm for a three InGaN quantum dot layer stack.

HL 86.9 Fri 12:30 FOE Anorg

Correlating different characterization methods on individual Carbon Nanotubes — •Robert Frielinghaus[1,2], Karin Goss[1,2], Christian Spudat[1,2], Lothar Houben[2,3], Matthias Müller[4], Christian Thomsen[4], Stefan Trellenkamp[2,5], Carola Meyer[1,2], and Claus M. Schneider[1,2] — [1]Peter-Grünberg-Institut (PGI-6), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]JARA Fundamentals of Future Information Technologies, Forschungszentrum Jülich, 52425 Jülich, Germany — [3]Peter-Grünberg-Institut (PGI-5) und Ernst-Ruska-Centre for Microscopy and Spectroscopy with Electrons, Forschungszentrum Jülich, 52425 Jülich, Germany — [4]Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany — [5]Peter-Grünberg-Institut (PGI-8-PT), Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

Carbon nanotubes (CNTs) can serve as model systems for molecular interactions in (quantum) transport experiments. Their properties are greatly affected by their chemical modification as, e.g., filling with

fullerenes. Yet standard samples do not allow for a direct structural observation. Here we present an approach to perform transport, transmission electron microscopy (TEM) as well as optical Raman measurements all on a single CNT. Windows are etched in a Si_3N_4 TEM membrane on which CNTs are grown by means of chemical vapour deposition. They can then be contacted via standard electron beam lithography. The TEM measurements provide the structural information that is needed for the interpretation of the transport data. This process may readily be applied to other material systems such as nanowires.

HL 86.10 Fri 12:45 FOE Anorg

Cell-internal structure of hexagonal polytypes in III-V semiconductors — •Christian Panse[1], Dominik Kriegner[2], and Friedhelm Bechstedt[1] — [1]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Germany — [2]Institute for Semiconductor and Solid State Physics, Johannes Kepler University Linz, Austria

Semiconductor nanowires (NW) play a key role in future nanotechnology. Despite of the zinc-blende (3C) bulk structure III-V nanowires exhibit a mixture of wurtzite (2H) and zinc-blende (3C) layers. With better control over the crystal structure it became possible to grow not only pure 3C or 2H layers but also small segments of the hexagonal 4H polytype. This offers a new degree of freedom for NW device design, like polytypic superlattices. Therefore, we investigate the structural properties of the different polytypes (3C, 2H, 4H, 6H). We perform *ab-initio* calculations within the density functional theory for different III-V compounds (GaAs, InAs, InP, InSb). The structural properties are calculated versus the hexagonality of the polytypes using the LDA exchange-correlation functional. Experiment (XRD) and theory show that hexagonal bilayers tends to increase the layer thickness along the c-axis, while simultaneously reduce the in-plane distances. Thereby, the change of the lattice parameters scales linearly with the hexagonality of the polytype. Overall an increase in the relative aspect ratio of the 2H structure by 0.6% compared to the ideal structure is observed. It turns out that only a careful treatment of the cell-internal parameters could guarantee a correct description of the structural properties.

HL 86.11 Fri 13:00 FOE Anorg

Model and applications of local droplet etching — •Christian Heyn — Institut für Angewandte Physik, Jungiusstr 11, 20355 Hamburg

The self-organized in situ drilling of nanoholes into semiconductor surfaces by using liquid metallic droplets as local etchant represents a new degree of freedom for the design of heterostructure devices.[1,2] The process is fully compatible with conventional molecular beam epitaxy (MBE) technology and does not require additional equipment. A model of this local droplet etching (LDE) is presented that is based on a core-shell structure of the droplets. With the model, the evolution of the droplet and substrate surface morphology is calculated. We demonstrate quantitative agreement between model results and measured surface morphologies. Furthermore, also the influence of the process temperature is correctly reproduced by the model. A brief overview on recent applications of the LDE method will be given, including the self-assembly of GaAs quantum rings and dots as well as the fabrication of air-gap heterostructures.

[1] Zh. M. Wang, B. L. Liang, K. A. Sablon, and G. J. Salamo, Appl. Phys. Lett. 90, 113120 (2007).

[2] Ch. Heyn, A. Stemmann, and W. Hansen, Appl. Phys. Lett. 95, 173110 (2009)

HL 87: ZnO: Growth and Defects

Time: Friday 10:15–13:30 Location: POT 51

HL 87.1 Fri 10:15 POT 51

Structural parameters of ZnMgO from first principles and experiment — •Marcel Giar[1], Thomas Wassner[2], Bernhard Laumer[1,2], Martin Eickhoff[1], and Christian Heiliger[1] — [1]I. Physikalisches Institut, Justus-Liebig-Universität, D-35392 Giessen, Germany — [2]Walter Schottky Institut, Technische Universität München, Am Coulombwall 3, D-85748 Garching, Germany

Recent experimental research on the variation of the lattice parameters of wurtzite ZnMgO with the Mg content x(Mg) show that the lattice parameter a strongly depends on the thickness of the prepared thin films. For layers with a thickness of about 300nm grown by molecular beam epitaxy a is found to be independent of x [1] whereas for thin films of 1μm we find an increase in a with increasing x. We conduct cell relaxations keeping the lattice parameter a fixed in the basal plane as well as complete cell relaxations using the LDA and a supercell approach to account for both effects known from experiment. We further employ alloy statistics to consider different alloy configurations inside the supercell. Theoretical and experimental results for the lattice constants a and c and related parameters are compared showing a good qualitative agreement.

[1] T. A. Wassner, B. Laumer, S. Maier, A. Laufer, B. K. Meyer, M. Stutzmann, M. Eickhoff, J. Appl. Phys. 105, 023505 (2009)

HL 87.2 Fri 10:30 POT 51

Defect Reduced Growth of Pulsed Laser Deposited ZnO — •Fabian Budack, Marc A. Gluba, Lars-Peter Scheller, and N.H. Nickel — Helmholtz-Zentrum Berlin für Materialien und Energie, Kekuléstr. 5, 12489 Berlin, Germany

Zinc oxide is a transparent semiconductor with a pronounced doping asymmetry. While electron conduction is easily achieved even in nominally undoped material reliable and stable p-type doping was not yet realized. Beside hydrogen, intrinsic defects have been discussed as the origin of the prevailing n-type conduction. Understanding the conditions for the formation of native donor-like defects is a necessary step towards obtaining stable p-type ZnO.

Nominally undoped, albeit n-type, ZnO thin films have been deposited by pulsed laser ablation (PLD) on sapphire and MgO substrates under varying oxygen partial pressures. Both, structural parameters like growth rate as well as electrical properties, were investigated. It is found that the carrier concentration shows a distinct minimum at oxygen partial pressures of 5 to $7 \cdot 10^{-4}$ mbar while the mobility is nearly constant over a broad range of partial pressures. The decrease of the electron concentration is accompanied by an increasing growth rate, indicating a defect reduced growth mode in the presence of oxygen. However, a further increase of the deposition pressure leads to the formation of nanostructures, which results in new defects. This trade-off and its impact on the doping asymmetry of ZnO will be discussed.

HL 87.3 Fri 10:45 POT 51

Electrochemical deposition of ZnO for Flexible Electronic Devices — •Miriam Schwarz and Veit Wagner — School of Engineering and Science, Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

Electrochemical deposition from aqueous zinc nitrate ($Zn(NO_3)_2$) solution provides a simple way to deposit crystalline ZnO at low temperatures. Thus, it is a suitable process for flexible substrates like polyethylenterephthalat (PET) foil and makes ZnO to an interesting alternative in the field of flexible electronics in comparison to organic counterparts. The electrochemical approach allows to strongly influence the morphology of the ZnO layer by many well defined deposition parameters like the applied voltage, temperature, time and electrolyte concentration. This correlation is investigated by atomic force microscopy (AFM) and scanning electron microscopy (SEM) for the morphology of the ZnO layer, while Raman spectroscopy is applied to evaluate the crystalline quality of the layers. It reveals that ZnO crystallites of hexagonal shape with diameters depending on the deposition parameters are achieved. In order to study the correlation between the ZnO morphology and its electrical performance in devices, Schottky diodes and field-effect transistors were manufactured and systematically analyzed.

HL 87.4 Fri 11:00 POT 51

Incorporation of dopant atoms into zinc oxide surface layers using ultrashort laser pulses — •Andreas Schneider, Apurba Dev, Kathrin Sebald, and Tobias Voss — Institut für Festkörperphysik, Bremen, Germany

The exposure of semiconductors to ultrashort laser pulses can lead to

ultrafast melting and ablation of their surfaces. These non equilibrium processes create quasi-periodic surface structures. For silicon, these micro-structured surfaces - often called black silicon - show a strong increase of the absorption above and below its bandgap in a sulphurous environment creating an extremely highly doped surface layer. We apply a similar approach for zinc oxide. A thin layer of antimony is vapor-deposited on a bulk c-plane wafer followed by structuring the sample with amplified 100fs laser pulses. After multiple pulses, the zinc oxide surface shows a ripple pattern. Steep trenches run down to 3μm into the bulk. Cross sectional TEM measurements reveal a 200nm thick polycrystalline layer on top of the ripple structure. Below this layer the ripples are single crystalline. EDX measurements show that antimony was incorporated to the first 260nm, resulting in the tracing of antimony even in the single crystalline region. The exact amount of incorporation and the surface morphology strongly depend on the applied structuring parameters. Using SEM we find that increasing the laser fluence also increases the observed ripple period. In contrast to this a larger number of pulses leads to smaller ripple periods as well as steeper and deeper trenches. Our results are a promising step towards doping zinc oxide surface layers by ultrashort laser pulses.

HL 87.5 Fri 11:15 POT 51

Dominant Laplace DLTS peaks E280 and E290 in melt-grown ZnO — •Leopold Scheffler, Vladimir Kolkovsky, and Jörg Weber — Technische Universität Dresden, 01062 Dresden, Germany

In the present study single-crystal ZnO grown from the melt was investigated by electrical measurements such as DLTS and high-resolution Laplace DLTS. A peak E280 dominates the DLTS spectrum in the wide temperature range of 20-450 K. Using high-resolution Laplace DLTS this peak was found to consist of two levels with activation energies of 280 meV and 290 meV below the conduction band, respectively. The relative intensities of these peaks depend on the measurement temperature. The thermal stability of the defects in oxygen and oxygen-lean atmosphere is analyzed. The origin of these defects will be discussed.

HL 87.6 Fri 11:30 POT 51

Metastable state of the $V_{Zn}H_2$ defect in ZnO — •Dirk Bastin, Edward Lavrov, and Jörg Weber — Technische Universität Dresden, 01062 Dresden, Germany

The Zn vacancy passivated by two hydrogen atoms in ZnO $V_{Zn}H_2$ was studied by IR absorption spectroscopy. It was shown that in addition to the ground state comprising two inequivalent O-H bonds aligned parallel and 'perpendicular' to the c-axis of the crystal, there is a metastable state of the defect ($V_{Zn}H_2^*$). $V_{Zn}H_2^*$ consists of two equivalent O-H bonds oriented 'perpendicular' to the c-axis. The metastable state of the Zn vacancy decorated with two hydrogen atoms reveals two local vibration modes at 3329.0 and 3348.4 cm^{-1} which represent antisymmetric and symmetric combinations of the two separate O-H stretch modes, respectively. The energy difference between the ground and the metastable states of the complex was found to be 75±9 meV. It was also established that the activation energy of the hydrogen motion within the Zn vacancy is 0.96±0.09 eV.

15 min. break

HL 87.7 Fri 12:00 POT 51

Ion-beam Induced Luminescence in n-type Zinc Oxide — •Ronald Stübner[1], Matthias Allardt[1], Daniel Severin[2], Markus Bender[2], and Jörg Weber[1] — [1]Technische Universität Dresden, 01062 Dresden, Germany — [2]GSI Helmholtzzentrum für Schwerionenforschung, 64291 Darmstadt, Germany

Ion implantation of semiconductors introduces a wide variety of defects. Their concentration and depth profile depends on the energy and the fluence of the ions as well as on the temperature of the sample during the irradiation. The in-situ monitoring of these defects helps to understand the creation mechanism and kinetics of the different kinds of defects. The design and assembly of an ionoluminescence measurement system was done during a diploma thesis. The system has been installed at the M-Branch of the ion accelerator at the GSI Helmholtz Centre for Heavy Ion Research in Darmstadt where samples of n-type ZnO single crystals have been irradiated at room temperature and low temperatures, respectively. In this talk, the results of these measurements as well as the results of subsequent photoluminescence investigations will be presented.

HL 87.8 Fri 12:15 POT 51

$Zn_{1-x}Cd_xO$ thin films and heterostructures grown by pulsed laser deposition — •Martin Lange, Christof P. Dietrich, Holger von Wenckstern, Michael Lorenz, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Semiconductor Physics Group, Linnéstr. 5, D-04103 Leipzig, Germany

Effecient optoelectronic devices are based on heterostructures which require band gap engineering. A reduction of the ZnO bandgap is possible when Cd is incorporated.[1] Here, we present an ansatz allowing the incorporation of up to 24 % Cd in ZnO without a phase separation using pulsed laser deposition. Therefore, we applied low substrate temperatures down to room temperature. A red-shift of the near band-edge luminescence down to energies of approximately 2.6 eV was achieved.

We used mixed targets of ZnO and CdO and were therefore able to grow the $Zn_{1-x}Cd_xO$ directly on the a-plane saphire substrates without surrounding ZnO layers. The thin films exhibit a wurtzite crystal structure with the c-axis parallel to the growth direction. With increasing Cd-content the c-axis constant increases in agreement with literature.[2] The bandgap energy decreases with increasing Cd-content, which was verified by a red-shift of the luminescence maximum and the absorption edge of the $Zn_{1-x}Cd_xO$.

Finally, $Zn_{1-x}Cd_xO$ was combined with ZnO thin films and ZnO nanowires in various heterostructures.

[1] S. Sadofev *et al.*, Appl. Phys. Lett. **89**, 201907 (2006)
[2] K. Yamamoto *et al.*, J. Cryst. Growth **312**, 1703 (2010)

HL 87.9 Fri 12:30 POT 51

Strain-related defects in $Mg_xZn_{1-x}O$ thin films — •Florian Schmidt, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Abteilung Halbleiterphysik, Linnéstraße 5, 04103 Leipzig

We investigated the influence of tensile and compressive strain, respectively, on the incorporation of deep levels defects in $Mg_xZn_{1-x}O$ thin films grown by pulsed-laser deposition on a-plane sapphire substrates. For ZnO it was recently shown that tensile strain induces a new defect level traceable via photoluminescence by the recombination line I_{12} [1]. In order to investigate thin films under tensile and compressive strain, respectively, we chose Al-doped ZnO as buffer layer, which has a larger a-lattice constant than that of ZnO and can be used as an ohmic back-contact due to its low resistivity. The a-lattice constant of $Mg_xZn_{1-x}O$ increases with x, so the Mg-content can be used to change the strain state of the thin film from tensile to compressive strain. Therefore, we changed the Mg-contents in the samples from $x = 0$ to 0.02. In concordance with ref. [1] we observe the I_{12} transition in low temperature photoluminescence measurements only if the samples are under tensile strain. Further we have found by deep level transient spectroscopy (DLTS) and Laplace DLTS that the two deep level defects, labelled T2 and E3' in the literature, are detectable only in thin films under tensile strain. The E3' defect level is most likely an extended defect formed to relief stress. Independent of the strain state the two defect levels E100 and E3 are detected.

[1] M. Brandt *et al.*, Phys. Rev. B **81**(7) 073306 (2010)

HL 87.10 Fri 12:45 POT 51

Strain distribution in ZnO microwires — •Christof P. Dietrich, Martin Lange, Fabian J. Klüpfel, Rüdiger Schmidt-Grund, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Abteilung Halbleiterphysik, Institut für ExperimentellePhysik II, 04103 Leipzig, Germany

We present a direct experiment to determine the strain dependence of semiconductor energy bands with high precision. For this purpose we benefit from the unique properties of self-organized grown ZnO microwires with respect to their excellent crystal quality and the possibility to easily adjust the strain in such objects by bending, opposite to thin films or bulk single crystals. In order to study the band gap energy variation with strain we measure the related photoluminescence (PL) of the exciton recombination spatially resolved at low temperatures on mechanically bent ZnO microwires fabricated by carbothermal reduction. We show that mechanical bending leads to a significant blue and red-shift of the wire luminescence due to the formation of compressive and tensile strained parts of the wire, respectively. Linescans perpendicular to the wire axis showed maximum energetic shifts of the dominant recombination peaks of ±30 meV due to strain values of ±1.5 %. The compressive and tensile strain inside the wires turned out to be symmetrically distributed perpendicular to the wire axis meaning that the neutral fibre coincides with the central wire axis. From these experiments, we are able to precisely determine the deformation

parameter that connects the energetic shift of the wire luminescence and the applied uniaxial stress.

HL 87.11 Fri 13:00 POT 51

On the T2 deep level in zinc oxide thin films — •Matthias Schmidt[1,2], Robert Karsthof[1], Florian Schmidt[1], Holger von Wenckstern[1], Martin Ellguth[1], Rainer Pickenhain[1], Marius Grundmann[1], and Gerhard Brauer[2] — [1]Universtity of Leipzig, Institute for Experimental Physics II, Linnéstraße 5, D-04103 Leipzig — [2]Forschungszentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Postfach 51 01 19, D-01314 Dresden

For the majority of deep levels studied in n-type conducting ZnO by means of capacitance spectroscopy only the activation energy and the high temperature limit of the electron capture cross-section are known since these quantities can be evaluated easily from the temperature dependence of the trap's thermal electron emission rate.

We focused on the T2 level present in ZnO thin films grown by pulsed laser deposition. In order to tune the T2 concentration in the samples, we employed different growth and annealing conditions as well as the implantation of oxygen and zinc ions, respectively. The physical properties of T2 were studied by different deep level transient spectroscopy and photo- capacitance experiments. These experiments revealed a strong dependence of the thermal activation energy, 185meV<E<280meV, on the concentration of T2 in the sample as well as on the electric field (Poole-Frenkel effect). T2 was found to be preferentially generated under zinc rich conditions as both, the implantation of zinc ions and thermal annealing at low oxygen partial pressures increase its concentration. From photo- capacitance transients the photo- ionisation cross- section spectrum was calculated.

HL 87.12 Fri 13:15 POT 51

Low temperature CVD-synthesis of nitrogen doped ZnO thin films — •Sebastian Eisermann, Stefan Lautenschlaeger, Michael N. Hofmann, Andreas Laufer, Melanie Pinnisch, Christian Reindl, Julian Benz, Peter J. Klar, and Bruno K. Meyer — I. Physikalisches Institut, Justus-Liebig-Universität Giessen, Heinrich-Buff-Ring 16, 35392 Giessen

We report on the growth of nitrogen doped ZnO thin films prepared at low temperatures by chemical vapour deposition. As substrates, polar and non-polar ZnO single crystals were used. The successful incorporation of nitrogen into the ZnO matrix was confirmed by Secondary Ion Mass Spectrometry (SIMS) and Raman measurements. The optical features were examined by photoluminescence (PL) analysis. Furthermore, ZnO diode structures were fabricated and investigated by IV-measurements. The PL spectra of the nitrogen doped films show a pronounced Donor-Acceptor-Pair-Recombination (DAP) in the energy-region of 3.25 eV. The intensity of this luminescence feature increases with increasing nitrogen content. The IV-measurements reveal typical diode-like behaviour of the ZnO diode structures.

HL 88: Lasers

Time: Friday 10:15–13:30 Location: POT 151

HL 88.1 Fri 10:15 POT 151

Effects of Many-Body Coulomb Effects on Injection-Locked Quantum Dot Lasers — •Benjamin Lingnau[1], Kathy Lüdge[1], Eckehard Schöll[1], and Weng W. Chow[2] — [1]Institut f. Theo. Physik, Sekr. EW 7-1, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Sandia National Laboratories, Albuquerque, New Mexico 87185-1086, USA

We simulate a single-mode quantum dot semiconductor laser device under the injection of an external optical signal into the laser cavity. For a certain range of parameters, the laser will be frequency-locked to the injected signal. In the past, many-body Coulomb effects were found to influence laser dynamics[1]. With our simulations, we now investigate how many-body Coulomb effects influence the locking behavior of the device, and the parameter range for which frequency locking occurs. The theory used in the simulations is based on a semiclassical approach, where the laser field and active medium are described by the Maxwell-semiconductor-Bloch equations. Many-body Coulomb effects are described within the screened Hartree-Fock approximation. Carrier-carrier and carrier-phonon collisions are treated within the effective relaxation rate approximation. Inhomogeneous broadenening of the quantum-dot distribution is taken into account.

[1] B. Lingnau, K. Lüdge, E. Schöll, and W. W. Chow, "Many-body and nonequilibrium effects on relaxation oscillations in a quantum-dot microcavity laser", Appl. Phys. Lett. 97, 111102 (2010)

HL 88.2 Fri 10:30 POT 151

Optical Gain, Thermal Resistance and Antiguiding Factor of GaN-based Laser Diodes from UV to Green — •Wolfgang Scheibenzuber[1], Ulrich Schwarz[1], Teresa Lermer[2], Stephan Lutgen[2], and Uwe Strauss[2] — [1]Fraunhofer IAF, Tullastrasse 72, D-79108 Freiburg, Germany — [2]Osram Opto Semiconductors GmbH, Leibnizstrasse 4, D-93055 Regensburg, Germany

For highly efficient GaN-based laser diodes emitting from UV to green, suitable for projection applications or ultra short pulse generation, a detailed knowledge of the internal device properties optical gain, internal losses, thermal resistance and antiguiding factor is required. We measure these properties on state-of-the-art laser diodes emitting from UV to green. Optical gain and internal losses are determined from the modulation depth of the longitudinal modes in the electroluminescence spectrum below threshold using the Hakki-Paoli method. The measurements show an increase of the spectral width of the gain spectra towards longer laser wavelength, which is related to the larger inhomogeneous broadening and band-filling in InGaN quantum wells with high indium content. The thermal resistance of the devices is determined from the shift of the longitudinal modes above threshold. From the wavelength-shift of the longitudinal modes with increasing current at a constant device temperature we extract the charge carrier induced refractive index change and calculate the antiguiding factor of the laser diodes. All three examined samples have an antiguiding factor of 4 +- 0.5.

HL 88.3 Fri 10:45 POT 151

Implementing 330 nm UV-output by frequency doubling of a miniaturized red AlGaInP-VECSEL emitting at 660 nm — •Hermann Kahle, Thomas Schwarzbäck, Marcus Eichfelder, Wolfgang-Michael Schulz, Robert Rossbach, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen, Universität Stuttgart, Allmandring 3, 70569 Stuttgart, Germany

Vertical external cavity surface-emitting lasers (VECSELs) have emerged as an important category of power-scalable and frequency tunable semiconductor lasers. Using external cavities, optical pumping and intra-cavity optical elements, VECSELs provide the possibility of intra-cavity frequency doubling. We present a VECSEL-Chip design, based on a multi-quantum-well structure with 20 compressively-strained $GaInP$ quantum wells (QWs) grown by metal-organic vapour-phase epitaxy on $GaAs$ substrates for an operation wavelength of around 660 nm. Five QW packages are placed in $(Al_{0.55}Ga_{0.45})_{0.51}In_{0.49}P$ cladding layers, which are lattice matched to $GaAs$, in a resonant periodic gain design. Each package consists of four QWs embedded in $(Al_{0.33}Ga_{0.67})_{0.51}In_{0.49}P$ barriers. The 3 λ thick cavity is fabricated on an $Al_{0.50}Ga_{0.50}As/AlAs$ distributed Bragg reflector. By inserting a BBO-crystal into the cavity, we present an UV-emitting laser. Frequency-tuning using a birefringent filter will be presented. To improve pump photon absorption in the active region of the VECSEL-Chip, a design with 20 QWs, grouped in pairs, is also possible.

HL 88.4 Fri 11:00 POT 151

Thermal properties of high power vertical-external-cavity surface-emitting lasers — •Alexej Chernikov[1], Jens Herrmann[1], Maik Scheller[1], Martin Koch[1], Bernadette Kunert[1], Wolfgang Stolz[1], Sangam Chatterjee[1], Stephan W. Koch[1], Tsuei-Lian Wang[2], Yushi Kaneda[2], Joe M. Yarborough[2], Jörg Hader[2], and Jerome V. Moloney[2] — [1]Faculty of Physics and Material Sciences Center, Philipps-Universität Marburg, Renthof 5, D-35032 Marburg, Germany — [2]College of Optical Sciences, The University of Arizona, 1630East University Boulevard, Tucson, AZ 85721, USA

Vertical-external-cavity surface-emitting lasers (VECSELs), developed in the late 90s, have received much attention in the scientific community due to the unique combination of high output power and excellent beam quality. VECSELs provide light across a broad spectral range, efficient intra-cavity frequency mixing as well as the possibility for pulsed operation. The majority of the applications rely on the high output power of the device. Since overheating generally limits the laser performance, efficient cooling concepts as well as careful choice of the pump profile are crucial. Here, we focus on the thermal properties of a high-power VECSEL. Spatially resolved temperature measurements are performed under simultaneous monitoring of the output characteristics of the device. Our results illustrate the substantial importance of three-dimensional heat transfer in the structure, limiting the VECSEL performance for large spot sizes. Finally, the heat-removal concept is optimized for a maximum output power above 70 W.

HL 88.5 Fri 11:15 POT 151

Red-emitting, highly polarized vertical-cavity surface-emitting lasers as lighting module for active microoptics — •Susanne Weidenfeld[1], Michael Wiesner[1], Marcus Eichfelder[1], Frederik Schaal[2], Christof Pruss[2], Wolfgang Osten[2], Robert Rossbach[1], Michael Jetter[1], and Peter Michler[1] — [1]Institut für Halbleiteroptik und Funktionelle Grenzflächen, Universität Stuttgart, Allmandring 3, 70569 Stuttgart, Germany — [2]Institut für Technische Optik, Universität Stuttgart, Pfaffenwaldring 9, 70569 Stuttgart, Germany

AlGaInP-based vertical-cavity surface-emitting lasers (VCSELs) are attractive candidates for optical data transmission via polymer optical fibers (POF) meeting the POF's attenuation minimum at around 650 nm. For different applications the fundamental mode is desirable as well as a stable linear polarization. This is especially essential for the implementation of the VCSEL as a lighting module in a device that spatially resolved controls the polarization of incident light. With the monolithic integration of an oxide aperture, the transverse beam profile can be defined. The vertical structure of these lasers and thus the on-wafer processing offers also the opportunity to implement beam shaping optics monolithically in the surface. We present detailed analysis of the transverse beam profile and polarization characteristics of VCSELs. We demonstrate that oxide aperture sizes smaller than 6 μm are required for emission in fundamental mode and that the devices are highly linearly polarized. We further show first steps towards integrating beam shaping optics into the top mirror of the VCSEL.

HL 88.6 Fri 11:30 POT 151

Laser Diode Self-Mixing Velocimetry of Solid and Liquid Targets — •Thomas Gläßer[1], Wolfgang Elsässer[1], and James O'Gorman[2] — [1]Institut für Angewandte Physik, Technische Universität Darmstadt, Schloßgartenstraße 7, 64289 Darmstadt — [2]previously with Eblana Photonics, Dublin (Ireland)

The laser diode self-mixing (or optical feedback) interferometry technique is a contactless measurement technique based on a very simple configuration. The setup consists only of a laser diode (LD), the focusing optics and the target to be probed. The laser beam is scattered by the target and partly back reflected into the laser cavity. This leads to a interferometric carrier and power modulation of the LD containing information about the velocity of the target. For signal detection a monitor photodiode included in the LD package could be used.

Compared to the widely established laser doppler velocimetry (LDV), which is based on Mach Zehnder or Michelson interferometers, the self-mixing approach provides advantages in its setup size and wight and allows much easier adjustment at very low cost.

We present velocity measurements on different flowing liquids using near infrared discrete mode LDs at 1300 nm and 1550 nm.

15 min. break

HL 88.7 Fri 12:00 POT 151

Single-mode Quantum Cascade Lasers Employing a Candy-cane Shaped Fabry-Perot Cavity — Peter Q. Liu[1], •Kamil Sladek[1,2], Xiaojun Wang[3], Jen-Yu Fan[3], and Claire F. Gmachl[1] — [1]Department of Electrical Engineering, Princeton University, Princeton, NJ 08544 USA — [2]Institute of Bio- and Nanosystems (IBN-1), Jülich Aachen Research Alliance (JARA), Forschungszentrum Jülich, 52425 Jülich, Germany — [3]AdTech Optics, 18007 Cortney Court, City of Industry, CA 91748 USA

Quantum Cascade (QC) lasers are versatile mid-infrared light sources for spectroscopic molecular sensing. Most of the applications require single-mode operation of the QC lasers, which is usually achieved by either integrating distributed feedback gratings into the laser cavity or making use of an external cavity. However, both approaches require more complicated fabrication and/or coating processes. Previously we demonstrated single-mode QC lasers employing a folded FP cavity which is essentially a monolithic coupled-cavity fully compatible with simple (no Bragg gratings) ridge waveguide laser fabrication. Those lasers have single-mode performance, high throughput and relatively lower cost. Here we present an even simpler monolithic coupled-cavity design, a candy-cane shaped FP cavity, to achieve single-facet, single-mode QC lasers. It demonstrates a straightforward path to achieving single mode operation of QC lasers. Single-mode emission from QC lasers up to ~500 mA (~70%) above the threshold current is achieved in pulsed mode operation at 80 K with a SMSR of ~25dB. Mode-hop free temperature tuning of the emission wavelength is also demonstrated.

HL 88.8 Fri 12:15 POT 151

Three-section DBR lasers based on surface defined gratings for high speed telecommunication applications — •S. Afzal[1], F. Schnabel[1], W. Scholz[1], J. P. Reithmaier[1], A. Capua[2], E. Shumakher[2], G. Eisenstein[2], O. Parillaud[3], M. Krakowski[3], I. Montrosset[4], and M. Vallone[4] — [1]INA, University of Kassel. — [2]Technion, Israel. — [3]Alcatel-III-V Lab, France. — [4]Politecnico di Torino, Italy.

To combine low-cost fabrication and high-speed data communication like 100 GBit/s, multi-section DBR lasers are developed with nanoimprint compatible surface defined gratings. This laser design has the potential to enhance the modulation bandwidth by exciting a higher order optical mode, the so-called photon-photon resonance (PPR). ICP-RIE etching was used to transfer the e-beam exposed surface pattern in one step into the semiconductor. High aspect ratios of $>$ 1:15, vertical trenches with a width of about 140 nm and an etch depth of $>$ 2 um were obtained for the lateral gratings. The three-section lasers are fabricated on a MOVPE grown 1.5 um InP laser material exhibiting CW threshold currents of 94 mA for a 0.9 mm long device. A side mode suppression ratio of $>$ 50 dB could be achieved demonstrating a high enough coupling strength of the lateral gratings. The influence of different operation conditions (currents, temperature) and dependence on the grating period on threshold current and emission wavelength are studied and will be discussed. First high frequency measurements in operation conditions without PPR enhancement show a -3dB bandwidth of about 15 GHz.

HL 88.9 Fri 12:30 POT 151

2.3 μm GaSb-based semiconductor disk laser with sub-MHz linewidth — •Sebastian Kaspar, Benno Rösener, Marcel Rattunde, Tino Töpper, Christian Manz, Klaus Köhler, and Joachim Wagner — Fraunhofer-Institut für Angewandte Festkörperphysik, Tullastrasse 72, D-79108 Freiburg, Germany

Semiconductor disk lasers, also known as vertical-external-cavity surface-emitting lasers (VECSELs) can be regarded as a hybrid of classical semiconductor lasers and solid state lasers, offering an almost free choice of wavelength, high output power and diffraction-limited circular beam. VECSELs emitting in the $2-3\,\mu$m wavelength range are of special interest for a variety of applications such as materials processing and laser surgery. Other applications like spectroscopy and optical data transmission require narrow linewidth laser sources.

We report on the realization of narrow-linewidth GaSb-based VECSELs emitting in the $2.0-2.3\,\mu$m range. Single frequency emission is realized by inserting a quartz plate as birefringent filter into the external resonator for wavelength control and by optimizing the cavity for TEM_{00} mode operation. By using a high-finesse Fabry-Pérot interferometer (FPI), stable single frequency operation was verified with an output power above 200 mW. Coarse wavelength tuning of up to 118 nm is achieved by rotating the quartz plate. Modehop-free fine-tuning of the laser wavelength of over 5 GHz was possible by mounting the output coupling mirror to a piezoelectric transducer. By stabilizing the emission wavelength to the edge of a FPI transmission maximum, a linewidth of less than 400 kHz was achieved.

HL 88.10 Fri 12:45 POT 151

2.0 μm GaSb-based semiconductor disk lasers optically pumped at different wavelengths — •Tino Töpper, Benno Rösener, Marcel Rattunde, Sebastian Kasper, Christian Manz, Klaus Köhler, and Joachim Wagner — Fraunhofer IAF, Tullastrasse 72, D-79108 Freiburg, Germany

Semiconductor disk lasers, also known as vertical-external-cavity surface-emitting laser (VECSEL), combine the wavelength versatility and efficiency of diode lasers with the capability of a high output power emitted in a nearly diffraction-limited circular beam inherent to solid-state lasers. VECSEL in the wavelength range of 2-3μm are of interest for a broad range of applications including material processing, medical therapy and trace gas sensing.

We will report on the direct comparison of two GaSb-based VECSEL structures, both with an emission wavelength of 2.0μm but with different active region designs, optimized for barrier-pumping at 1.0μm (AlGaAsSb-barriers) and 1.5μm (GaSb-barriers). Both structures were characterized in pulsed mode in order to reduce thermal heating effects. At room temperature, the power efficiency of the 1.5μm-pumped structure is 1.43-times higher than the 1.0μm-pumped structure, reflecting directly the reduced quantum deficit due to the longer pump-wavelength. Temperature dependant measurements revealed that the decrease in power efficiency and increase in threshold pump power with increasing temperature is more pronounced for the 1.5μm-pumped structure. We attribute this effect to the reduced barrier height of the latter structure and thus increased heterobarrier leakage.

HL 88.11 Fri 13:00 POT 151

Investigation of heat dissipation in Mid-Infrared quantum cascade lasers — •Stefanie Mayer, Christian Schilling, Ralf Ostendorf, Quankui Yang, Rainer Lösch, Wolfgang Bronner, and Joachim Wagner — Fraunhofer Institut für Angewandte Festkörperphysik IAF, Freiburg, Deutschland

The output power and efficiency of quantum cascade lasers (QCL) is severely limited by self-heating effects of the device during operation. Therefore, a fundamental knowledge of the heat dissipation is essential for further device optimization.

We present modelling of heat transfer processes in GaInAs/AlInAs/InP-based QCLs by finite elements analysis. The influence of different mounting techniques and of different heat spreaders on the temperature of the active region has been studied. The results indicate a significant reduction of the temperature (by about 40-50 %) inside the device by using diamond heat-spreaders and epi-down mounting due to improved heat dissipation. In addition we extended our analysis to QCL arrays and investigated thermal crosstalk between adjacent emitters of the array.

These results are confirmed by electro-optical measurements performed on QCL emitting at a wavelength of 4.7 μm. Here, an enhancement of 148.47 % in optical peak output power was observed in pulsed operation mode with 10 % duty cycle by using diamond heat-spreaders and epi-down mounting.

HL 88.12 Fri 13:15 POT 151

Spin induced polarization oscillations in vertical-cavity surface-emitting laser devices — •Mingyuan Li[1], Henning Soldat[1], Hendrik Jähme[1], Nils C. Gerhardt[1], Martin R. Hofmann[1], and Thorsten Ackemann[2] — [1]Chair of Photonics and Terahertz-Technology, Ruhr University of Bochum, Germany — [2]SUPA and Department of Physics, University of Strathclyde, Glasgow, Scotland, UK

The capabilities of spin controlled vertical-cavity surface-emitting lasers (VCSELs) such as high-speed modulation and amplification of spin information due to the nonlinearity at threshold offer a promising method of communication with enhanced bandwidth. We investigate the polarization dynamics of electrically pumped vertical-cavity surface-emitting lasers after additional spin injection at room temperature. The experimental results demonstrate a stable polarization oscillations with a frequency in the high GHz range, which is determined by device parameters such as linear birefringence and linear dichroism. A theoretical calculation on the basis of a rate equation model is performed, in order to understand the underlying mechanism for coupling between the dynamics and device parameters. The calculation reveals a possibility to control the frequency of the oscillations by tuning the birefringence.

HL 89: Optical Properties II

Time: Friday 10:15–13:30 Location: POT 251

HL 89.1 Fri 10:15 POT 251

Electric-field-induced second harmonic generation in GaAs — •Marco Lafrentz[1], David Brunne[1], Benjamin Kaminski[1], Dmitri R. Yakovlev[1,2], Victor V. Pavlov[2], Roman V. Pisarev[2], and Manfred Bayer[1] — [1]Experimentelle Physik 2, Technische Universitaet Dortmund, D-44221 Dortmund, Germany — [2]Ioffe Physico-Technical Institute, Russian Academy of Sciences, 194021 St. Petersburg, Russia

We report on electric-field-induced second-harmonic generation (SHG) in the GaAs semiconductor in the vicinity of the band gap. The light has been send along 001-crystallographic direction. In this geometry SHG is forbidden in electric-dipole approximation. In applied electric field the SHG signal arises due to field-induced symmetry breaking causing new optical nonlinearities. Electric-field and temperature investigations assign the strong signal at $E(2\omega) = 1.517$ eV for $T = 2$ K to excitonic resonance. This phenomenon is a supplementary tool for detailed investigation of complex suscebtibilities we have reported on in the past [1,2].

[1] V. V. Pavlov, A. M. Kalashnikova, R. V. Pisarev, I. Sänger, D. R. Yakovlev, and M. Bayer, Phys. Rev. Lett. **94**, 157404 (2005)

[2] I. Sänger, D. R. Yakovlev, B. Kaminski, R. V. Pisarev, V. V. Pavlov, and M. Bayer, Phys. Rev. B **74**, 165208 (2006)

HL 89.2 Fri 10:30 POT 251

Optical third-harmonic spectroscopy of the magnetic semiconductor EuTe — •David Brunne[1], Marco Lafrentz[1], Benjamin Kaminski[1], Victor Pavlov[2], Andre Henriques[3], Roman Pisarev[2], Dmitri Yakovlev[1], and Manfred Bayer[1] — [1]TU Dortmund — [2]A. F. Ioffe physical-technical Institute — [3]Instituto de Fisica, Universidade de Sao Paulo

EuTe possesses the centrosymmetric crystal structure m3m of rock-salt type in which the second harmonic generation (SHG) is forbidden in electric-dipole approximation, but the third harmonic generation (THG) is allowed. We studied the THG spectra of this material and observed several resonances in the vicinity of the band gap at $2.2 - 2.5$eV and at higher energies up to 4eV, which are related to four photon THG processes. The observed resonances are assigned to specfic combinations of electronic transitions between the ground $4f^7$ state at the top of valence band and excited $4f^6 5d^1$ states of Eu^{2+} ions, which form the lowest energy conduction band. Temperature, magnetic field and rotational anisotropy studies allowed us to distinguish crystallographic and magnetic field induced contributions to the THG. A strong modification of the THG intensity was observed in applied magnetic fields at particular resonances due to interference of crystallographic and magnetic field induced contributions. A microscopic quantum mechanical model of the THG response was developed and its conclusions are in good agreement with the experimental results.

HL 89.3 Fri 10:45 POT 251

A simulated reflectivity experiment: theoretical optical spectrum of strained-lattice bulk SrTiO3 — •Lorenzo Sponza[1,2], Valérie Véniard[1,2], Adriano Verna[3], and Stefano Nannarone[3,4] — [1]LSI - Ecole Polytechnique, 91128 Palaiseau, France — [2]European Theoretical Spectroscopy Facility (ETSF) — [3]IOM-CNR lab. TASC Area Science Park, Basovizza, Italy — [4]Università di Modena e Reggio Emilia, Italy

Reflectivity and absorption measurements are powerful techniques to investigate microscopic properties of matter as structural configuration. An interpretation of measured data can be given through the macroscopic dielectric constant, even if such an interpretation is complicated.

Here we present a theoretical study carried on the optical properties of bulk SrTiO3 (STO) with two different lattice structures: one is the cubic structure (a=3.905 Angstrom) and one is a strained configuration. We present the computation of the macroscopic dielectric tensor of STO performed in the framework of Time Dependent Density Functional Theory (TDDFT) and Many Body Perturbation Theory (MBPT) in the G0W0 approximation and solving Bethe-Salpeter equation. Comparison with experimental data has been also carried out.

Using a C++ code written ad hoc to compute the reflectivity of

anisotropic materials, we will display the difference in signal due to the structural strain and we will link it to the difference between the two theoretical dielectric tensors.

HL 89.4 Fri 11:00 POT 251

Air-Gap Heterostructures — •Jochen Kerbst, Matthias Schmidt, Stephan Schwaiger, Andrea Stemmann, Stefan Mendach, Wolfgang Hansen, and Christian Heyn — Institut für Angewandte Physik, Jungiusstr 11, 20355 Hamburg

We demonstrate the fabrication of a novel type of heterostructure providing epitaxial semiconductor layers which are separated by thin air gaps. The air gaps with thickness ranging from 4 to 8 nm are stabilized by low-density nanopillars. The nanopillars are generated by a combination of self-assembled droplet etching (LDE) [1,2] during molecular beam epitaxy (MBE) and post-growth selective etching. In particular, first a thin AlAs layer is grown on a GaAs substrate. Afterwards, local etching with Ga droplets forms nanoholes deeper than the thickness of the AlAs layer. The nanoholes are filled with GaAs and finally overgrown with a 50 or 100 nm thick GaAs film. After removal of the samples from the MBE system, wet chemical selective etching of only the AlAs layers yields the formation of the air-gab heterostructures. The thickness of the air gaps is precisely controlled by the thickness of the initial AlAs layers. Reflectivity measurements confirm the existence of the air gaps and the gap thickness.

[1] Zh. M. Wang, B. L. Liang, K. A. Sablon, and G. J. Salamo, Appl. Phys. Lett. 90, 113120 (2007).

[2] Ch. Heyn, A. Stemmann, and W. Hansen, Appl. Phys. Lett. 95, 173110 (2009)

HL 89.5 Fri 11:15 POT 251

Refractive Index matching of $BaTiO_3/SrTiO_3$ Heterostructures — •Tammo Böntgen, Jan Zippel, Rüdiger Schmidt-Grund, Michael Lorenz, and Marius Grundmann — Universtät Leipzig, Institut für Experimentelle Physik II, Linnéstr. 5

By altering the growth parameters for $BaTiO_3/SrTiO_3$ heterostructures we achieved matching of the refractive index for selected wavelengths. Using spectroscopic ellipsometry we have determined the optical properties of these heterostructures and their constituting layers. By systematically varying the growth parameters, the refractive index of the STO layer was tuned such that it crosses the refractive index of BTO. The index matching leads to a vanishing reflectivity at the crossing wavelength. The crossing wavelength varies with the choice of the growth parameters. X-Ray diffraction measurements were carried out on the heterostructures to probe the effect of the growth conditions on the STO lattice parameters. A dependence of the lattice constant on the growth parameters was found, linking the change in the optical properties to the lattice deformation. This kind of index matching can in principal also be achieved for other perovskite $ATiO_3$ hetero- or multilayer structures. This work was supported by Deutsche Forschungsgemeinschaft in the framework of Sonderforschungsbereich 762 "Functionality of Oxidic Interfaces".

HL 89.6 Fri 11:30 POT 251

Effect of localized boron impurities on the line shape of the fundamental band gap transition in photomodulated reflectance spectra of (B,Ga,In)As — •Thomas Sander[1], Jörg Teubert[1], Peter J. Klar[1], Andrew Lindsay[2], and Eoin P. O'Reilly[2,3] — [1]Institute of Experimental Physics I, Justus-Liebig-University Giessen, Germany — [2]Tyndall National Institute, Lee Maltings, Cork, Ireland — [3]Department of Physics, University College Cork, Ireland

Photomodulated reflectance (PR) spectra of (B,Ga,In)As epilayers reveal unusual changes of the fundamental band gap PR line shape with temperature and hydrostatic pressure. We show that these changes arise because temperature variation or hydrostatic pressure shifts the conduction band edge (CBE) into resonance with boron-related cluster states. The resulting line shape changes are described by a level repulsion model which yields states of mixed character with an exchange of oscillator strengths. This model is corroborated by theoretical calculations which show a finite density of boron cluster states above the CBE at room temperature, with appropriate symmetry to couple to the CBE states.

15 min. break

HL 89.7 Fri 12:00 POT 251

Surface acoustic wave induced electron tunneling from an InGaAs/GaAs wetting layer — •Jens Pustiowski[1], Florian J.R. Schülein[1], Dirk Reuter[2], Andreas D. Wieck[2], Max Bichler[3], Kai Müller[3], John J. Finley[3], Achim Wixforth[1], and Hubert J. Krenner[1] — [1]Lehrstuhl für Experimentalphysik I, Universität Augsburg, 86159 Augsburg, Germany — [2]Lehrstuhl für Angewandte Festkörperphysik, 44780 Bochum, Germany — [3]Walter-Schottky-Institut, 85748 Garching, Germany

We report on a stroboscopic technique to probe the dynamic modulation controlled by a surface acoustic wave (SAW) of the photoluminescence (PL) of a wetting layer which is formed during the growth of InGaAs/GaAs quantum dots. A short laser pulse ($\tau < 100$ps) is actively phase locked to the frequency of the SAW and the relative phase between laser excitation and SAW can be precisely controlled [1]. Thus, we are able to map one complete cycle of the SAW and study the PL quenching and its modulation in the time domain. For low SAW powers the observed modulation with the fundamental period of the SAW arises from different mobilities of electrons and holes. This imbalance leads to different ionization efficiencies in the type-II band gap modulation induced by the SAW. At high SAW power levels, the modulation period doubles which can be readily explained by SAW induced tunneling induced by the vertical piezoelectric field component.

[1] S. Völk et al., arxiv:1011.1898 (2010).

HL 89.8 Fri 12:15 POT 251

Optical orientation of Mn^{2+} ions in GaAs — •Lukas Langer[1], Ilya A. Akimov[1,2], Roslan I. Dzhioev[2], Vladimir L. Korenev[2], Yuri G. Kusrayev[2], Victor F. Sapega[2], Dmitri R. Yakovlev[1,2], and Manfred Bayer[1] — [1]Experimentelle Physik 2, Technische Universität Dortmund, 44221 Dortmund, Germany — [2]A.F. Ioffe Physical-Technical Institute, Russian Academy of Sciences, 194021 St. Petersburg, Russia

We report on optical orientation of Mn^{2+} ions in bulk GaAs under application of weak longitudinal magnetic fields ($B \leq 150$ mT). The studied samples were grown by liquid phase epitaxy and Czochralski method and were doped with a low Mn acceptor concentration of $8 \times 10^{18}\,\mathrm{cm}^{-3}$. Time resolved measurements of circular polarization for donor-acceptor photoluminescence in Faraday geometry reveal nontrivial spin dynamics of donor localized electrons. Initially the degree of polarization of the electron spins is 40%. It then decays within some tens of ns to reach a plateau. The plateau is absent at $B = 0$ T and saturates at $B = 150$ mT reaching the value of 35%. It's sign changes with the helicity of incident light. It follows that the s-d exchange interaction with optically oriented electrons induces a steady state nonequilibrium polarization of the Mn^{2+} ions. The latter maintain their spin and return part of the polarization back to the electron spin system, resulting in the plateau. This provides a long-lived electron spin memory in GaAs doped with Mn. The dynamical polarization of ionized Mn acceptors was also directly monitored using spin flip Raman scattering spectroscopy, in agreement with time-resolved data.

HL 89.9 Fri 12:30 POT 251

Nanoscale Optical Imaging of Semiconductor Nanowires — •Miriam Böhmler[1], Anton Myalitsin[2], Alf Mews[2], and Achim Hartschuh[1] — [1]Department Chemie & CeNS, Ludwig-Maximilians-Universität München — [2]Department Chemie, Universität Hamburg

Inorganic semiconducting nanowires (NWs) feature size-related optical properties which make them interesting for a wide range of applications, e.g. nanoscale optoelectronics, sensors, and photovoltaics. Their relevant length scales that are determined by nanowire diameter and exciton Bohr radius, however, can not be resolved by conventional diffraction limited methods.

We illustrate the prospects of tip-enhanced near-field optical microscopy (TENOM) [1] as a method to investigate single nanowires. In TENOM a sharp metallic tip acts as optical antenna thereby enhancing the detected signal and increasing the optical resolution to about 15 nm. We present our investigations of CdSe NWs which have been grown by the wet chemical solution liquid solid technique [2]. Here, TENOM provides the possibility to simultaneously image photoluminescence (PL) as well as Raman scattering of individual NWs with nanoscale resolution. We observe spatial variations of the PL intensity and energy on a length scale of about 15 nm indicating crystal phase transitions and diameter fluctuations.

[1] A. Hartschuh, "Tip-enhanced near-field optical microscopy", Angew. Chemie (Int. Edition) 47, 8178 (2008). [2] Z. Li, et.al., "Controlled Synthesis of CdSe Nanowires by Solution-Liquid-Solid

Method", Adv. Funct. Mater. 19, 3650-3661 (2009).

HL 89.10 Fri 12:45 POT 251

Excitonic Absorption Spectra with Energetic Disorder — •Dirk Heinze, Jens Förstner, Matthias Reichelt, and Torsten Meier — Department of Physics and CeOPP, University of Paderborn, Warburger Str. 100, 33098 Paderborn

Using a time-domain real-space tight-binding approach[1], we calculate linear absorption spectra for a semiconductor quantum wire model system in the presence of energetic disorder. To model the energetic disorder a Gaussian distribution of random numbers is taken to represent a spatial disorder potential. The influence of the strength and spatial correlation of the energetic disorder is analysed. Extending previous studies, e. g. [2], a smooth spectrum is achieved by self-averaging over a sufficiently large system.

[1]T. Meier, P. Thomas, and S. W. Koch. Coherent Semiconductor Optics - From Basic Concepts to Nanostructure Applications. Springer, 2007

[2]I. Kuznetsova et al., Modeling excitonic line shapes in weakly disordered semiconductor nano-structures.. Phys. Rev. B 81, 075307 (2010)

HL 89.11 Fri 13:00 POT 251

Exciton dynamics in potential traps and the possibility of Bose-Einstein condensation — •Rico Schwartz[1], Nobuko Naka[2,3], Jan Brandt[4], Christian Sandfort[4], and Heinrich Stolz[1] — [1]Institut für Physik, Universität Rostock, D-18051 Rostock, Germany — [2]Department of Physics, Kyoto University, Kyoto 606-8502, Japan — [3]PRESTO, JST, 4-1-8 Honcho Kawaguchi, Saitama 332-0012, Japan — [4]Fakultät Physik, Technische Universität Dortmund, D-44221 Dortmund, Germany

Experiments on excitons in Cu_2O confined in a stress-induced potential trap [1] at subkelvin temperatures are reported. The paraexcitons were created by resonant excitation of orthoexcitons followed by ortho-para conversion. We excited with a pulsed laser (linewidth 1 GHz, repetition rate 1 kHz, pulse length 50 ns). With a gated CCD time dependent spatially resolved luminescence spectra were observed. A fit of the data with a simple rate equation model leads to bimolecular decay rates of the para- and orthoexcitons which are at least 5 orders of magnitude lower than those from literature [2]. Concomitant, we reached exciton numbers in the order of 10^9 in the trap. The effective temperature of the excitons was determined by fitting the high energy flank in the spectra with a Bose distribution. This temperature decreases after the excitation pulse to the bath temperature (0.15 K), which is well below the critical temperature of BEC at these exciton numbers. We also discuss whether the shape of the spectra points to an excitonic BEC.

[1] N. Naka and N. Nagasawa, Phys. Rev. B 65, 075209 (2002)

[2] K. Yoshioka et al., Phys. Rev. B 82, 041201(R) (2010)

HL 89.12 Fri 13:15 POT 251

Zero-magnetic-field spin-splitting and the warping in the valence band of highly p-doped asymmetric AlGaAs/GaAs Quantum Wells — •Michael Hirmer, M. Hirmer, D. Schuh, W. Wegscheider, T. Korn, and C. Schüller — Institut für Experimentelle Physik, Universität Regensburg, 93040 Regensburg

Zero-Magnetic-Field-Spin-Splitting (ZMFSS) in 2D quantum wells (QW) induced by the structure inversion asymmetry, and its control, are of major importance for both fundamental research and spintronic applications. In hole systems, the asymmetry leads to a ZMFSS of the heavy hole (HH) states in third order of the in-plane wave vector $k_{||}$ [1]. In our experiments, we focus on highly p-doped asymmetric AlGaAs/GaAs QW. We utilize electronic intersubband Raman measurements in backscattering geometry. In all samples we observe a low-energy spin-density excitation (SDE) with energies in the range of 0-3 meV. Samples with higher hole density show a two-component SDE. Comparing these excitation energies to 8 band k·p calculations [2] of the valence subbands , the SDE can be interpreted as an intersubband excitation of the spin-split HH ground state, reflecting directly the ZMFSS. The two components can be attributed to different HH dispersions in different crystallographic directions, the so-called warping. We found that the observed spin splitting increases systematically with increasing hole density p, or by an external electric field. Measurements of the Shubnikov de Haas oscillations showed similar results.

[1] R. Winkler, Phys. Rev. B 62, 073309 (2000).

[2] Nextnano^3 by Stefan Birner

HL 90: Intersectional Joint Session: Nano Plasmonic

Time: Friday 10:30–13:00 Location: BAR 205

Invited Talk HL 90.1 Fri 10:30 BAR 205

Plasmon Driven Higher Harmonics Generation — In-Yong Park, Seungchul Kim, Joon-Hee Choi, and •Seung-Woo Kim — Ultrafast optics for ultraprecision research group, KAIST, Daejeon, Republic of Korea

Plasmonic resonance enables field enhancement of a low-intensity fs pulse, permitting high harmonic generation without an additional amplifier. This new concept of generating ultrafast higher harmonic pulse was previously demonstrated using Au bow-tie antennas. The resulting intensity enhancement factor reached ~20 dB and successfully produced up to the 21st harmonic. Notwithstanding the high enhancement factor, the 2-dimensional configuration of the bow-tie nanostructure was found sensitive to thermal damages preventing practical usage. To cope with the problem, a 3-dimensional solid nanostructure is newly proposed and tested in this investigation. The newly designed nanostructure takes the shape of an ellipsoidal tapered waveguide fabricated in a cantilever micro-structure. The tapered waveguide functions as a plasmonic device that induces field enhancement by exploiting surface-plasmon polaritons being created as a femtosecond pulse propagates through. In comparison to bow-tie nano-antennas, the use of surface plasmon polaritons offers a much larger volume of enhanced laser field due to counter-propagating surface plasmon modes within the waveguide in response to the incident femtosecond pulse. The intensity of incident NIR pulses is enhanced by a factor of ~350, being strong enough to produce EUV harmonics up to the 43rd order directly from a modest input intensity of 1012 Wcm-2 in interaction with Xe gas.

Invited Talk HL 90.2 Fri 11:00 BAR 205

Structure and Dynamics of Free Nanoparticles: From Charging to Time-Resolved Photoemission — •Eckart Rühl — Physikalische Chemie, Freie Universität Berlin, Takustr. 3, 14195 Berlin

Nanoscopic systems prepared from nanoparticles as unique building blocks have the advantage that their properties depend critically on the single nanoscopic units and their assembly on substrates. Single nanoparticles show often size and composition dependent optical, electronic, structural, and dynamical properties. This includes quantum size effects, which are efficiently modified by the internal structure of the nanoparticles and their surroundings. Recent progress in chemical syntheses of structured nanoparticles as well as properties of single nanoparticles is presented. This includes controlled preparation of dimers or small aggregates of nanoparticles. Single, free nanoparticles without any contact to other particles or substrates are either prepared in traps or focused nanoparticle beams. These approaches allow us to study the intrinsic size- and composition dependent properties of isolated nanoscopic matter and their photon-induced dynamics. Results from a variety of different experimental approaches making use of synchrotron radiation and ultra-short laser pulses are presented. These provide specific information on the electronic structure, plasmonic excitations, the location of the emitted electrons in nanoparticles, the dynamics of electron emission and cation formation, as well as the dynamics of collective electronic excitations in the femtosecond time domain.

Invited Talk HL 90.3 Fri 11:30 BAR 205

Terahertz Nano Plasmonics — •Dai-Sik Kim — Center for Subwavelength Optics, Department of Physics and Astronomy, Seoul National University, Seoul, Korea

In this talk, we will focus on how terahertz electromagnetic waves, with wavelengths in the millimeter scale, can funnel through nano slits and nano slot antennas. The field enhancement is enormous, three orders of

magnitudes, which can be used for nonlinear processes and ultrasensitive probing of underlying structures. Optics in extreme subwavelength regime resembles electro-statics involving capacitors, in contrast to the electromangetic waves in free space.

Invited Talk HL 90.4 Fri 12:00 BAR 205

Coulomb complexes: Electron emission from clusters in strong FEL pulses — •Ulf Saalmann — MPI for the Physics of Complex Systems

The response of atomic clusters to short intense pulses at extreme-ultraviolet (XUV) and Xray wavelengths — as available from short-wavelength free-electron laser (FEL) sources like FLASH in Hamburg/Germany, the SCSS in Japan or LCLS in Stanford/California — is studied theoretically. Due to the high photon flux the clusters become multiply charged by massive electron emission. We device a model, which we call Coulomb complexes [1], in order to investigate the emission process. It turns out that the electron spectra strongly depend on the ionization rate. For low rates the electron release occurs sequentially and our model allows for an analytical description of the plateau-like electron spectra [1]. At high rates a dense nanoplasma is formed and ionization occurs through energy-exchanging collisions resulting in exponential electron spectra [2]. Both mechanisms can be understand in terms of our model containing only very few parameters available from experiments.

[1] Gnodtke, Saalmann, Rost, New J. Phys. in press (2011).
[2] Bostedt et al., New J. Phys. 12, 083004 (2010).

Invited Talk HL 90.5 Fri 12:30 BAR 205

Appearance of Surface and Volume Plasmons in Fullerenes — •Sanja Korica[1], Axel Reinköster[1], Markus Braune[1], Jens Viefhaus[1], Daniel Rolles[1], G. Fronzoni[2], D. Toffoli[2], M. Stener[2], P. Decleva[2], O. Al-Dossary[3], Burkhard Langer[4], and Uwe Becker[1,3] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Universitá di Trieste, Italy — [3]King Saud University, Riyadh, Saudi-Arabia — [4]Freie Universität Berlin

Since the discovery of the C_{60} molecule in 1985 many studies have been performed to investigate its fundamental properties. These properties are mainly driven by its unique molecular structure like its spherical shell. One of the important characteristics of this molecule is the collective response of its valence electron cloud to electromagnetic radiation. This collective behavior gives rise to the occurrence of the giant dipole resonance a surface plasmon in the absorption spectrum centered around 20 eV, which has been analyzed theoretically by various authors. In addition, our photoionization cross-section measurements reveal a resonance near 40 eV, a volume plasmon analogous to observations made for C_{60} ions. Time-dependent density functional calculations confirm the collective nature of this feature as corresponding plasmon excitation. A third excitation of this kind is predicted but not experimentally confirmed. Concerning photoelectron emission, plasmonic excitations are characterized by a particular intensity behavior near threshold. They follow the threshold behavior law predicted for the first time by Thomas Derrah. Our measurements of the C_{60} plasmon excitations above the C 1s ionization threshold confirm this law very well and are in unexpectedly good agreement with the corresponding behavior of K-shell satellite excitations in atoms such as neon.

HL 91: Joint Focussed Session: Theory and Computation of Electronic Structure: New Frontiers VIII

Time: Friday 11:15–12:45 Location: TRE Phy

Topical Talk HL 91.1 Fri 11:15 TRE Phy

Tunable bandgaps and excitons in doped semiconducting carbon nanotubes made possible by acoustic plasmons — •Catalin Spataru and Francois Leonard — Sandia National Laboratories, Livermore, California, USA

Doping of semiconductors is essential in modern electronic and photonic devices. While doping is well understood in bulk semiconductors, the advent of carbon nanotubes and nanowires for nanoelectronic and nanophotonic applications raises some key questions about the role and impact of doping at low dimensionality. Here we show that for semiconducting carbon nanotubes, bandgaps and exciton binding energies can be dramatically reduced upon experimentally relevant doping, and can be tuned gradually over a broad range of energies in contrast to higher dimensional systems. The later feature, made possible by a novel mechanism involving acoustic plasmons, establishes new paradigms for the understanding and design of nanoelectronic and nanophotonic devices.

HL 91.2 Fri 11:45 TRE Phy

Electronic Excitations in Single-Wall Carbon Nanotubes: Building-Block Approach — •Ralf Hambach[1,2], Christine Giorgetti[1,2], Xochitl Lopez-Lozano[3], and Lucia Reining[1,2] — [1]LSI, Ecole Polytechnique, CNRS, CEA/DSM, Palaiseau, France — [2]European Theoretical Spectroscopy Facility — [3]University of Texas at San Antonio, United States

Parameter-free calculations of electron energy-loss spectra for low-dimensional systems like single-wall carbon nanotubes can become numerically very demanding or even unfeasible for large diameters.

We overcome this problem by means of a building-block approach: Combining effective-medium theory and ab-initio calculations we can describe the collective excitations in nanostructures (like carbon nanotubes) starting from the microscopic polarisability of their building blocks (bulk graphite). To this end, Maxwell's equations are solved using the full frequency- and momentum-dependent microscopic dielectric function $\epsilon(\mathbf{q}, \mathbf{q}', \omega)$ of the bulk material. The latter is calculated from first principles within the random phase approximation [1].

Besides an important gain in calculation time this method allows us to analyse the loss spectra of nanostructures in terms of their normal-mode excitations. We apply the building-block approach to study angular-resolved loss spectra for graphene and single-wall carbon nanotubes and find a very good agreement with full ab-initio calculations of these systems and corresponding experiments.

[1] AbInit: www.abinit.org, DP-code: www.dp-code.org

HL 91.3 Fri 12:00 TRE Phy

Functionalized Tips Leading to Atomic-Resolution Force Microscopy — •Nikolaj Moll, Leo Gross, Fabian Mohn, Alessandro Curioni, and Gerhard Meyer — IBM Research – Zürich, Säumerstrasse 4, CH-8803 Rüschlikon, Switzerland

Performing atomic force microscopy (AFM) with a molecule or an atom at the tip the resolution can be dramatically enhanced as the resolution crucially depends on the chemical nature of the tip termination. A pentacene molecule is imaged with atomic resolution with a tip functionalized with a CO molecule. The interactions between the CO tip and the pentacene are studied with first principles calculations. The different energy contributions are analyzed, and the Pauli energy is computed. The source of the high resolution is Pauli repulsion, whereas van-der-Waals and electrostatic interactions only add a diffuse attractive background. To validate the usefulness of AFM with functionalized tips the natural product cephalandole A is studied.The measurements together with first principle calculations demonstrate that the direct imaging of an organic compound with AFM facilitates the accurate determination of its chemical structure. The method might be developed further towards molecular imaging with chemical sensitivity, and could solve certain classes of natural product structures.

[1] Leo Gross, Fabian Mohn, Nikolaj Moll, Peter Liljeroth, and Gerhard Meyer, Science 325, 1110-1114 (2009).

[2] Leo Gross, Fabian Mohn, Nikolaj Moll, Gerhard Meyer, Rainer Ebel, Wael M. Abdel-Mageed, and Marcel Jaspars, Nat. Chem. 2, 821-825 (2010).

HL 91.4 Fri 12:15 TRE Phy

Impact ionization rates from ab initio calculations — •Marton Voros[1], Dario Rocca[2], Gergely Zimanyi[3], Giulia Galli[2,3], and Adam Gali[1,4] — [1]Budapest University of Technology and Economics, Department of Atomic Physics — [2]UC Davis, Department of Chemistry — [3]UC Davis, Department of Physics — [4]Hungarian Academy of Sciences, Research Institute of Solid State Physics and Optics

Achieving multi exciton generation (MEG) in semiconducting nanocrystals may lead to overcome the well-known Shockley-Queisser

limit when building semiconductor-based solar cells. A thourough, theoretical understanding of the experiments that reported MEG in e.g. Si and PbSe nanocrystals, is still missing and could significantly contribute to clarify the several controversial results in the field. Several theoretical and numerical studies have addressed the origin of the MEG formation, mostly supporting an impact ionization mechanism. However, impact ionization rates have only been evaluated for model nanocrystals by using empirical pseudopotentials fitted to bulk properties or by applying tight binding wavefunctions, and model dielectric functions to describe the screened Coulomb interaction. We present a full ab-initio scheme based on Density Functional Theory in a plane-wave pseudopotential implementation that includes static screening within the random-phase approximation. As a first application, we will discuss how impact ionization rates are affected by the size of small Si nanocrystals.

HL 91.5 Fri 12:30 TRE Phy

Selective Excitation of Molecular Vibrations by Tunneling Electrons — •Jessica Walkenhorst[1], Marius Wanko[1], Alberto Castro[2], and Angel Rubio[1] — [1]Nano-Bio Spectroscopy group and ETSF Scientific Development Centre, Dpto. Física de Materiales, Universidad del País Vasco, Centro de Física de Materiales CSIC-UPV/EHU-MPC and DIPC, San Sebastián, Spain — [2]Institute for Biocomputation and Physics of Complex Systems (BIFI), University of Zaragoza, Spain

Tunneling electrons can be used to excite vibrations in molecules. By combining scanning electron microscopy (STM) with inelastic electron tunneling spectroscopy (IETS) one can obtain vibrational spectra of single molecules adsorbed on a surface. Interestingly in large molecules the vibrational spectrum depends on the impact point of the electrons on the molecular surface. Selective excitation of vibrational modes by the STM tip has been proposed to explain these experimental findings (the so-called 'excitation of local vibrations' model). Therefore, we want to simulate the dynamical response of Schiff base (CNH4+) to tunneling electrons. To this end, we perform molecular dynamics simulations based on time-dependent density functional theory (TDDFT). Vibrational spectra are then obtained by Fourier analysis of the velocity autocorrelation function. This way, we study the relative strength of the excited molecular vibrations in dependence on the impact point of the tunneling electrons. Finally, a comparison between numerical results and experimental findings is attempted and the validity of the 'excitation of local vibrations' model is discussed.