Semiconductor Physics Division
Fachverband Halbleiterphysik (HL)

Overview

[Contact and location details for Jürgen Christen and Erich Runge]

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)
Organization: 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)
Organization: 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 Manthei, Wadim Quiring, Mohammad 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 — Shibeghsa Tanaka, Jun-Ichi Kasai, Sumiko Furisaki, Ryuichi Akimoto, Takeshi Kikawa, Shinji Tsuji, Haruhiiko 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 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
Semiconductor Physics Division (HL) Overview

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 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 Foucussed Session: Thin Film Chalcogenide Photovoltaics I
HL 9.1–9.4 Mon 11:15–13:00 WIL A317 Joint Foucussed Session: Transparent Conductive Oxides 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 14.1–14.11 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 Foucussed Session: Thin Film Chalcogenide Photovoltaics II
HL 24.1–24.6 Mon 16:00–17:30 GER 37 Joint Foucussed Session: Thin Film Chalcogenide Photovoltaics III
HL 25.1–25.9 Mon 15:45–18:15 POT 151 Interfaces and Surfaces
HL 26.1–26.7 Mon 16:00–17:45 POT 06 Invited Talk: Martin Wagner
HL 27.1–27.1 Mon 17:00–17:30 POT 51 THz Physics
HL 28.1–28.5 Mon 17:30–18:45 POT 51 Organic Photovoltaics II: mainly Phthalocyanine
HL 29.1–29.4 Mon 17:45–18:45 POT 151 Nano Wires: Growth and Characterization
HL 30.1–30.6 Tue 10:15–11:45 FOE Anorg III-V-Compounds: Nitrides
HL 32.1–32.6 Tue 10:15–13:00 POT 151 Spin-dependent Transport I
HL 33.1–33.12 Tue 10:15–13:30 POT 251 Interfaces and Surfaces
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 Foucussed Session: Transparent Conductive Oxides II
HL 38.1–38.5 Tue 12:00–13:15 FOE Anorg Polaritons and Polariton Lasing
HL 40.1–40.5 Tue 14:00–15:15 ZEU 222 Photovoltaics: Chalcopyrites I
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 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)
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<td>HL 52.1–52.6</td>
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<td>POT 51</td>
<td>Nonpolar and Semipolar Nitrides</td>
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<td>HL 53.1–53.4</td>
<td>Wed</td>
<td>12:30–13:30</td>
<td>POT 251</td>
<td>Optical Properties I</td>
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<td>HL 54.1–54.10</td>
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<td>14:00–17:00</td>
<td>ZEU 222</td>
<td>Joint Session: Organic Semiconductors IV: Excitations and Charges</td>
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<td>HL 56.1–56.1</td>
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<td>HL 57.1–57.4</td>
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<td>POT 151</td>
<td>ZnO: Optical Properties</td>
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<td>HL 58.1–58.1</td>
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<td>HL 59.1–59.5</td>
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<td>SKM Symposium: Semiconductor Nanophotonics - Quantum Optics and Devices (SYNP)</td>
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<tr>
<td>HL 60.1–60.5</td>
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<td>15:00–16:15</td>
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<td>Quantum Dots: Transport</td>
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<td>HL 61.1–61.7</td>
<td>Wed</td>
<td>15:00–17:00</td>
<td>TRE Phy</td>
<td>Joint Focussed Session: Theory and Computation of Electronic Structure: New Frontiers IV</td>
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<tr>
<td>HL 62.1–62.6</td>
<td>Wed</td>
<td>15:15–16:45</td>
<td>POT 51</td>
<td>Nitrides: Advanced Characterization Techniques</td>
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<tr>
<td>HL 63.1–63.10</td>
<td>Wed</td>
<td>15:45–18:30</td>
<td>POT 151</td>
<td>II-VI-Compounds</td>
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<td>HL 64.1–64.11</td>
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<td>16:30–19:30</td>
<td>POT 251</td>
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<td>HL 65.1–65.4</td>
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<td>17:00–18:00</td>
<td>POT 51</td>
<td>Nitrides: AlGaN</td>
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<td>HL 66.1–66.8</td>
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<td>17:15–19:15</td>
<td>GER 38</td>
<td>Joint Session: Plasmonics and Nanophotonics</td>
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<td>HL 67.1–67.6</td>
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<td>FOE Anorg</td>
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<td>HL 68.1–68.12</td>
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<td>10:15–13:30</td>
<td>FOE Anorg</td>
<td>Photovoltaics: Chalcopyrites II</td>
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<td>HL 69.1–69.5</td>
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<td>10:15–11:30</td>
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<td>Nitrides: LEDs</td>
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<td>HL 70.1–70.13</td>
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<td>HL 71.1–71.11</td>
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<tr>
<td>HL 72.1–72.6</td>
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<td>HL 73.1–73.4</td>
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<td>12:00–13:00</td>
<td>GER 38</td>
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<td>HL 74.1–74.9</td>
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<td>10:30–13:00</td>
<td>HSZ 02</td>
<td>Joint Session: Quantum Optics of Solid State Photon Sources</td>
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<td>HL 75.1–75.6</td>
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<td>TRE Phy</td>
<td>Joint Focussed Session: Theory and Computation of Electronic Structure: New Frontiers V</td>
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<td>HL 76.1–76.6</td>
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<td>POT 51</td>
<td>Nitride-based Green Lasers</td>
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<td>HL 77.1–77.8</td>
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<td>14:00–16:00</td>
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<tr>
<td>HL 78.1–78.6</td>
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<td>16:15–17:45</td>
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<td>HL 79.1–79.10</td>
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<td>14:30–17:15</td>
<td>FOE Anorg</td>
<td>Photovoltaics: Mainly Silicon</td>
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<td>HL 80.1–80.5</td>
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<td>14:30–17:15</td>
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<td>Focussed Session: Novel Green Laser Diodes</td>
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<td>HL 81.1–81.10</td>
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<td>Graphene: Transport</td>
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<td>HL 82.1–82.10</td>
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<td>Ultrafast Phenomena</td>
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<td>HL 83.1–83.6</td>
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<td>TRE Phy</td>
<td>Joint Focussed Session: Theory and Computation of Electronic Structure: New Frontiers VI</td>
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<td>HL 85.1–85.130</td>
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<td>Poster Session II</td>
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<td>HL 86.1–86.11</td>
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<td>FOE Anorg</td>
<td>Quantum Dots: Growth and Characterization</td>
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<td>HL 87.1–87.12</td>
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<td>ZnO: Growth and Defects</td>
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<td>HL 88.1–88.12</td>
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<td>HL 89.1–89.12</td>
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<td>HL 90.1–90.5</td>
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<td>BAR 205</td>
<td>Intersectional Joint Session: Nano Plasmonic</td>
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**Annual General Meeting of the Semiconductor Physics Division**

**Thursday 17:15–18:00 POT 051**

- Bericht
- Wahl
- Verschiedenes
Invited Talk

HL 1.1 Mon 10:15 FOE Anorg
Self-organized quantum dots as single and entangled photon emitters — Erik Stock
Waldemar Unrat, Anatol Lochmann, Andrei Schliwa, Murat Oztürk, Achsath Bakarov, Aleksandr Toporov, Ilja Derer1, Vladimir Haisler, and Dieter Bimberg
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 several quantum dot (QD) superlattice. 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 RLED 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. Micro-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.


15 min. break

HL 2: Electronic Structure Theory

HL 2.1 Mon 10:15 POT 51
Quasiparticle band offsets at heterojunctions from GW superlattices 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 a hierarchy of absolute GW corrections. For this, relative GW corrections are proposed an alternative route which circumvents the transferability issue.


15 min. break

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 (DFT). 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 — Bohn 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 calculations.

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 10^6 - 10^10 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 Düsseldorf

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 geometry.
Semiconductor Physics Division (HL)

Monday

HL 2.6 Mon 11:30 POT 51
Holographic view on nanostructure wave functions
- Gabriel Bester1, Jie Peng1, Wen Lei1, Christian Nothapho2, Axel Lowiek2, Dirk Reuter3, and Andreas Wieck3 — Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, 70569 Stuttgart, Germany — 2Department of Physics and CeNIDE, University of Duisburg-Essen, Bismarckstr. 81, D-47057 Duisburg, Germany — 3Elektrotechnik and CeNIDE, Universität Duisburg-Essen, Lotharstraße 1, 47048 Duisburg, 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 Bz. The states of the so-called p-shell, which show distinct orientations along the crystal axes for Bz = 0, can be modified to become more axially 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.


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

Time: Monday 10:15-11:45

Location: POT 515

HL 3.1 Mon 10:15 POT 151
Dynamic nuclear polarization in n-GaAs - free versus local electrons
- Jie Huang1, Yuanfan Chen1, A. Ludwig2, D. Reuter2, A. D. Wieck2, and Gerd Bacher1 — 1Werkstoffe der Elektrotechnik und CeNIDE, Universität Duisburg-Essen, Bismarckstr. 81, D-47057 Duisburg, Germany — 2Department of Physics and CeNIDE, University of Duisburg-Essen, Lotharstraße 1, 47048 Duisburg, Germany

In this work we study charge carrier spin dynamics in doped GaAs/AlGaAs quantum wells.

HL 3.2 Mon 10:30 POT 151
Electron g-Factor Anisotropy in Symmetric (110)-oriented GaAs/AlGaAs Quantum Wells
- Jens Hübscher1, Huy Vinh Thanh Duc2, Sergei Kunz1, Stefan Oertel1, Michal Pochwala3, Dieter Schuh2, Thorsten Meier3, and Michael Ostreich1 — 1Institut für Theoretische Physik — Universität Regensburg, 93040 Regensburg, Germany — 2Department 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 Lande-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 D2h to C2v 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 well described within 14 x 14 band k·p theory and identify the intermixing of different 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 Oertel1, Jens Hübscher1, Dieter Schuh2, Werner Wegscheider2, and Michael Ostreich1 — 1Institut für Theoretische Physik — Universität Regensburg, 93040 Regensburg, Germany — 2Department of Physics, University of Paderborn, Warburger Str. 100, D-33098 Paderborn, Germany

In this contribution 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-
Controlling the charge state of nitrogen-vacancy centers in diamond — •Moritz Haup1, Bernhard Grotz2, Boris Naydenov2, Magali Ros1, Fedor Jelezko2, Jörg Wrachtrup2, Martin Stutzmann1, Jörg Wrachtrup2, Martin Stutzmann1, Friedemann Reinhard2, and José Garrido1 — 1Walter Schottky Institut, TU München, Garching, Germany — 2TH 4.5 Mon 11:15 POT 251

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

In bioelectronic hybrids, composed of photoactive 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.

VL 4: Carbon: Diamond, Nanotubes, and Graphene

Time: Monday 10:15–13:30

Location: POT 251

Two dimensional hole gases (2DHG) with high carrier mobilities are required for both fundamental research and possible future ultrafast spintronics. 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 cm²/Vs which are achieved after illumination. In contrast, the dsd-structure hosts a 2DHG with mobility up to 2.05 × 10^5 cm²/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 AlGaAs/As on carrier concentration and mobility were investigated and are presented here.
Dielectric photorefractive assembly of field-effect transistors using sorted semiconducting carbon nanotubes — **Juliane Posseckardt**¹, Yann Battie², Romain Flurier², and Michael Mertic³ — ¹TU Dresden, Professor für Physikalische Chemie, Mess- und Sensortechnik, 01062 Dresden, Germany — ²LEM 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 fractions 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

Time-resolved picosecond photocurrents in contacted carbon nanotubes — **Leonard Prechtl**¹, Li Song², Stephan Manus², Dieter Schuh³, Werner Wegscheider³, Nadine Erhard¹, and Alex W. Holleitner¹ — ¹Walter Schottky Institut and Physik-Department, TU München — ²Fakultät für Physik und die Center for NanoScience (CeNS), LMU, München — ³Institut für Experimentelle und Angewandte Physik, Universität Regensburg — 4Laboratorium für Festkörperforschung, ETH Zürich

We introduce coplanar stripe 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.

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

Raman spectroscopy is a powerful tool to study defects in sp² 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 allows for the characterization of carbon nanotubes via Raman spectroscopy [2].


Excited state spectroscopy on a bilayer graphene double quantum dot — **Christian Volk**¹,², Stefan Frings³, Bernat Terres³,⁴, Jan Dauber³, Stephan Engels³, Stefan Trellenkamp³, Uwe Wichmann¹, and Christoph Stamper-Kurn³ — ¹JARA-FIT and II. Institute of Physics B, RWTH Aachen, 52074 Aachen, Germany — ²Institute 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).

Disorder induced energy gaps in graphene nanoribbons — **Jan Dauber³, Bernat Terres³,⁴, Christian Volk²,², Stefan Trellenkamp³, Uwe Wichmann¹, and Christoph Stamper-Kurn³ — ¹JARA-FIT and II. Institute of Physics B, RWTH Aachen, 52074 Aachen, Germany — ²Institute for 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 PAVONE1,2, ROSTAM GOLESORKHITARI2, JÜRGEN SPITALER1,2, and CLAUDIA AMBROSCI-DRAUX1

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**

**HL 5.1 Mon 10:15 POT 06 Memristive switching in vanadium dioxide thin films** — DANilo BÜRGER, VARUN JOHN, GYÖRGY KOVÁCS, ILONA SKORUPA, MANNFRED HELM, and HEIDEMARIE SCHMIDT-CROGH, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

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 modulated 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 (001)-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 pinned 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.


**HL 5.2 Mon 10:30 POT 06 Disorder induced localization in crystalline phase-change materials** — PETER JOST1, THEO SIEGRIST1,2, HANNÖ VOLKEN1, MICHAEL WODA1, PHILIPP MEREKELBACH1, CARL SCHLOCKERMANN1, and MATTHIAS WÜTTI1 — 1) 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 Sb2Te3. The insulating state results from a degree of disorder which is unexpectedly 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.


**HL 5.3 Mon 10:45 POT 06 Electronic Transport Properties of Nb/InAs-Nanowire/Nb Josephson Junctions** — YUSUF GÜNEL1, IGOR E. BATOY2, HILDE HARTDIEGEN1, KAMIL SLADEK1, ANDREAS PENZ1, GREGOR PANATOV1, NETLEY GRÜTZMACHER1, and THOMAS SCHMIDT-CROGH1, Dresden-Rossendorf, Bautzner Landstraße 400, 01314 Dresden, Germany

Metal-oxide-semiconductor (MOS) devices on lithographically defined and etched graphene nanoribbons and structural arrangement as compared to amorphous SiO2. The radial distribution function (rdf) curve of porous SiCOH indicates a significant difference in density and structural arrangement as compared to amorphous SiO2 and low-k dielectrics. Careful investigation of electron energy-lumo spectroscopy (EELS) combined with TEM, provides information about the elemental composition, chemical bonding, band structure, dielectric functions, valence, and conduction electron densities. The rff curve of porous SiCOH indicates a significant difference in density and structural arrangement as compared to amorphous SiO2.

In this study, we report on a metal insulator transition (MIT) in the pseudo-binary alloys between GeTe and Sb2Te3. The insulating state results from a degree of disorder which is unexpectedly 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.


**HL 5.4 Mon 11:00 POT 06 low-k dielectric and amorphous SiO2 - a comparative TEM/EELS analysis** — PRADEEPSINGH1, SVEN ZIMMERMANN2, STEFFEN SCHULZ2, STEFAN SCHULZE2, and MICHAEL HIETSCHOLD1

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 network; 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
Quantitative Characterization of Dielectric and Electronic Properties on the Nanometer Scale — Matthias Fenner¹, Ferry Kienberger¹, Hassan Tanbakuchi¹, Hans-Peter Huber², and Markus Hochleitner²
Agilent Technologies Inc.,
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 atomically sharp tips.
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 cases) from 10^14 atoms/cm^3 to 10^20 atoms/cm^3. We present the methods for calibration as well as applications of SMM.

Si-InAs heterojunction Esaki tunnel diodes with high current densities — Cedric Bessire, Mikael Björk, Heinrich Fluckiger, Kirsten Moselund, Hesham Ghoneim, 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 of 0.3 eV between Si and InAs of 130 mV 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/cm^-2 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/cm^-2 at 0.5 V reverse bias.

Invited Talk — Uwe Rait and Thomas Kirchartz
IEK-5: Photovoltaics, Forschungszentrum Jülich, Germany
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 p-n junction solar cell. 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. The differences have immediate consequences on the limitations, the practical design and the technical realization of the various types of devices.

Invited Talk — Sodium-chloride axial nanowire heterostructures as Bio-FETs — Sebastian Pregl¹, Walter Weber², and Gianluca Coletti³
Max Bergmann Center of Biomaterials, Dresden University of Technology, 01062 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 synthesized 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.
involve experiments conducted under various conditions. We observe that the 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.


We have investigated ultralow-density InP quantum dots (QDs) in In0.48Ga0.52P. The QDs were grown using gas-source molecular-beam epitaxy (GSMBE) with ultralow growth rate. InP QDs emiting 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 an energy difference of $\Delta E \approx 2 \mu eV$. This splitting can be qualitatively compared to 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.**
Excitation pulse width dependence of triggered single-photon emission from InP/(Al,Ga)InP quantum dots — Christian Keßler1, Matthias Reischle2, Wolfgang-Michael Schulz1, Marcus Eichfelder1, Robert Roschach1, Michael Jetten1, Paul Gartner1, Matthias Florian2, Christopher Giers1, Frank Jahnke2, and Peter Michler1 — 1Institut für Halbleiteroptik und Funktionelle Grenzflächen, Universität Stuttgart, Allmandring 3, 70569 Stuttgart — 2Institut 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 single quantum dot (QD) devices 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 \( \Gamma \). 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)

Spectroscopy of electrically controlled intentionally positioned and shape engineered single InAs quantum dots — Minisha Mehta1, Dirk Reuter1, Andreas D. Wieck2, Stefan Michaelis de Vasconcellos1, Artur Zrenner1, and Cerdik Meier1 — 1Physics Department, Paderborn, Germany — 2Applied 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 quantum source by integrating 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 \( 2 \times 2 \) \( \mu m^2 \). 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 show similarity in terms of structure and their dependence on injection current is presented. Thus, these results slightly suggest a promising potential for quantum devices [1]. 1 M. Mehta et al., Appl. Phys. Lett. 97, 143101 (2010).

Topical Talk — HL 8.1 Mon 11:00 — 12:00

Topical Talk

HL 8.1 Mon 11:00 — 12:00

Cubic (In,Ga)Se2 solar cells: the importance of lateral variations of the absorber quality — Susanne Strehlitt1, University of Siegen, Germany — Dirk Reuter1, Andreas D. Wieck2, and Stefan Michaelis de Vasconcellos1, University of Paderborn, Germany — Cerdik Meier1 — 1Physics Department, Paderborn, Germany

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 \( \text{Cu(In,Ga)}\text{Se}_2 \) show the highest efficiencies in the lab as well as in industry. Record efficiencies above 20\% have been reached with these polycrystalline solar cells. Among these technologies solar cells based on \( \text{Cu(In,Ga)}\text{Se}_2 \) show the highest efficiencies in the lab as well as in industry. Record efficiencies above 20\% have been reached with these polycrystalline solar cells. Among these technologies solar cells based on \( \text{Cu(In,Ga)}\text{Se}_2 \) show the highest efficiencies in the lab as well as in industry. Record efficiencies above 20\% have been reached with these polycrystalline solar cells. Among these technologies solar cells based on \( \text{Cu(In,Ga)}\text{Se}_2 \) show the highest efficiencies in the lab as well as in industry. Record efficiencies above 20\% have been reached with these polycrystalline solar cells.

This talk will provide an overview over the general characteristics 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 cadmium and copper to form the kesterite compound \( \text{Cu}_2\text{ZnSnS}_4 \). 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 measurements gives 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 photovoltaics.

Topical Talk

HL 8.2 Mon 11:30 — 12:00

Efficient Photovoltaic Devices using Multinary Chalcogenide Semiconductors — Hans-Werner Schock and Thomas Unold — Helmholtz Zentrum Berlin für Materialien und Energie, Hahn-Meitner Plats, 1, 14190 Berlin, Germany

Multinary compounds like \( \text{Cu(In,Ga)}\text{Se}_2 \) or \( \text{Cu(In,Ga)}\text{S}_2 \) are very promising materials for thin film solar cells currently reaching photovoltaic efficiencies beyond 20\% for small device areas. The tolerance of chalcopyrite semiconductors regarding grain structure and defects allows to fabricate 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 cadmium and copper to form the kesterite compound \( \text{Cu}_2\text{ZnSnS}_4 \). 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 measurements gives 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 photovoltaics.
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**

**Title:** Electrical Characterization of Cu(In,Ga)(Se,S)₂-Based Solar Cells at Low Temperatures

**Authors:** Udo Rehblöhn, Friedrich-Schiller-Universität Jena, Physikalisch-Astromonische 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 bandgap 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**

**Title:** Surface and Bulk Properties of Post-Transition Metal Oxide Semiconductors

**Authors:** Philip D.C. King, Sepher Vasheghani Farahani, James B. Pendry

**Institute:** 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 as 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 semiconductor in the future form. Here, the surface and bulk electronic properties of epitaxially grown high-quality oxide semiconductors (In₂O₃, CdO, and SnO₂) will be discussed. Optical, electronic and structural properties of these semiconductor 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**

**Title:** Ab-initio calculation of electronic and optical properties of transparent conductive oxides

**Authors:** André Schieffer, Claudia Rödl, Frank Fuchs, Jürgen Fürnholzl, Benjamin Höfﬄing, Karsten Hannewald, Patrick Rink, Joel Varley, Anderson Janott, Chris G. Van de Walle, and Friedhelm Bechtoldt

**Institutes:** 1IPTO and ETSF, FSU Jena, Germany 2MPI-FKF, Berlin, Germany 3Materials 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: GaW₀ 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, SnO₂, In₃O₇, and Ga₂O₃. The origin of these phenomena will be discussed in terms of 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**

**Title:** Bulk semiconductor oxides: crystal growth and physical properties

**Authors:** Roberto Forneri, Leibniz Institute for Crystal Growth, IKZ, Max-Born-Str. 2, 12489 Berlin

**Institute:** Leibniz-Institut für Kristallzüchtung, Max-Born-Str. 2, 12489 Berlin, Germany

Semicontrolling 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 epixial 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 epitaxial layers 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 semiconductor Ga₂O₃ single crystals will be reviewed. Single crystals with diameter of 18 mm and 50-60 mm length were grown along the b-axis from an Irudid crucible under a dynamic protective atmosphere. The transmission in the visible 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 = 2-5×10¹⁴ 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, dilatation density studies, ICP-OMS, DTA, EPR and High Resolution TEM are also presented.

**Topical Talk**

**Title:** The electronic properties of β-Ga₂O₃

**Authors:** Mansour Mohamed, Christoph Janowitz, Isaak Unger, Zbigniew Galazka, Just R. Weiner, and Riccardo Manzer

**Institutes:** 1Humboldt-Universität zu Berlin, Institut für Festkörperphysik, Newtonstr. 15, 12489 Berlin, Germany 2Leibniz-Institut für Kristallzüchtung, Max-Born-Str. 2, 12489 Berlin, Germany 3Materials Department, University of California, Santa Barbara, California 93106-5050, USA

β-Ga₂O₃ belongs to the group of transparent conducting oxides (TCOs) with a wide band gap. It exhibits the largest band gap with E₉ = 4.9 eV [1] and thus a unique transparency from the visible into the UV region. The n-type high-quality β-Ga₂O₃ 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-Ga₂O₃ 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 functional exchange-correlation potentials 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 \(\beta\)-Ga2O3 is compared and discussed with the theoretical calculations. The effect of changing the temperature from 300K to 20K on the experimental band structure \(\beta\)-Ga2O3 was studied.

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

**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 functional theory calculations 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 new explored paths 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".


**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 Nanoflux 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 \(C_6\) [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**, Robert A. DiStasio Jr., Roberto Car, and Matthias Scheffler — Fritz-Haber-Institut der MPG, Berlin, Germany — 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.


**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**, Joachim Paier, Patrick Rinke, Andreas Grüneis, Georg Kresse, Gustavo E. Scuseria, and Matthias Scheffler — Fritz-Haber-Institut der MPG, Berlin — University of Vienna (Vienna) — 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 HTBH8/04 and NHTBH8/04 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, 1212 (2005).

**HL 10.5 Mon 12:30 TRE Phy**

**Au\(_X\) clusters (\(N=1\ldots6\)) supported on MgO(100) surfaces: the effect of exact exchange and dispersion interactions on adhesion energies**. — **Lauro Oliver Paz-Borbón**, Giovanni Barcaro, Alessandro Fortunelli, Sergey Levchik, and Matthias Scheffler — Fritz-Haber-Institut der Max Planck-Gesellschaft, Berlin. — 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\(_X\) clusters (\(N=2\ldots6\)) 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\(_X\) clusters.

One dimensional model systems in time-dependent density functional theory — •Nicole Helbig, Joanna I. Fucks, Ilya V. Tokatly, and Angel Rubio — 1ETSF Scientific Development Centre and Universidad del Pais Vasco, San Sebastian, Spain — 2IKERBASQUE, Basque Foundation for Science, Bilbao, Spain — 3Fritz-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

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 $S_{\text{corr}}(\omega, \omega') = \langle I(\omega)I(\omega') \rangle - \langle I(\omega) \rangle\langle I(\omega') \rangle$ up to 90 MHz, with $I(\omega)$ being the frequency dependent intensity of the time dependent signal [2]. $S_{\text{corr}}$ allows to distinguish between the homogenous and inhomogeneous broadening. We discuss a broad range of application for $S_{\text{corr}}$ including the detection of critical dynamics at second order phase transitions and the detection of coherent signals on a large background of noise.


Direction Dependence of Spin Relaxation in Confined 2D Systems — •Paul Wenc and Stefan Kettemann — 1School of Engineering and Science, Jacobs University Bremen, Bremen 28759 — 2Asia 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 directional 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, PRD81.125308), the relaxation due to cubic Dresselhaus spin orbit coupling is reduced and the linear part shifted with the number of transverse channels.

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.
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 12.1** Quantum Dots and Wires: Arsenides

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

Calculation of the Diameter dependent Polytypism in GaAs Nanowires — Volker Pankoke, Peter Kratzler, 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, supported 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.

Spatially resolved photocurrent spectroscopy on a single pn-doped GaAs nanowire — Daniel Sager, Christoph Gutseitz, Andrej Lysov, Matthias Offer, Ingo Regolin, Werner Prost, Franz-Josef Tegude, Axel Lorke, and Gerhard Bacher  
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 & Halbleitertechnologie, 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 photo-generated current, is measured as a function of the laser spot position. A photocurrent, which is proportional to the photo-generated current, is measured as a function of the laser spot position. A photocurrent, which is proportional to the photo-generated current, is measured as a function of the laser spot position. A photocurrent, which is proportional to the photo-generated current, is measured as a function of the laser spot position.

We demonstrate maximum photocurrent generation directly at the pn-junction, which is strongly increasing if the laser spot is placed outside the junction.


Dynamic and directional modulation of the optical emission of individual GaAs nanowires using surface acoustic waves — Jörg B. Kienzl, Daniel Rudolph, Gerhard Abstreiter, Jonathan J. Finley, Gregor Kohlmlüller, Achim Wixforth, and Hubert J. Krenner  
Würzburg University, 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 direction. 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 ≈ 50 – 100 nm is significantly smaller than 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.

1. Institute of Bio- and Nanosystems (IBN-1), Forschungszentrum Jülich, 52428 Jülich, Germany
2. GfE, Gemeinschaftsbau 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.

Strain-tuning of the excitonic fine structure splitting in semiconductor quantum dots — Johannes D. Plumbhof, Vlastimil Krapek, Fred Ding, Klaus D. Jöns, Robert Hafnerkrah, Petr Klenovský, Andreas Herklotz, Kathrin Dörk, Armando Rastelli, Peter Michler, and Oliver G. Schmidt  
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 compatible to the emission linewidth. We employ a piezoelectric actuator (PMN-PT) to manipulate the excitonic linewidth 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 nm. 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.

Fabrication and optical properties of GaAs quantum dots by filling of self-assembled nanoholes — David Sonnenberg, Andreas Graff, Christian Heyn, and Wolfgang Hansen  
Institut für Physik Universität Duisburg-Essen, Lotharstr. 1, 47048 Duisburg, Germany

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.

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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 demonstrated by photoluminescence (PL) linewidths of less than 10 meV. Micro-PL measurements of single QDs show sharp excitonic lines and linewidths comparable 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.


Semiconductor Physics Division (HL)

HL 13: Invited Talk: Bernd Kästner

Invited Talk

Semiconductor quantized current and voltage standard — •Bernd Kästner — 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 \( \hbar \). 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 \( V = f \ast (h/e) \) 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.


HL 14: Invited Talk: Karl W. Böer

Invited Talk

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-quantening 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 leakage. 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

Topical Talk

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 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].


Highly efficient vacuum processed BHJ solar cell based on merocyanines — •Vera Steinhäuser, Hannah Bürckstümmer, Nils M. Kronenberg, Martin R. Lenze, Dirk Hertel, Frank Wöhrnlein, and Klaus Meerholz — 1Institut für Organische Chemie und Röntgenstrukturanalyse der Universität Würzburg, Germany — 2Institut für Physikalische Chemie der 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 stack 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.

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**15 min. break**

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**Efficiency-Limiting Processes in Bulk Heterojunction Organic Solar Cells** — Ian Howard, Ralf Maurer, Fabian Etzel, Valentin Kam, 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, potential intermediates of free charge carrier generation, is debated. In this contribution we directly observe charge generation and recombination processes in state-of-the-art polymer:mehtanofullerene photovoltaic blends by transient absorption spectroscopy and compare polystyrene (PSHT) of varying regioregularity and low-bandgap polymers as electron donor materials. We observe a common feature of these blends is 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. Maurer, M. Meister, F. Laquai, J. Am. Chem. Soc. 2010, 132, 14866. [2] I.A. Howard, F. Laquai, Macromol. Chem. Phys. 2010, 211, 2063.

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**Biased-Dependent Transient Absorption on Organic Solar Cells: Connection to Device Performance?** — Ian Howard, Ralf Maurer, Valentin Kam, Michael Meister, and Frédéric Laquai — Max Planck Forschungsgruppe für Org. Optoelektronik, Max-Planck-Institut für Polymerforschung, Mainz, Deutschland


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**Characterization of trap states in small-molecule organic solar cells by using Impedance Spectroscopy.** — Lorenzo Bur-Tone, Debudatta 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 recombination 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 $1 \times 10^{17}$ cm$^{-3}$. Moreover we observe from the impedance analysis the presence of dopants in the intrinsic layer with an estimated effective concentration of about $8.4 \times 10^{15}$ cm$^{-3}$. This value is in agreement with very low doping concentration and suggests the formation of a non-arupt junction between intrinsic and doped layers.

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**The effect of energetic disorder on open-circuit voltage in organic photovoltaics** — James C Blakeley, 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. Blakeley and N. C. Greenham, J. Appl. Phys. 106, 034507 (2009).

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

Current-voltage curves allow to determine both fill-factor and efficiency of bulk transport layers, poly(3,4-ethylenedioxythiophene) : poly(styrene sulfonate) (PEDOT : PSS) and poly(aniline) : 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.
cy 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 non-linear 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.

We present investigations on the coherence of the emission from the first-order field-correlation function \(g(1,t)\) and \(\tau_2\) down to the thermal regime. We conclude that the influence of morphology and temperature on the charge carrier recombination and mobility on a microscopic scale can thus be investigated.
quantum dot coupled to two distinct micropillar cavity modes — <<STEFANIE WEILER1, ATA ULHAK1, SVEN MARCUS ULRICH2, STEPHAN RETTIESEN2, ANDREAS LÖFFLER3, ALFRED FORCHEL1, and PETER MÜHLER1 — 1Universität Stuttgart, Allmandring 3, 70569 Stuttgart 2Universität Würzburg, Am Hubland, 97074 Würzburg Quantum dots (QDs) are promising candidates for quantum information processing. Exciting them resonantly to as high energy as possible is important for 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 detuning for all detunings. When exciting the QD resonantly, we could demonstrate nonresonant coupling to the nearby mode and with increasing detuning for all detunings. When exciting the QD resonantly, we could demonstrate nonresonant coupling to the nearby mode and with increasing detuning for all detunings.

Whispering gallery mode lasing in electrically driven quantum dot micropillars — FEHRDINAND ALBERT, TRISTAN BURA, TOBIAS HEINDEL, CHRISTIAN SCHNEIDER, STEPHAN RETTIESEN, SVEN HÖFLING, LUKAS WÖRSCHE, 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 electrodynamic (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 (WGM) 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

Whispering gallery mode lasing in electrically driven quantum dot micropillars — FEHRDINAND ALBERT, TRISTAN BURA, TOBIAS HEINDEL, CHRISTIAN SCHNEIDER, SVEN HÖFLING, LUKAS WÖRSCHE, and ALFRED FORCHEL — Technische Physik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — Naval Research Laboratory, Washington, D.C. 20735, USA Devices for applying vertical electric fields to quantum dot layers (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 microcavities. 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 contacted the 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 1.6 meV. Moreover, first studies show a reduction of the exciton fine structure splitting, which is interesting for the generation of entangled photons.

Site-controlled quantum dots in an electrically driven single-micropillar cavity — SEBASTIAN MAIER, CHRISTIAN SCHNEIDER, ALEXANDER HUGGENBERGER, TOBIAS HEINDEL, STEPHAN HECKELMANN, STEPHAN RETTIESEN, SVEN HÖFLING, LUKAS WÖRSCHE, 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 allow for directed and highly efficient light emission. The bottom (top) distributed Bragg reflector (DBR) consists 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.

Optical properties of monolithic InGaN quantum dot pillar microwatt — KATHRIN SERBAUL, MORITZ SEVFRIEND, JOSHUA KALDEN, HEIKO DARTSCH, CHRISTIAN TESSAREK, STEPHAN FIGGE, CARSTEN KRUSE, DEITLF HOMMEL, and JÜRGEN GUTOWSKI — Institute of Solid State Physics, University of Bremen, Germany The realization of monolithic microwatt cavities (MCs) with InGaN quantum dot (QD) pillars is attracting considerable attention with respect to efficient light sources. For instance they allow for the realization of efficient monolithic MCs as well as the single-mode emission of pillar structured MCs. In this contribution, we present the successful implementation of InGaN QDs into fully epitaxial monolithic MCs showing discrete resonant 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 2.73 eV 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.

Experimental realization of high-Q AlAs/GaAs micropillar cavities with submicrometer diameters

Am Hubland, D-97074 Würzburg, Germany — Forchel — 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 Al2O3 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.


ZnO mesa-structures in planar microcavities — •Helena Hilmer, Christian Sturm, Steve Linke, Rödiger 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 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-light, 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-photon-polaritons. 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 £ = 10 K a superlinear dependence of the exciton-polariton occupation on the excitation density for an intermediate detuning regime (|£| ≤ 20 meV).


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 agreement compared with the strain dependent band structures. The present unknown band offset in non-polar cubic GaN/AlN superlattices has been derived from photoluminescence and infrared 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 the band offset from the GW approximation and 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.

HL 18.1 Mon 14:30 POT 151

**Huge Magnetoresistance in a High Mobility Two-Dimensional Electron Gas** — Lina Bockhorn1, Patrick Barthold4, Dietmar Schur2, Werner Wegscheider2, and Rolf J. Haug1 — 1Institut für Festkörperphysik, Leibniz Universität Hannover — 2Institut für Experimentalle und Angewandte Physik, Universität Regensburg — 3ETH 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 superlattice and a 2DEG, with a mobility of \( \mu = 1.19 \times 10^6 \text{cm}^2/\text{Vs} \) at a temperature of 1.5 K. The 2DEG have an electron density of \( n_e = 3.1 \times 10^{11} \text{cm}^{-2} \).

The experiment was performed using a magnetic field of 10 T and 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 30%. 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 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](http://arxiv.org/abs/1012.0168)

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HL 18.2 Mon 14:45 POT 151

**THz photoresponse of quantum Hall edge channels** — Christian Nottroff1,2, Kevin Rachor3, Detlef Heitmann3, Dirk Reuter4, Andreas Wieck4, and Axel Lorch2 — 1Technische Universität Chemnitz, Germany — 2Institute for Applied Physics, Leibniz Universität Hannover, Germany — 3Forschungszentrum Dresden-Rossendorf e.V., P.O. Box 510119, 01314 Dresden, Germany — 4Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany

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 and a Fourier spectrometer is used as a broad band, black-body source. In the presence of a THz laser, the photocurrent shows a clear peak at the THz frequency. In the absence of a laser, the photocurrent is negligible.

We find an exchange enhancement of the spin splitting at odd fillings. 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.


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HL 19.1 Mon 14:30 POT 251

**Phase Separation and Size Controlled Nanocrystal Formation in GeO** — Christoph Sahl1, Christian Sternewald2, Alexander Nyrov1, Alexander Schwamberger3, Florian Wieband1, Manuel Zschiesche2, Johannes Borany2, Achim Hohi3, and Metin Tolan1 — 1Fachbereich Physik, Universität Duisburg-Essen, Lotharstr.1, D-47048 Duisburg — 2Institut für Angewandte Physik, Universität Hamburg, Jungiusstr. 11, D-20355 Hamburg — 3Lehrstuhl für Festkörperforschung, Ruhr-Universität Bochum, Universitätsstraße 150, D-44780 Bochum

We investigate the formation of size controlled Ge NCs using a GeO metal-organic precursor. The precursors were synthesized using a GeO metal-organic precursor. The precursors were synthesized using a GeO metal-organic precursor. 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 30%. 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 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.

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, the phase separation of GeO\(_2\) (\( \gamma \approx 1\)) 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\(_2\)/SiO\(_2\) superlattice approach. The influence of reducing hydrogen in the annealing ambient on the phase separation process and resulting NC density is discussed.

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HL 19.2 Mon 14:45 POT 251

**Theory of the microwave induced zero resistance states in two-dimensional electron systems** — Sergey Mikhailov4 — 1Institute of Physics, University of Aarhus, D-86135 Aarhus, 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.


Structural modifications of low energy heavy ion irradiated Ge — Tobias Steinbach, Jan Wernerke, 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 sample sets were irradiated with different ion species and angles of incident angle. Angle resolved X-ray reflectivity 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 Schneggenschügle1, Alexander Chriennoz2, Cosma Schuster3, and Robin Grimes1 — 1PESE Division, KAUST, Dhahran 23955-6900, Kingdom of Saudi Arabia — 2Department of Materials, Imperial College London, London SW7 2BP, United Kingdom — 3Institut 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.


HL 19.7 Mon 16:00 POT 251
In-situ incorporation and distribution of boron dopants in silicon nanowires — Pratyush Das Kanungo1, Xin Ou2, Reinhard Koeniger1, Alexander Tonkikh1, Wolfgang Skorupa3, and Peter Werner1 — 1Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle, Germany — 2Forschungszentrum Dresden - Rossendorf, FWHM, 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 thin (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 microscope on doped semiconductor nanostructures with local, carrier-depleted space charge regions — Christine Baumgart1, Anne-Dorothea Müller2, Falk Müller3, Manfred Helmi1, and Heidemarie Schmidt1 — 1Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Institut für Ionenkristallphysik und Materialforschung, P.O. Box 510119, 01314 Dresden — 2Anfatec Instruments AG, Melanchthonstr. 28, 08606 Oelsnitz

We present optical investigations of two dimensional silicon photonic crystal defect nanocavities with high density (10^6 cm^-2) germanium islands acting as an internal light source. Power and time dependent micro photoluminescence (μ-PL) spectroscopy at a lattice temperature of 295K 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.
Failure analysis and optimization of semiconductor 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.


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 Hückmann, 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 at 800 °C and a subsequent high-stress deformation at 300 MPa at 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 gives 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 H2 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 H2 depends on the temperature.

HL 19.11 Mon 17:15 POT 251
Thermally stimulated current in solid phase crystallized poly-Si thin films — •Markus Moerer, Lars-Peter Scheller, and Norbert Nickel — Helmholtz-Zentrum Berlin für Materialien und Energie, Kekulèstr. 5, 12489 Berlin, Germany

Poly-crystalline 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 Gisipel1, Kay-Michael Günther1, Anna Lena Baumann2, Augustinias Rubys2, Stefan Kontermann2, and Wolfgang Schade1,2 — 1Clausthal University of Technology, EFZN, Energie-Campus, Am Stollten 19, 38640 Goslar — 2Fraunhofer Heinrich Hertz Institute, Energie-Campus, Am Stollten 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 0.1µm and a sulphur content of about 1 at. % which influences the mechanical adhesion and contact resistances. Deposition techniques like screening, 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 — •Augustinias Rubys1, Christian Lehmann2, Thomas Gisipel2, Anna Lena Baumann1, Stefan Kontermann2, and Wolfgang Schade1,2 — 1Fraunhofer Heinrich Hertz Institute, Energie-Campus, Am Stollten 19, 38640 Goslar — 2FU Berlin, Fachbereich für Experimentalphysik, Arnimallee 14, 14195 Berlin — 3Clausthal University of Technology, EFZN, Energie-Campus, Am Stollten 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 wavelength range 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 cone shaped 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 104 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

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 Gedefaw, Ingo Paulowicz, Arnim Schuchardt, Sebastian Wille, and Rainer Aderung — Functional Nanomaterials, Institute for Materials Science, Faculty of Engineering, Christian-Albrechts-University, Kaisersstrasse 2, 24143 Kiel, Germany

Recent studies on the growth of semiconductor and ceramic nanocrystals 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-
tures 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.

Self assembly of 1D-nanoparticles at interfaces using external fields — ANINDYA MAJUMDER1,2, OLIVER JOß2, JÖRG OPPS1,2, GIANUALELIO CUNIBERTI3, and ECKHARD BEYER1,2 — 1Institute of Surface and Manufacturing Technology, Dresden University of Technology, 01062 Dresden, Germany — 2Fraunhofer IWS, Winterbergstrasse 28, 01277 Dresden, Germany — 3Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, 01062 Dresden, Germany — 4Fraunhofer IFFZ, 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 recent technological applications, the self assembly of nanoparticle interfaces by manipulating the particle surface energy is an upcoming area with great potential for applied and fundamental research.

Properties of annealed RF-sputtered Cu2O thin films — DANIEL REPPII, ANDREAS LAUFER, ANGELIKA POLITY, DETLEF 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. Cu2O thin films were sputtered from a copper and a Cu2O 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 showed a decreased carrier concentration by a factor of 0.00 (25 - 1017 cm−3) to 2.5 · 1015 cm−3 while the mobility increases from 0.37 to 35 cm2/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 Cu2O. The results using the Cu2O-target will be discussed at the conference.

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 get lost at the metal-semiconductor interface. We investigate epitaxial growth as well as structural, magnetic, and electrical properties of Heusler/semiconductor hybrid systems. In particular, we focus on Ni2MnIn 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.

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.

**HL 22.4 Mon 16:00 TRE Ma**

Spin Seebeck effect in metals and insulators - **KON-ICHI UCHIDA and EHI 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 currents, a potential for driving nonequilibrium spin currents. The analysis of the complete mode spectrum using electron-beam spectroscopy is an ideal tool for the determination and imaging of the mode spectrum of complex plasmonic cavities, including the elusive dark modes.

**HL 22.5 Mon 16:45 HSZ 01**

Plasmonic nanocavities: New design concepts and determination of the complete mode spectrum using electron-beam spectroscopies — **STEPHAN 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 22.6 Mon 17:00 TRE Ma**

Heat conduction of low-dimensional quantum magnets — **CHRISTIAN HERR**, **NIKOLAI HLUKER**, **PATRICK RIBEIRO**, **BERND BÜCHNER**, **SURJEET SINGH**, **ROMUALD SAINT-MARTIN**, and **ALEXANDRE REVCOLEVSKY** — Leibniz-Institute for Solid State and Materials Research, IFW Dresden, Institute for Solid State Research, 01171 Dresden, Germany — Laboratoire de Physico-Chimie de L’Etat Solide, ICMP, UMR8182, Université Paris-Sud, 91405 Orsay, France

Some years ago, a new, magnetic mode of heat transport which occurs in low-dimensional quantum magnets has been discovered. It is comparable to that of metals. The magnetic heat conductivity $\kappa_{mag}$ of such quantum magnet materials can be exceptionally large (even at room temperature), dwarfs the phonon heat conduction and is intensely studied since then. The magnetic heat conductivity $\kappa_{mag}$ is a phenomenon enabling the conversion of heat currents into spin currents, a potential for driving nonequilibrium spin currents. The analysis of the complete mode spectrum using electron-beam spectroscopy is an ideal tool for the determination and imaging of the mode spectrum of complex plasmonic cavities, including the elusive dark modes.
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

**Topical Talk**

HL 23.1 Mon 14:45 GER 37

Dünnschicht-Chalcopyrit-Solarzellen: Überblick und Forschungsfelder — •MICHAEL POWALLA — Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg


Am ZSW wird eine Kleinzellinie 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.

**Thin film solar cells based on the ternary compound CuInSnS3** — •DOMINIK M. BERG, PHILLIP J. DALE, and SUSANNE SIEBENTRUTT

University of Luxembourg, Laboratory for Photovoltaics, 41 rue du Brill, L-4422 Belvaux, Luxembourg

Thin films of kesterite (Cu2ZnSnS4) 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 CuInSnS3 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 Vmax 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 CuInSnS3 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 CuInSnS3 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 CuInSnS3 based solar cell devices so far. Loss mechanisms and ways to increase efficiency will be discussed.

**Investigation of lattice defects and compositional gradients in Cu(In,Ga)Se2 thin films for solar cells** — •JEAN-DIEURICH1, DANIEL ABOU-RASS2, THORSTEN RISSOM2, THOMAS USOLI2, HANS-WERNER SCHICK2, and CHRISTIAN BOIT1 — 1Department of Semiconductor Devices, Berlin University of Technology, Einsteinufer 19, 10587 Berlin — 2Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14199 Berlin

Cu(In,Ga)Se2 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)Se2/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 imaging along the lengths of the Cu(In,Ga)Se2 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 µm). We assume that these dislocations compensate for lattice mismatch due to the change in composition in this area of the lattice.

**Time dependent capacitance voltage measurements on Cu(In,Ga)Se2 Solar Cells** — •THOMAS ADLER1, WOLFRAM WITTE2, DIMITRIOHS HARISKO2, and ANDREAS KLEIN1

1Darmstadt University of Technology, Institute of Materials Science, Petersenstrasse 32, D-64287 Darmstadt, Germany — 2Zentrum 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)Se2 (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.

**Characterisierung der elektrischen Eigenschaften von Korn- grenzen an polykristallinen Chalkopyriten** — •SEBASTIAN LINKE, THORSTEN RISSOM, DANIEL ABOU-RASS, MARTHA CH. LUXSTEINER and SASCHA SADEWASSER — Helmholtz-Zentrum für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin

Polykristalline CuInx1−xGa2Se3 (CIGSe) Absorberchichten bilde die Grundlage der Dünnschicht-Solarzellen mit dem momentan höchsten Wirkungsgrad. Eine Besonderheit ist, dass polykristalline CIGSe Solarzellen, im Gegensatz zu Dünnschichtzellen auf Siliziumbasis, höhere Wirkungsgrade für Dünnschichtsolarzellen von 20,3 % erreicht. Aktuelle Forschungsergebnisse wie z. B. die Erreichung des weltbesten Wirkungsgrades für Dünnschichtsolarzellen von 20,3 % mit einer CIGS/Cds-Diode werden präsentiert.

**Thin film solar cells based on the ternary compound CuInSnS3** — •DOMINIK M. BERG, PHILLIP J. DALE, and SUSANNE SIEBENTRUTT

University of Luxembourg, Laboratory for Photovoltaics, 41 rue du Brill, L-4422 Belvaux, Luxembourg

Thin films of kesterite (Cu2ZnSnS4) 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 CuInSnS3 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 Vmax 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 CuInSnS3 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 CuInSnS3 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 CuInSnS3 based solar cell devices so far. Loss mechanisms and ways to increase efficiency will be discussed.

**Investigation of lattice defects and compositional gradients in Cu(In,Ga)Se2 thin films for solar cells** — •JEAN-DIEURICH1, DANIEL ABOU-RASS2, THORSTEN RISSOM2, THOMAS USOLI2, HANS-WERNER SCHICK2, and CHRISTIAN BOIT1 — 1Department of Semiconductor Devices, Berlin University of Technology, Einsteinufer 19, 10587 Berlin — 2Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin

Cu(In,Ga)Se2 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)Se2/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 imaging along the lengths of the Cu(In,Ga)Se2 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 µm). We assume that these dislocations compensate for lattice mismatch due to the change in composition in this area of the lattice.
resists 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)Se₂ 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 ultra-short laser pulses — Matthias Domke, Gerhard Heise, and Heinz Huber — Hochschule München
Laser lift-off processes have been observed during structures 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 Rölling — Accurion GmbH, Stresmannstr. 30, 37079 Göttingen
The setup consists 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 images 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 25: Transport

Time: Monday 15:45–18:15

HL 25.1 Mon 15:45 POT 151
Transport properties of BiTe-SbTe superlattices — Bogdan Yavorsky², Nicki Hinsche¹, Peter Zahn², Martin Gradhand², Michael Zerner¹, and Ingrid Mehr¹² — ¹Institut für Festkörperphysik, Friedrich Schiller Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany; ²Institut für Materialwissenschaften, Technische Universität Dresden, 01062 Dresden, Germany

During the last decade Bi-Te-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 (Bi₂Te₃)_x(Sb₂Te₃)_1-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.
within the framework of density functional theory. The property
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 power-
factor at a given temperature can be enhanced slightly by strain for
p-doping, while no enhancement is obtained for n-doping.

References

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Georg Barzola-Quiquia, Andreas Ganczarczyk, 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 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 disadvantageous 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.

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Thermal Probing of Heat Generation in Biased Silicon Nanowires — •Fabian Menger1,2, Heike Riel1, Andreas Steummer2, and Bernd Gotsmann1 — IBM Research - Zurich, 8033 Rueschlikon, Switzerland — 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 heater 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, nanoscale 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.

Controlling the transport properties of InAs nanowires by Si doping — •Karl Weis1,3, Stephan Würthli1,3, Andreas Winden1,3, Kamil Sladek1,3, Thomas Weirich2,3, Thomas Schäpers1,3, Hilde Harthdegen1,3, Hans Lütj1,3, Nataliya Demsarina1,3, and Detlev Grützmacher1,3 — Institut für Bio- und Nanosysteme (IBN) 1, 2, 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 SiH4 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 SiO2 back gate, we get a clear positive correlation between doping level and conductivity/capacitance/mobility. This conduction/transport properties 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 4K, the I-V characteristics show indications of single electron tunneling.

Field dependent transport properties and conductance fluctuations of InSb nanowires — •Huifan Yao1, H. Yusuf Günel1, Christian Blömers1, Weis Karl1, Yennai Wang2, Zia Grace Lu3, Detlev Grützmacher1, and Thomas Schäpers1,3 — Institute of Bio- and Nanosystems (IBN) 1, and JARA-FIT Jülich-Aachen Research Alliance, Research Center Jülich GmbH, D-52425 Jülich, Germany — 2Department of Physics & Astronomy, University of Southern Californi-
Semiconductor Physics Division (HL)

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 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 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 Dumphich, and Frank-J. Meyer zu Heringsdorf

Address: Faculty of Physics and Center for NanoIntegration Duisburg-Essen (CeNIDE) University Duisburg-Essen, 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 crystalline orientations Ag(001) and Ag(111). While FIB structuring of Ag wires has promising prospects, there are some downsidess 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.


**HL 26.2 Mon 16:15 POT 06**

**Time Scaling of Silver Nano-Crystal Growth at the Interface of Silver Thick Film Electrodos on n-Type Silicon**

Stefan Kontermann, Alexander Rup, and Ralph Preu

Fraunhofer Institute for Solar Energy Systems, Heidenhofstr. 2, 79110 Freiburg, Germany

The interface of silver thick film contacts on n-type silicon features nanoscale silver crystals. They carry the current across such surfaces 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 sputtering process. 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 on Silicon Surfaces**

David Knix, Hafice 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 Froh Schmidt

Theoretische Physik, Universität Paderborn, 33095 Paderborn, Germany

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].

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-distance of about 0.5 eV between the two sites. Also, we investigate the possibility of a dissociation of the molecule on the LN surfaces.


HL 26.6 Mon 17:15 POT 06
Photoemission spectroscopy studies of SrTiO$_3$ and its interface to gold — Sush Wintz$^1$, Mandy Grobosch$^1$, Martin Knupfer$^1$, Juliane Sehit$^2$, Florian Hanzic$^2$, Hartmut Stöcker$^2$, and Dirk C. Meyer$^2$ — IWF Dresden, P.O. Box 127011, 01171 Dresden, Germany — 1Institut für Experimentelle Physik, TU Bergakademie Freiberg, Leipziger Str. 20, 09506 Freiberg, Germany

HL 27: Invited Talk: Martin Wagner

Invited Talk: Martin Wagner, Harald Schneider, Dominik Stehr, Stephan Winnerl, Aaron M. Andrews, Stephan Schartner, Gottfried Strasser, and Manfred Helm — 1Helmholtz-Zentrum Dresden-Rossendorf, P.O. 510119, 01314 Dresden — 2Micro Nanostructure Center, Flerzagasse 7, 1040 Vienna, Austria

HL 28: THz Physics

Density Dependence of the Excitonic 1s-2p Transition Energy in THz Spectroscopy — Benjamin Breddermann, Mackillo Kir, and Stephan W. Koch — Department of Physics and Materials Science 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 $n_{ex}$ 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 $n_{ex}$ 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.

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 photo-switches. We further detect a photo-thermoemitter 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 divergence, 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, these oscillations are only observed 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**

―Thun Uyen-Khanh Dang, Sebastian Eisen, Andreas Kron, Martin Richter, Wilhelm Kühn, Matthias Nowack, and Martin Jakob—1Institut für Theoretische Physik, Technische Universität Berlin, Germany. 2European Space Research Institute, Frascati, Italy. 3Department of Chemistry, University of California Irvine, USA. 4Max 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-photon interaction [2], its influence on the two-dimensional intersubband absorption spectrum is investigated. Experimentally observed signatures are reproduced in the theoretical simulations.


**HL 28.5 Mon 18:30 POT 51**

**Generation of tunable 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 tunable 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 TES 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 beat with an adjustable time delay - recombined and are focused on the antenna. By using this technique we generated THz pulses tunable from 0.35 to 2.5 THz with adjustable spectral widths (FWHM) of 200 to 500 GHz.


**HL 29: Organic Photovoltaics II: mainly Phtalocyanine**

**HL 29.1 Mon 17:45 FOE Anorg**

**Band gap states of copper phthalocyanine thin films induced by nitrogen exposure**

―Tomoki Sueyoshi, Haruya Karuta, Masaki Ono, Kazuuki Sakamoto, Satoshi Kera, and Nobuo Ueno—1Graduate School of Advanced Integration Science, Chiba University, Chiba, Japan. 2Peter 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 external 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.
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 Puech, Wolgang Tress, Selina Olthof, Max Thietze, Jan Messer, 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:C60 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:C60) to 1:6 by volume, we observe significant changes of Voc from 0.54 to 0.63 V. To exclude that this increase with higher C60 content is caused by the increased contact area of C60 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 C60), Voc is not affected significantly. Hence, we attribute the changes in Voc 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 C60 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 Derick Schlettwein — Institute of Applied Physics, Justus-Liebig-University Giessen, Germany. email: schlettwein@uni-giessen.de

Blends of F16PCuC6 and PCuC6 were prepared on glass by physical vapour deposition. The acquired thin films had a thickness of around 20nm. The co-evaporation of PCuC6 and F16PCuC6 was varied to obtain different molecular mixtures. High adimixtures of PCuC6 to F16PCuC6 were 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 PCuC6 in F16PCuC6 (moderate per cent range) disturbed the charge flow in the films. Very little admixture of PCuC6 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 F16PCuC6 solid state structure. The dominant substrate—structure of pure F16PCuC6 (highly conductive) was partly changed to the herringbone β-structure (less conductive). Consequences for photoconduction in the films will be discussed.

HL 30.1 Tue 10:15 FOE Anorg
Autocatalytic growth of GaAs nanowires on Si (111) using different SiO templates — Daniel Rudolph1, Simon Hertenberger1, Xiaodong Wang1,2, Watcharapong Paosangthong3, Max Bichler1, Gerhard Abstreiter1, Jonathan J. Finley1, and Gregor Kohlhuber1 —1) Walter Schottky Institut, Technische Universität München, Garching, Germany — 2) Pohi 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 SiO2, (b) an ultrathin layer of thermal SiO2, and (c) a layer of thermal SiO2 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 zinchenelle 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 (BN-I) and JARA-Fundamentals 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 silsesquioxane (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 Wallay1, Florian Furtmayr1,2, Rudolph Matz3, Marcus Rohrke3, and Martin Eickhoff3 — 1) Physikalisches Institut, Justus-Liebig-Universität Giessen — 2) Physikalisch-Chemisches Institut, Justus-Liebig-Universität 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-aging is addressed.

HL 30.4 Tue 11:00 FOE Anorg
Effects of doping profile on the optoelectronic properties of GaN nanowires — Friedrich Limbach1,2, Tobias Gottschek1,2, Tomi Stoica1,3, Carsten Pfeiffer1,2, Oliver Brandt2, Achim Tempez2, Sebastain Geburt3, Carsten Ronning3, and Raffaella Calarco1,2 — 1) Institute of Bio- and Nanosystems (IBN-1), Research Centre Jülich GmbH, 52425 Jülich, Germany, and 2) JARA-FIT Fundamentals of Future Information Technology — 3) Paul-Drude-Institute for Solid State Electronics, Hausvogteiplatz 5-7, 10117 Berlin, Germany.

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
Furthermore, the samples exhibit no significant strain indicating that the In flux was pulsed by opening and closing the In shutter periodically. With the intention to improve the quality of these thin films, we have doped with Zn and Sn for p- and n-type doping, respectively, in 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.

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.


HL 30.6 Tue 11:30 FOE Anorg

Microstructures and electronic properties of one-dimensional ZnO nanostructures — Peter Hess, Yong Lei, Martin Peter-Lechner, 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

HL 31.1 Tue 10:15 POT 51

Direct measurement of the band gap and Fermi level position at InN(1120) — Philipp Ebert1, Sarah Scharphauser1, Andrea Lens2, Aizhan Sabitova1, Lena Ivanova1, Mario Dähne2, Yu-Liang Hong3, Shangji Gwo3, and Holger Eisele4 — 1Institut für Festkörperforschung, Forschungszentrum Jülich GmbH, 52425 Jülich — 2Institut für Festkörperphysik, Technische Universität Berlin, 10623 Berlin — 3Department 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 $E_G = 0.7 \pm 0.1$ eV. The Fermi energy is pinned 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 Hangelter — Technische Universität Braunschweig, Institut für 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 Koukourakis1, Dominic Funk2, Nils C. Gerhardt2, Martin R. Hofmann2, Sven Liebich3, Christina Beicken2, Steffen Zinskann2, Martin Zimprich2, Kerstin Volz4, Stefan W. Koch2, Wolfgang Stolz2, and Bernadette Kuner2 — 1Photonics and Terahertztechnology, Ruhr-Universität Bochum, Bochum, Germany — 2Material Science Center and Faculty of Physics, Philips-University Marburg, Marburg, Germany — 3NAP 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 demonstrated high modal gain values at room temperature, 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 — Darja Sukridina1, Duc Dinh2, Michael Kneissl1, Norbert Esser2,3, and Patrick Vogt4 — 1TU Berlin, Institute of Solid State Physics, Hardenbergstr. 36, 10623 Berlin, Germany — 2TAS 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 films with thicknesses even below 100 nm. Our measurements confirm valence band spectra we could determine the polarity of c-plane InN Semiconductor Physics Division (HL) Tuesday growth direction of the columns on semi-polar InN surface.

Die Bandlücke von AlGaN variiert von 3,4eV – 6,2eV und ermöglicht physik, Hardenbergstr. 36, 10623 Berlin, Germany

Suszeptortemperatur von 1100

Nukleationschicht direkt auf (10¯10) m–plane Saphir mittels metallor-...
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 $p = 1.06 \times 10^{12}$ cm$^{-2}$ and a hole mobility of 7.26 $\times$ 10$^3$ cm$^2$/Vs. Magnetotransport measurements on L-shaped Hall bars along [011], [01-1], [010] and [001] crystal directions and related work developed by Shubnikov-de-Haas oscillations and quantum Hall plateaus, indicating the high quality of the material. In the field range from minus 67 to 67 the longitudinal resistance is superimposed with a negative parabolic magnetoresistance background. The minimum of the longitudinal resistance at $B=0$T decreases with increasing temperature, and hence, is a sign for weak antilocalization.

**Invited Talk**

**HL 32.1 Tue 10:15 POT 151**

**Self-assembled monolayers on zinc oxide** — **Craig L. Perkins** — National Renewable Energy Laboratory, 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 crystallized with 1-hexanethiol and 1-hexanephosphonic acid were examined with a novel quartz crystal microbalance (QCM)-based flow spectroscopy, and contact angle measurements. A means of using ammonium chloride as a probe of molecule-ZnO interactions is introduced. These findings define a new route towards the realization of novel hybrid systems for optoelectronics and photonics.

**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.

**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 nanocrystal structures were prepared on oxidised silicon samples using nanoprobe 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 hybrid 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 counterelectrode, 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, Waltermann, Stefan Kontermann, and Wolfgang Schade — Clausthal University of Technology, EFZN, EnergieCampus, 38640 Goslar — 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 photoabsorance 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 seepage 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 33.1** Tue 10:15 POT 251

**Time-resolved Kerr detection of acoustic spin transport in GaAs (110) quantum wells**

- Alberto Hernández-Minguez, Klaus Hermann, Snežana Lazic, Rudolph Hey, and Paulo V. Santos — Paul-Drude-Institut für Festkörperphysik, 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 incoherent 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 $\delta P$ in polarization of a probe pulse delayed by $\tau$ with respect to the pump. Spatial profiles of $\delta P$ during acoustic transport show a peak at $x = \varphi_{SAW}\tau$, 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 $\mu$m, 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**

- Haucke Lehmann, Till Benter, Alexander Bühl, and Jan Jacob — Institut für Angewandte Physik und Zentrum für Mikrostrukturforschung, Universität Hamburg, Jungiusstraße 11, 20555 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 rattlewegung. 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].


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 magnetic field 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.

Semiconductor Physics Division (HL)  
Tuesday

HL 33.10 Tue 12:45 POT 251  
Perpendicular Spin Injection and Polarization Features in InAs Quantum Dots — •ANNE LUDWIG1, HENNING SOLDAT2, FRANK STROMBERG2, ASTRID ESBERING1, ANNE WAPLUND3, MINGYUAN LI4, NLS C. GERHARDT2, DIRK REUER4, OLEG PETRACH4, MARTIN HOFFMANN4, HEIKO WEND5, WERNER KEUNE6, and ANDREAS D. WIECK3  — 1Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum — 2Lehrstuhl für Photonik und Terahertztechnologie, Ruhr-Universität Bochum — 3Fachbereich Physik and Center for Nanointegration Duisburg-Essen, Universität Duisburg-Essen — 4Experimentalphysik 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 inverting 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 KUHLEN1,2, KLAUS SCHMALBACH1,2, MARKUS HAGEDORN1,2, MIHAIL LEPKA3,2, THOMAS SCHÄPERS3,2, GERNOT GÜNTERHÖLZEL1,2, and BERND BESCHOTEN1,2  — 1II. Physikalisches Institut A, RWTH Aachen University, 52056 Aachen — 2JARA: 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 eplayers, which favorably does not require any ferromagnetic electrodes. An electric field is found to create a Dresselhaus-type internal magnetic field, which is perpendicular to the applied field \([100]\) at \(4 \times 10^5 \text{V/m}\). 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 GÖBBERIS1,2, PHILIPP SCHÄPERS1,2, KLAUS SCHMALBCH1,2, THOMAS SCHÄPERS3,2, MIHAIL LEPKA3,2, GERNOT GÜNTERHÖLZEL1,2, and BERND BESCHOTEN1,2  — 1II. Physikalisches Institut A, RWTH Aachen University, 52056 Aachen — 2JARA: Fundamentals of Future Information Technology, 52074 Aachen

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-spectroscopic photocurrent effect [1]. However, no direct proof of the spin polarization of these currents has been reported yet.

We present photovoltage measurements on n-InGaAs eplayers 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.


This work has been supported by DFG through FOR 912.

HL 34: Joint Session: Solid State Photon Sources

Time: Tuesday 10:30–13:00

Optical Processes in OLEDs: Molecular Photonicics

•MICHAEL FLÄMMICH, DIRK MICHAELS, 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 coupling out 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.

Single Photon Source with Diamond Nanocrystals on Tapered Optical Fibers

•ALIKAU TÖRÖLER1, JULIANE HERMELBRACHT1, MARKUS WEBER1, WENJIANI ROSENFIELD2, ARJANE STIEBEINER3, ARNO RAUSCHENBREUTEL3, JAMES RABEAU4, and HARALD WEINFURTER1,2  — 1Ludwig-Maximilians-Universität, München — 2Max-Planck-Institut für Quantenoptik, Garching — 3Johannes-Gutenberg-Universität, Mainz — 4Macquarie 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.

Fiber-integrated diamond-based single photon source — •TIM SCHRÖDER, ANDREAS WOLFGANG SCHELL, GÜNTER KWESES, THOMAS ASCHELE, and OLIVER BENSON — Nano Optronics 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

Scattering-type 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 dot excitons in the near-field configuration. 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 µm 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 dots [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.


**HL 34.5** Tue 11:45 HSZ 02
Quantum-Dot Pyramidal Micracavities as Candidates for Electrically Pumped Efficient Single-Photon Sources — Daniel Rükel, Christoph Reinheimer, Florian Stockmar, Daniel M. Schaadt, Heinz Kaut, and Michael Hetterich — Institut für Angewandte Physik and DFG Center for Functional Nanoscale Metrology, Karlsruhe Institute of Technology (KIT), Wolfgang-Gaede-Straße 1, 76131 Karlsruhe (Germany)

We have investigated InAs-QDs embedded in reversed pyramidal GaAs micracavities 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 combination of e-beam lithography and a selective wet-chemical etching process. In order to pump QDs electrically they were embedded in the intrinsic layer of a pin-junction and induced excitons by means of their ribbons connected via nanowires to a large 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 Olav Berenson — 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 demonstrated 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 the 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 3mm by 3mm by 30mm makes this device interesting for robust and low cost single photon implementations.

**HL 34.7** Tue 12:15 HSZ 02
A spatially circularly-polarized single-photon source — Andreas Merz, Paolo Anshoff, Robin Schwerdt, Heinz Kaut, 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 well as single photon source. With an applied magnetic field of 2T, a pronounced spin-polarization of ∼ 65% is achieved, while at B = 6T 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 — Snezana Lazic, Rudolf Hey, and Paulo Santos — Paul-Drude-Institut für Festkörperphysik, 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 the QW photon source. With an applied magnetic field of 2T, an emission of non-classical light from QD arrays was investigated by analysing the statistics of the emitted photons using the Hanbury Brown and Twiss approach.

**HL 34.9** Tue 12:45 HSZ 02

Electrically pumped InGaAs/GaAs quantum dot (QD) based Resonant-Cavity LED (RC-LED) 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.
HL 35: Joint Session: Organic Semiconductors II: Solar Cells B

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 perpyrrolimidines,2 tri-angurally shaped polyaromatic hydrocarbons,3 Aleg,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). 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.


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 — ●VICTOR ATTALA, MINA YOONS1,2, and MATTHIAS SCHEFFLER — 1Fritz-Haber-Institut der MPG, Berlin, Germany — 2Oak 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 individual 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 transferred charge is strongly functional dependent - in particular all semilocal functionals have significant artificial charge transfer in the asymptotic limit.


HL 35.3 Tue 11:15 ZEU 222
Sub-Bandgap Absorption in Polymer-Fullerene Solar Cells — ●MARTIN PRESSL, FELIX HERREMA, MARKO SERELAND, MARK BÄRENKLAU, ROLAND RÖSCH, WICHARD J. D. BEENKEN, ERICH RUNGE, SVITOSLAV SHOKHOVETS, HARALD HOPPE, and GERHARD GORSCH — 1Experimental Physics I, Institute of Physics & Institute of Micro- and Nanotechnologies, Ilmenau University of Technology, Weimarer Str. 32, 98693 Ilmenau, Germany — 2Theoretical 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 STEVUELMUTHNER, 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-C61-butyric acid methyl ester (PCBM) are known to depend largely on the morphology of the interface between the donor and acceptor materials. A recent study of optical spectra and SBG EQE signals of 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 could not provide information about the fraction of crystallized chains, the width of the aggregate, and the energetic disorder of 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 increased in PCBM aggregation.


HL 35.5 Tue 11:45 ZEU 222
Influence of Phase Segregation on the Dynamics of Charge Carriers in Organic Solar Cells — ●ANDREAS BAUMANN, TOM J. SAVENJEE, DHARMAPURA H. K. MURTHY, MARTIN J. HERENY, CARSTEN DEIBHLL, and VLADIMIR DYAKONOV — 1Experimental Physics VI, Physical Institute, Julius-Maximilians-University of Würzburg, Am Hubland, D-97074 Würzburg — 2Bavarian Center for Applied Energy Research (ZAE Bayern), Am Hubland, D-97074 Würzburg — 3Optoelectronic Materials Section, Department of Chemical Engineering, Delft University of Technology, 2628 BL Delft, The Netherlands — 4Department 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 gemicante 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 OPTIT, JULIA WAGNER, MARK GUBER, URICH 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 acceptor.
films when mixing CuPc or DIP with C mixed films in the case of the two phthalocyanines to phase-separated nar and mixed films as well as for their performance in photovoltaic – Fent donor (copper phthalocyanine – CuPc, diindenoperylene – DIP) acceptor materials.

Semiconductor Physics Division (HL) Tuesday

HL 35.7 Tue 12:15 ZEU 222
Towards Ideal Morphology of Polymer Bulk Heterojunction Solar Cells — CHETAN RAI SINGH, MICHAEL SOMMER, MARCEL Himmerlich, ANDRE WICKLEIN, STEFAN KRISCHOK, MUKUNDAN THELLAKKAT, AND HARALD HOPPE — Institute of Physics, Ilmenau University of Technology, Germany — 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 KOE RNER, HANNAH ZIEHLKE, ROLAND FITZNER, EUGEN REINOLD, PETER BAUERLE, KARL LEO, AND MORITZ RIEDER — Institute for Angewandte Photophysik, Technische Universität Dresden — 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.

We use photoinduced absorption spectroscopy (PIA) to probe the long-living (µs-ms) excited states (triplet excitons, cations) after photoexcitation of DCV-nT/C60 blends. With PIA, their generation and recombination behaviour can be investigated. Here, we report our results obtained on a series of DCV-nTs 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 C60.

HL 35.9 Tue 12:45 ZEU 222

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 unper- turbated (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.

HL36: Joint Focussed Session: Transparent Conductive Oxides II

Time: Tuesday 11:15–13:15

Topical Talk

HL 36.1 Tue 11:15 WIL B122
Experimental Electronic Structure of In2O3 and Ga2O3 — 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 -In2O3 and Ga2O3 from the group of TCO’s showing the smallest respectively largest optical gap- will be explored experimentally. The investigations of optical and electronic properties were performed on high quality n-type single crystals showing carrier densities of 1019 cm−3 (In2O3) and 1017 cm−3 (Ga2O3). 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 ARCES and a combination of X-ray photoemission and X-ray absorption complementarity it is shown that 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.

Location: WIL B122

Topical Talk

HL 36.2 Tue 11:45 WIL B122
Transparent Electronics Using Oxide Materials — MARCUS 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 semiconductor 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 — AXL 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 comparison of study of different ZnO single crystals and doped and undoped ZnO films reveals pronounced differences in the free and bound excitation.
Electronic and Optical Excitations in Magnetic Insulators

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

Fe/Au(001) thin films excitonic states within the fundamental band gap is investigated. However, describing the excitation freedom, magnetic materials attract more and more interest due to potential technological applications. With the advent of electronic devices exploiting also the spin degree of freedom, magnetic materials are expected to play a key role in future technology. Here, we focus on the antiferromagnetic transition-metal oxides as typical representatives for the class of magnetic insulators.

The combination of the local spin density approximation (LSDA) and the dynamical mean field theory (DMFT) provide a powerful tool to treat correlations beyond the local density approximation (LDA). 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 tunneling microscopy images are presented and discussed in the light of previous experiments.

HL 36.4 Tue 12:45 WIL B122 Thermodynamic stability, stoichiometry and electronic structure of bcc-In$_2$O$_3$ surfaces — Peter Agorton and Karsten Albre — TU Darmstadt, Petersenstr. 32, 64287 Darmstadt

The thermodynamic stability of all experimentally observed low index surfaces of bcc-indium oxide (In$_2$O$_3$) have been investigated by means of density-functional theory calculations. The effect of a changing environment has been studied 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$_3$O$_5$ single crystals — Valentina Scherrer, Peter Hlawenka, Christoph Janowitz, Allica Krapp, Helmut Dwelik, and Recardo Manzke — Institut für Physik, Humboldt-Universität zu Berlin

The scientific interest in transparent conducting oxides (TCOs) such as ZnO, Ga$_2$O$_3$, In$_3$O$_5$ 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 quality In$_3$O$_5$ single crystals and substrates for homoepitaxy, which also limits the attainable progress in device production. High quality In$_3$O$_5$ single crystals were grown using the chemical vapor transport method (CVT). The crystals were of body centered cubic bixbyte-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 $\Gamma$-point yielded a direct band gap of $\sim 3$ eV. The weak conduction band emission near the Fermi edge enabled the 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

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 $\Gamma$ point. Further, the occurrence of spin-allowed and spin-forbidden Frenkel-type-like bound excitonic states within the fundamental band gap is investigated.

HL 37.2 Tue 11:45 TRE Phy LSDA+DMFT calculations of Fe/Ni disordered alloys and Fe/Au(001) thin films — Jan Minar, Jurgen Blaun, Aria 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 the local density approximation (LDA). 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.


HL 37.3 Tue 12:00 TRE Phy Effective on-site Coulomb interaction in transition metals from constrained RPA — Ersos Saboglu, Christoph Friedrich, and Stephan 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 3$d$, 4$d$, and 5$d$ 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 $U$ parameter 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 3$d$ 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 3$d$ transition metals. This work has been supported in part by DFG-FOR-1346.

[1] www.flapw.de

HL 37.4 Tue 12:15 TRE Phy
Ab-initio description of spin-dependent transport in disordered alloys — DIEMO KÖDERTITZSCH, STEPHAN LOWITZER, and HUBERT EBERT — Ludwig-Maximilians-Universität München, Departement 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 extrinsic contributions, on equal footing. We use an implementation of the Kubo-Streda equation employing the fully relativistic Korringa-Kohn-Rostoker (KKR) Green’s function method in conjunction with the Coherent Potential Approximation (CPA) theory. For discussing spin currents we employ our recently devised relativistic spin projection scheme [1] and a corresponding generalization of the Kubo-Streda equation. We illustrate the power and versatility of the approach by giving several examples.


HL 37.5 Tue 12:30 TRE Phý Applying hybrid-functional and many-body methods to rare earths: a study of Cerium — MARCO CASADU1, XINGUO REN2, JOACHIM PAIER, PATRICK RINKE, ANGEL RUBIO1,2, and MATTHIAS SCHIEFFLEIN1 — Fritz-Haber-Institut der MPG (TH), Berlin, Germany — 2Humboldt Universität (Institut fuer Chemie), Berlin, Germany — 3UPV/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 isostructural 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+e-RPA). 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+e-RPA – a physically meaningful screening of exact-exchange – achieves the same effect from first principles.
function $g(\tau)$ 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 occurrence of two distinct transitions.

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 meV and diamagnetic coefficients up to 0.025 meV/T 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.

We study the propagation of lower branch exciton polaritons in 200 μm - 800μm thick Cd$_0.8$Zn$_{0.2}$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 $h\nu_0 = 1.664$ eV. The lifetimes of the exciton polaritons in the upper and lower branches are 1.5 ns and 3 ns, respectively.

In time of flight measurements we observe significant delay of 1 ps optical pulses, which increases to 350 ps at $h\nu = 1.661$ 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.

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 spectrally resolved excitonic component of artificial contrasts due to the Zeeman effect.

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.
ied the thickness variation of ZnO:Al films used as window layer in Cu(In,Ga)(Se,S) (CIGS) thin film solar cells. Thin ZnO:Al layers (200nm) on glass exhibit significantly enhanced transmission at wavelengths \( < 400 \text{nm} \) while a considerable sub-bandgap absorption at \( > 800 \text{nm} \) appears in thicker films which is attributed to free charge carrier absorption. The IV-characteristics of CIGS solar cells with \( d_{\text{ZnO:Al}} = 200 \text{nm} \) exhibit a strong enhancement of the short-circuit current density \( J_{SC} \) (\( \Delta J_{SC} = 3 \text{mA} \)) 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 CIGS-module. XRD-diffractionograms 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 of the involved elements.

HL 39.6 Tue 14:45 FOE Anorg
Spatially and time resolved cathodoluminescence spectroscopy of CuGaSe2 — Thorsten Rissom, Matthias Müller, Frank Bertram, Jürgen Christen, Daniel Abou-Ras — Helmholtz-Zentrum Berlin für Materialien und Energie, Germany
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 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 Kam, Glauco Battaglinari, Ian A. Howard, Michael Hansen, Hans W. Spiess, Alexey Mavrinetskii, Woutchon Pisula, Chen Li, Klaus Müller, and Frédéric Laguë — 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 excitation 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 Wang1, Hamed Azimi1, Hanne-Gaeg Mac2, Mauro Morana2, Hans-Joachim Schlueter2, Alfred J. Meixner1, and Dai Zhang2 — 1Institute of Physical and Theoretical Chemistry, Auf der Morgenstelle 18, University of Tübingen, Germany; 2Konarka Austria F&E GmbH, Linz, Austria; 3Konarka Technologies GmbH, Nürnberg, Germany
We present the study of the influences of the additive 1,8-octanethiol (ODT) on the nanometer scale morphology and local photophysics of low band-gap polymer blends, PCDTDFTB 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 PCDTBT:PCBM blend film induced by OTD by the dramatically increased PL emission from PCDTBT 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 properties and the morphology of the blend film with/without OTD 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. Pascu1,2,3, Ruth Lohwasinnen2, Michael Sömmers2, Mukundan Thelakkat4, Thomas Thurn-Albrecht1, and Kay Saalwächter4 —

1Institut für Physik, Martin-Luther-Univ. Halle-Wittenberg, Halle, Germany —
2Makromolekulare Chemie I, Universität Bayreuth, Germany —
3Experimentelle Physik III, TU Dortmund, Germany

Molecular weight and stereoregularity affect the morphology and the crystallinity of conjugated polymers and are thus pivotal for the mobility of charge carriers in electro-optical device applications. We use 13C solid-state NMR to determine the crystallinity and details on crystal-crystal phase transitions 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 around 64% upon increasing MW, corresponding to a corrected maximum value for the reference melting enthalpy of $\Delta H_m \approx 37 \text{ J/g}$ 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.


**HL 40.4 Tue 14:45 ZEU 222**

Self-Assembled Ultralong Organic Semiconducting Nano/Microwires — Julia Lambricht, Torbat P. I. Saragi, and Josef Salebeck —

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 34122 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 Handloser1, Ricky Dunbar2, Philipp Altpeper2, Lukas Schmidt-Mende1, and Achim Hartschuh2 —

1Department Chemie und CeNS, Ludwig-Maximilians-Universität, München, Germany —
2Department Physik and CeNS, Ludwig-Maximilians-Universität, München, Germany

Plasmons 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

**HL 41.1 Tue 14:15 POT 51**

Systematics of nonradiative recombinations in blue and green emitting GaN1/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 GaN1/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 $x_{\text{In}}$ 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 $x_{\text{In}}$ and thicker QWs, a strong reduction of nonradiative lifetimes $\tau_{nr}$ occurs for high $x_{\text{In}}$ ( > 25%). As the experiments were performed in the low carrier density regime, the nonradiative recombination rate $R_{nr} \propto 1/\tau_{nr}$ is of defect-related nature following an exponential temperature dependence $R_{nr} \propto \exp (-E/kT)$ 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 In0.53Ga0.47N(0001) surfaces —

C. Friedrich1, A. Biermann2, V. Hoffmann2, N. Esser1,3, M. Kneissl4, and P. Vogt1 —

1TU Berlin, Inst. f. Festkörperfysik EW6-1, Hardenbergstr. 36, 10623 Berlin, Germany —
2Ferdinand-Braun-Institut, Leibniz-Institut, Gustav-Kirchhoff-Str. 4, 12489 Berlin, Germany —
3Leibniz-Inst. für Analytische Wissenschaften - ISAS e.V., Albert-Einstein Str. 9, 12489 Berlin, Germany

The In0.53Ga0.47N(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 In0.53Ga0.47N(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 In0.53Ga0.47N(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 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.
Electrical Spin injection into Zinc Oxide

2

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

the internal electric fields at the heterointerface between InGaN and quantum wells shift from 2.60 eV to 2.75 eV with decreasing indium content. This indicates a decrease in effective mass of the conduction band as a function of indium content. The shift in energy levels is accompanied by a change in the bandgap, which also affects the luminescence efficiency.

We have investigated the feasibility of electrically injecting spin-1/2 carriers into heterostructures. Spin injection into InGaN quantum wells was observed at low temperatures, demonstrating the potential for use in spintronics applications. The spin injection was confirmed by measuring the spin relaxation time, which is important for the development of high-speed spintronic devices.

In summary, our results provide insights into the internal electric fields and their implications for the electronic properties of InGaN/GaN heterostructures, as well as the potential for spin injection at low temperatures. These findings will guide future research on the development of promising applications in spintronics.

Invited Talk

HL 42.1 Tue 14:15 POT 151

Interfacial charge-carrier energetics probed by electrode-mulated 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 studies. In this talk, I will discuss the use of electrode-mulated 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.

HL 43: Spin-dependent Transport II

Time: Tuesday 14:30–15:15

Electrical Spin injection into Zinc Oxide — Christoph Schwara, Christian Weyen, Gehry Güntheroth, Matthias Althammer, Sebastian T.B. Goennenwein, Matthias Opel, Rudolf Gross, and Bernd Bischof — 1II. Physikalisches Institut A, RWTH Aachen University, Aachen, Germany — 2Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — 3JARA - 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.

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

GaN is a prototypical wide-gap semiconductor with wurzite 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 wurzite GaN samples by time-resolved Kerr-rotation measurements up to a density of $1.5 \times 10^{19}$ 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.

Long room-temperature electron spin lifetimes in highly doped cubic GaN — ●Jörg Rudolph1, Jan Heye Buss1, Thorsten Schuppe2, Donat As3, Klaus Lischka2, and Daniel Hägeli1

1AG Spektroskopie der kondensierten Materie, Ruhr-Universität Bochum, Germany — 2Universität 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 d-n-doped cubic GaN (nT = 1 × 1019 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.


HL 44: Poster Session I

Time: Tuesday 18:00–21:00

Location: P3

HL 44.1 Tue 18:00 P3

Antiferromagnetic semiconductor LiMnAs — Vit Novák1, Tomas Jungwirth1, Miroslav Cukr1, Stephan Svoboda1, Zbyněk Soban1, 2, Xavier Marty3, Vaclav Holý3, Petra Břístová3, 2, and Petr Nemeček2

3Institute of Physics AS CR, Cukrovarnická 10, Praha, Czech Republic — 2Charles University, Ke Karlovu 5, Praha, Czech Republic — 3Czech Technical University, Technická 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 MnV compounds. Drift in pairs. 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 materials 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.

Drift in amorphous phase change materials — Rüdiger M. Schmidt1, Gunnar Bruns1, Jennifer Luckas2, Karl Schlockermann1, Martin Salanga2, and Matthias Wuttig1 — 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.

Visibility of graphene on gadolinium and dysprosium oxide thin films — Ole Petrov1, Tomáš Tádor2, C. Bock2, U. Kunze1, A. Milanov2, A. Devíš2, R. A. Fischer3, L. Thérekárka3, D. Schmidt2, and M. Havuč3 — 1Institute of Physics AS CR, Cukrovarnická 10, Praha, Czech Republic — 2Charles University, Ke Karlovu 5, Praha, Czech Republic — 3Czech Technical University, Technická 2, Praha, Czech Republic

In this work we study the visibility of monolayer graphene exfoliated on gadolinium (Gd2O3) and dysprosium oxide (Dy2O3), respectively. The rare earth oxides are deposited by thermal chemical vapour deposition on top of a highly oriented silicon substrate. Due to the higher dielectric constant of the rare earth oxides (εr ≈ 8–9) compared to SiO2 (εr ≈ 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.


Phonon dynamics in graphite observed with time-resolved terahertz spectroscopy — Martin Schuch 1,2, Konrad von Volkmann 1,3, Luca Perfetti 4, Tobias Kampschmidt 1,2, Christian Frischkorn 1,2, and Martin Wolf 4,1

Fachbereich Physik, Freie Universität Berlin, Arnamfelde 16, 14195 Berlin — 2Fritz-Haber-Institut der MPG, Faradayweg 4-6, 14195 Berlin — 3APE GmbH Plauer Str. 163-165 Haus N, 13053 Berlin — 4Laboratoire des Solides Irradiés, École 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 ɛ(x) 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 A1g and Eg phonons. The results are in agreement with theoretical predictions [2] and show that the A1g mode at the K point provides the dominant relaxation channel. Additional measurements on naturally grown graphite show no differences to HOPG.


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 1, Achim Wixforth 2, and Achim Hartshorn 3

1Department of Chemistry, CSU, Northridge, CA, U.S.A. 2Department of Materials Science and Engineering, Northwestern University, Evanston, Illinois, USA

Single-walled carbon nanotubes (SWNTs) are quasi-one 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] and [2].

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.


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Semiconductor Physics Division (HL)

Stefanie Heydrich, Marc A. Wilde, and Dirk Grundler
1Lehrstuhl für Physikalische Schichtsysteme, Technische Universität München, Physik Department, James-Franck-Str. 1, D-85747 Garching b. München, Germany — 2Institut 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 $M = -\mu_B/\mathcal{B}$ for a temperature $T$ yields direct access to the ground state energy $\mathcal{U}$ 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 14.13 Tue 18:00 P3
Spin orbit mediated entanglement in graphene — Alexander Lopez1,2 and John Schliemann1
1Institute for Theoretical Physics, University of Regensburg, D-93040 Regensburg, Germany — 2Centro de Física, Instituto Venezolano de Investigaciones Científicas, 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 14.14 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 SiO$_2$ substrates in an argon gas flow at atmospheric pressure. The samples were prepatterned with antinodes lattice by electron beam lithography and reactive ion etching. The hexagonal form of the antinodes 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 layer graphene samples patterned by hexagons of antinodes from temperature dependent investigations of the clearly resolved weak localization peak we deduce the phase coherence length as well as lengths for inter- and intravalley scattering.


HL 14.15 Tue 18:00 P3
Fabrication of top gates with ALD deposited Al$_2$O$_3$ on graphene structures — Franz-Xaver Schrettenbrunner, Dieter Weiss, and Jonathan Eroms — Institut für Experimentelle und Angewandte Physik, Universität Regensburg, 93040 Regensburg

We report the fabrication and transport measurements of top gated graphene devices. The insulating Al$_2$O$_3$ 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$_2$O-process with low pressure of five seconds creates a stable top gate dielectric on graphene resulting in strong n-doping of the sample (impurity carrier density: $n_{\text{imp}} = 5.2 \times 10^{11}$ cm$^{-2}$). Now this process was improved by growing 10nm Al$_2$O$_3$ 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 $n_{\text{imp}} = 3.6 \times 10^{11}$ cm$^{-2}$.

HL 14.16 Tue 18:00 P3

Paramagnetic surface-states in μC-3C-SiC as efficient acceptor in solar cells — Andre Konopka, Siegmond Greulich-Weber, Uwe Gerstmann, Eva Raals, and Wolf Gerber 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 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 effects we use magnetic resonance (EPR) and magnetic susceptibility measurements. 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 not 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 14.17 Tue 18:00 P3
Stoichiometric defects in silicon carbide — Guido Roma1,2, Ting Liao2, and Olga Natalia Bedoya-Martínez3 — 1CEA-Saclay, Département de Recherche en Métallurgie et Physique Quantique, Savoie, France — 2Institute of Metal Research, Shenyang, China

Defect structures showing odd-membered rings are known features of several tetrahedral semiconductors as well as carbon nanostuctures; examples of them are bond defects in crystalline and amorphous silicon, Stone-Wales defects in fullerene 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 anti-SCD and anti-SC2D defects 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 14.18 Tue 18:00 P3
Spin Noise Spectroscopy and Selection Rules in Highly Purified 28SiC — Nils Scharnhorst1, Georg Müller2, Helge Riemann2, Jens Hübner3, and Michael Oestreich3 — 1Institut für Solide State Physics, Leibniz Universität Hannover, Appelstr. 2, D-30167 Hannover, Germany — 2Institut für Kristallzüchtung, Max-Planck-St. 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 28SiC and natural silicon. Isotopically pure 28SiC is promising very long spin-coherence times due the missing inhomogeneous spin decoherence via nuclear hyperfine-interaction. The fragile measurements on localized spins in 28SiC will be realized by spin-noise spectroscopy based upon weakly interacting off-resonant Faraday-rotation [1] while spin selective pump-probe measurements yield the selection rules at the Δ-band minimum in natural, slightly n-doped silicon.


HL 14.19 Tue 18:00 P3
Structural and electronic properties of silicon polymorphs — Tobias Sander, Claudia Rödl, Karol Skino, 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 underestimated in their atomic geometries. Due

HL 14.20 Tue 18:00 P3
Semiconductor Physics Division (HL)

Investigation of the direct bandgap-emission of highly doped strained germanium layers — \Michael J. Drexler 1, Niko S. Köstner 1, Kolja Kolata 1, Giovanni Isella 2, Daniel Christina 2, Hans von Kasel 1, Hans Sigg 1, and Sangam Chatterjee 1

1Faculty of Physics and Measurements, Center of Technical Physics and Material Research, Philipps-Universität Marburg, Marbenhof 5, D-35032 Marburg, Germany — 2Dipartimento di Fisica del Politecnico di Milano, Polo di Como, via Anzani 42, I-22100 Como, Italy — 3Labor für Micro- und Nanotechnologie, Paul Scherrer Institut, Switzerland

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 bandgap transitions. The system is pumped with a Q-switched laser at 1064nm with 70 ns pulses and the emitted light is spectrally resolved with a double monochromator and detected with a liquid nitrogen cooled Ge-detector.


Giant dynamical Stark shift in germanium quantum wells — \Ronja Woscholski 1, Niko Steffen Köstner 1, Kolja Kolata 2, Christoph Lange 1, 2, Giovanna Isella 2, Daniel Christina 2, Hans von Kasel 1, and Sangam Chatterjee 1

1Faculty of Physics and Materials Science Center, Philipps-Universität Marburg, Marbenhof 5, D-35032 Marburg, Germany — 2Dipartimento di Fisica del Politecnico di Milano, Polo di Como, via Anzani 42, I-22100 Como, Italy

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 wells structured in a way 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 150 meV is found for a sample temperature of 10 K, 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.

Structural modification of SHI irradiated amorphous Ge layers — \Tobias Steinbach 1, Claudia S. Schnoehr 1, Leonardo L. Araujo 1, Raquel Goulian 2, David J. Sprostoe 2, Mark C. Ridgway 2, Daniel Severin 2, Markus Bender 3, Christina Trautmann 3, and Werner Wersch 1

1Institute of Solid State Physics, Friedrich Schiller University Jena — 2Department of Electronic Materials Engineering, Australian National University, Canberra — 3GSI 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. So-called the effect of high electronic energy deposition $\varepsilon_e$ 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 $\varepsilon_e$. XSEM revealed the transformation of the a-Ge layer into a porous structure with irregularly shaped voids that establish 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.

Electronic and Optical Properties of Group-III Nitride Alloys from ab-initio Methods — \Eli Claudio de Carvalho, André Schleife, Abderrazak Elibashe, Claudia Rödl, and Friedhelm Bechstedt

1Institut für Festkörpertheorie 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. 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, QCQA, SRS and MDM, are applied in order to illustrate different preparation techniques. The calculations are performed using high performance clusters. Based on the LDA-1/2 method electronic structures, are derived optical absorption spectra including electron-hole interaction. The electronic properties are computed as a function of composition by solving the Bethe-Salpeter equation. The computed spectra are analyzed and compared to available experimental data.

Band Parameters of (Al, Ga, In)N Polytypes from Different XC Functionals — \Eli Claudio de Carvalho, André Schleife, Frank Fuchs, and Friedhelm Bechstedt

1Institut für Festkörpertheorie 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.
is the p-doping of nitriles 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. In this work we 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 efficiency. Additionally the acceptor activation energy is expected to decrease 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.

Tuesday

HL 44.29 Tue 18:00 P3

Temperatureabhängigkeit des elektrischen Feldgradienten in AlGaN-N-..—●Ronnie Simon1, Sahar Hamidi1, Patric Kessler1, Ségrio Miranda2, Katharina Lorenz2, Reiner Vianden1 and ISOLDE Collaboration3—Helmholtz Institut für Struktur- und Kornphysik, Universität Bonn1, 2Instituto Tecnologico e Nuclear, 2686-953 Sacavém, Portugal 3CERN, Genf, Schweiz.


HL 44.27 Tue 18:00 P3

Epitaxial growth and characterization of InN and GaN on C-face SiC(III)/(Si(111))—▪Anja Eisenhardt1, Marcel Hemmerlich1, Pierre Lorenz1, Katja Tonišch1, Jörg Prebold1, and Stefan Krischok2—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(III) film with C-polarity. As characterization techniques 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 Si(100) substrates, respectively, as well as InN(0001) and GaN(0001) grown on 6H-SiC(0001). The electronic properties of the InN and GaN films grown on carbonized C-face SiC(III)/(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(III)/(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) (∼4.6 eV) and InN(0001)/(6H-SiC) (∼4.8 eV) samples. All InN and GaN epitaxial films were tensile strained.

HL 44.28 Tue 18:00 P3

Ex-situ activation of magnesium acceptors in InGaN/LED-structures—▪Gunnar Kusch, Markus Frentrup, Joachim Stellemach, Tim Kolbe, Tim Wernicke, Markus Pristovsek1, and Michael Kneissl2—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) 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) (∼4.6 eV) and InN(0001)/(6H-SiC) (∼4.8 eV) samples. All InN and GaN epitaxial films were tensile strained.

HL 44.28 Tue 18:00 P3

Effect of nitridation on the MOVPE growth of InN on c-, r- and a-plane sapphire—▪Sergei Solopov, Duc Dinh, Markus Pristovsek1, and Michael Kneissl2—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 (1120), c-plane (0001), m-plane (1010) and r-plane (1012) using metalorganic vapor phase epitaxy (MOVPE).

To grow InN directly on the sapphire substrate, a nitridation process is required to improve crystal growth 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 [1010] || [1120]sapphire. On the a-plane sapphire we obtained c-oriented InN with in-plane relationship of [1100]a, || [0001]sapphire and [1120]InN || [1100]sapphire. For the InN grown by MetSchuller et al. [1] temperatures below 900°C and additional in-plane relationship by temperatures below 900°C. We have grown also a-oriented InN on r-plane sapphire at nitridation temperature higher than 800°C. At nitridation temperatures below 800°C this orientation disappears.

**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, 30167 Hannover, Germany

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 sensitive only to the transverse spin dephasing time $T_\perp^\alpha$. 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.


When the Schottky junctions of the metal-intrinsic-n-doped type are widely used to control the charge in quantum dots (QDs) that are coupled with 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 1 μm × 1 μm. In this contribution, we present a novel approach to create such μ-diodes: After growing the basic layer sequence by optical lithography and subsequent O 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 overlap region of both stripes. The diode characteristic was confirmed by I-V measurements at room temperature as well as at low temperature (4.2 K). It is intended to perform PL measurements at low temperature, and it is expected that the magnetic field will modulate the detected spin fluctuations with the Larmor frequency. This traditional experimental scheme is sensitive only to the transverse spin dephasing time $T_\perp^\alpha$. 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.

**Diffusionslängen in GaAs** — Sergei Markman, Markus K. Greff and 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 Diffusionslängen der Minoritätsladungsträger, die sowohl die Ladungsträgerbeweglichkeit als auch die Lebensdauer beinhaltet. Durch fokussierte Ionenstrahlen (FIB) können elegantere laterale pn-Übergänge geschrieben werden, die oberflächennah sind. Da dann vom eingestrahlten Licht keine hoch dotierten Schichten durchtrennt werden müssen und so eine potenzielle Absorption entfällt, kann die Effizienz der Ladungsträgerregeneration in...

**HL 44.38**
	**18:00**
	P3
	**Hole spin dynamics in 2D hole systems in [113]-grown GaAs/AlGaAs quantum wells at low temperatures**

- **Stephan Furrer**, Christian Schüller — 1Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Germany
- 2Solid State Physics Laboratory, ETH Zurich, Switzerland

Für die realisierbare skalable solid-state quantum-bit systems, spins in semiconductor quantum dots are promised 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 relaxation times in our sample at a temperature of 2 K. A complete angle-dependent series on the direction of the in-plane B with respect to the crystal axes is planned.


**HL 44.39**
	**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.


**HL 44.40**
	**18:00**
	P3
	**Exciton-mediated lattice distortions in InAs/GaAs quantum dots**

- **Sebastian Timeneyer**, Michael Böhmke, Michael Paulus, Christian Sternimann, D. C. Florian Wilbrand, Oliver H. Serck, Manfred Bayer, and Metin Tolan — 1Fakultät Physik / DELTA, TU Dortmund, Germany — 2Experimentelle Physik II, TU Dortmund, Germany — 3HASYLAB, 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 nanostructures with a discrete density of states. 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 investigations 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 (DELTAL, TU Dortmund) and P08 (HASYLAB, DESY Hamburg).

**MOVPE grown InAs quantum dots: Towards long wavelength emission**

- **Matthew 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, Almamannring 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 and 1.55 μm 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 1.3 μm and 1.55 μm, 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 core/shell 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**
	**18:00**
	P3
	**Einfluss von höherer Gate-Spannung und Lichteinfluss auf die Ladespektroskopie von InAs-Quantenpunkt-Proben**

- **Patrick Labud, Arne Ludwig, Dirk Reuter, and Andreas D. Wieck** — Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, D-44780 Bochum


**HL 44.43**
	**18:00**
	P3
	**In-situ TEM mechanical testing of InAs nanowires**

- **Marat Mukhametshin**, Vadim Migunov, Zdenek Fata, Marat Mukhametshin, Andrew Lysov, Werner Prost, Ingo Regolin, Franz-Josef Tegude, and Michael Farle — 1Fakultät für Physik and CeNIDE University Duisburg-Essen, 47048 Duisburg, Germany

Recently, it became possible to measure the elastic properties of nanomaterials in-situ by Transmission Electron Microscopy (TEM). The characteristic elastic strain of nanowires was determined 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 modulus by directly imaging the bending curvature in the TEM. The Metal Organic Chemical Vapor Deposition (MOCVD) method was used to grow InAs nanowires (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
with increasing ion fluence (up to $1.5 \times 10^{14}$ cm$^{-2}$) irradiated continuously, show a moderate increase of the step height in air between subsequent irradiations. Samples followed by surface profilometry analysis in air, i.e. step height measurements, and additionally can be used with ultrasonic bonding which reduces the required size of the bonding pads by a factor of 3.


Homo- and heteroepitaxial GaP(100) surfaces in process gas ambients — Henning Döschner, Oliver Supplie, Peter Klein·schmidt, Anja Dobracht, Brückner, Christian Höhn, Antonio Müller, Claas Löbbel, and Thomas Hansappel — Heinz-Henn-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14190 Berlin, Germany

Phosphorus based III-V semiconductors like 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(2x2) and c(4x2) symmetries, and a flipping mechanism changing the orientation of the individual dimers. A step edge 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.

Development of porous structures in GaSb by ion irradiation — Tobias Steinbach, Carolin C. Jacob, and Werner Wernsch — 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 $1.5 \times 10^{14}$ cm$^{-2}$) followed by a much steeper increase for higher fluences up to a step height of $32 \mu m$. 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 $1.5 \times 10^{14}$ 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 in the behaviour of GaSb, which leads to this effect, is still an open question.

Lithography Optimization on HgTe — Els MAIER, Matthias J. MÜHLBAUER, Bruno KREFFT, Jiango YANG, Hartmut BUHMAN, and Laurens W. MOLENSKAMP — Physikalisches Institut (EPI), 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 very thin 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.


The results of the electron beam irradiation in Halbleitern mit großer Bandlücke — Patrick Kessler, Valentin Gerisch, Sergio M.C. Miranda, Katharina Lorenz, Reiner V. Kündig, and ISOLDE Collaboration — Heinz-Henn-Zentrum für Strahlen- und Kernphysik, Universität Bonn, Rheinland-Pfalz, Deutschland, 1Instituto Tecnológico e Nuclear, P-2686-953 Sacavém, Portugal — CERN, Genf, Schweiz

The samples used for the electron beam irradiation (EFG) and consequently the size of the ion beam (IB) are limited by the effective area of the beam, which is defined by the maximum acceptance angle. The dimensions of the ion beam (IB) in our case were limited by the size of the detector, which was a position sensitive Si detector with 50 mm diameter. The energy of the ions was limited by the maximum energy which can be obtained from the ISOLDE experiment. The energy of the ions used in our experiment was 14 MeV.

The results of the electron beam irradiation in Halbleitern mit großer Bandlücke — Patrick Kessler, Valentin Gerisch, Sergio M.C. Miranda, Katharina Lorenz, Reiner V. Kündig, and ISOLDE Collaboration — Heinz-Henn-Zentrum für Strahlen- und Kernphysik, Universität Bonn, Rheinland-Pfalz, Deutschland, 1Instituto Tecnológico e Nuclear, P-2686-953 Sacavém, Portugal — CERN, Genf, Schweiz

High quality ZnSe epilayers have been grown on GaP(100) by chemical vapor deposition using metallic zinc and selenium 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.

Group VII point defects in ZnSe — Leonardo S. dos Santos, Eva RAULS, and Wolf Gerhard 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 ZnS quantum wells doped with fluorine can emit indistinguishable photons, with possible applications in quantum computation. We have used Density Functional Theory calculations to study the electronic structure of ZnS quantum wells doped with chlorine.

High quality ZnS epilayers have been grown on GaP(100) by chemical vapor deposition using metallic zinc and sulphur 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.

Band Anticrossing in ZnSe, Te$_{1-x}$ and ZnS, Te$_{1-x}$ Alloys — Tobias Bertram, Christian Karcher, Henning Klaer, Sebastian Klaer, Detlef Hommel, and Wolfram Heimbrodt Department of Physics and Materials Science Centre, Philips University of Marburg, Germany — 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 successfully 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 is only slightly smaller than that of Silicon 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 height of the E- and E+ states with the BAC is smaller than that of 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 height of the E- and E+ states with the BAC is smaller than that of the ZnTe conduction band.
and absorption characteristics of the system and by that help to gain further insight into the way the bands are formed.

Influence of the Mn-concentration on the magnetotransport properties of Cl-doped ZnMnSe

- Christian H. Will
- Matthias T. Elm
- Jörg Teuber
- Peter J. Klär
- Michael Hettich

- Physikalisches Institut, Justus-Liebig-Universität, Heinrich-Buff-Ring 16, 35392 Giessen
- Institut für Angewandte Physik, Universität Karlsruhe, Wolfgang-Gaede-Str. 1, 76131 Karlsruhe

The incorporation of manganese ions in 1−x−Mn−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 ≈ 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 fixed at x = 0.5. The transport 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.

Tuning the Two-Dimensional Hole Gas Density in CdMnTe Quantum Wells by Near-surface Doping and Photoexcitation

- Franziska Frick
- Christian Kehl
- Georgy Astakhov
- Jean Geurts
- Wolfgang Ossau
- Yuri Kuskan
- Evgenii Yakovenko
- Tommaso Wotjowicz
- Grzegorz Karczewski

- University of Würzburg, Phys. Inst., EP3, 97074 Würzburg, Germany
- Institute of Chemistry, 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. 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 of 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 tunneling 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 (X0). We describe the observed 2DHG behaviour consistently by a model based on specific tunneling times of electrons and holes, which depend on the cap layer thickness and the photon energy of the optical excitation radiation.

Isotropical and heterostructural MgZnO and CdZnO alloys

- André Schleife
- Claudia Rödl
- Friderich Riedenbach

- Institut für Festkörpertheorie und -optik and European Theoretical Spectroscopy Facility, Friedrich-Schiller-Universität Jena, 07743 Jena, Germany

One important goal of material designs 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 these 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 isotropical and heterostructural MgZn1−x−O and CdZn1−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+G0W0 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.

Hydrothermal growth of ZnO nanorods for optoelectronic and photovoltaic applications

- Manuel H.W. Bauer
- Marcel Ruth
- Christiana A. Forder
- Christian Meier

- Universität Paderborn, Experimental Physics & CeOPP, Warburger Str. 100, 33098 Paderborn

Zinc oxide are grown in cubic and hexagonal 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 nanorripples 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.

Investigation of growth catalysts for ZnO nanopillar growth

- Manfred Mädels
- Ingo Tischer
- Benjamin Neuenschwander
- Tobias Meisch
- Martin Feitberg
- Uwe Röder
- 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.

Time-resolved photoluminescence spectroscopy on ZnO based films grown by molecular beam epitaxy

- Manuel H.W. Bauer
- Marcel Ruth
- Christiana A. Forder
- Christian 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.


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 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 recombinations with increasing temperature. 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. For that, we deduce an acceptor binding energy between 80 and 60 meV.


Thermal stability of ZnO/ZnCdO/ZnO double heterostructures — Martin Lange, Anna Reinhartd, Christoph P. Dietrich, Gabriele Brendorf, Michael Lorenz, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Semiconductors Group, Linnéstr. 5, D-04103 Leipzig, Germany

Band gap engineering is essential for the fabrication of efficient opto-electronic 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 c-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 were 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.


Defects in ZnO thin films studied by photo-capacitance measurements — Robert Karstoph, Matthias Schmidt, Holger v. Wencckstern, Rainer Pickelhain, and Marius Grundmann — University of Leipzig, Institute for Experimental Physics II, Linnétralke 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 intrinsic acceptor states or donor states 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°bar 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.

Microstructuring and characterization of Cu2O/ZnO heterostructures — Sören Zint, Julian Benz, Achim Kroenenger, 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 (Cu2O) is a promising candidate for photovoltaic applications due to its direct band gap in the visible spectral range. Moreover, Cu2O can be a non toxic and sustainable material. Thin Cu2O films can be deposited on different substrates by sputtering. Since the production of n-type Cu2O is a difficult task, ZnO can be employed for fabricating a p-n-junction. We report on the growth of lateral Cu2O/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.
Preparation of donor doped ZnO thin films — Achim Krongenberger, Philipp Schurig, Andreas Lauber, Hauck Metelmans, Jan E. Stehr, Jan Philipps, Benedict Kramm, Angelika Foliy, Detlev M. Hofmann, and Bruno K. Meyer — 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$_x$S$_{1-x}$ 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$_x$S$_{1-x}$ thin films were deposited from a ceramic Zn$_x$S$_{1-x}$ target by radio frequency sputtering on glass, sapphire and semi-insulating Si. The thickness of the films could be adjusted from 100 to 500 nm. From further investigations of Mg diffusion in ZnMgO proper comparison the preparation of many devices (>50) and statistical analysis of contact resistance between P3HT and several electrode materials on flexible substrates, 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.

Disorder Induced Metal-Insulator Transition in Crystalline Ge$_2$Sb$_2$Te$_4$ — Hanno Volker, Theo Siegrist$^{1,2}$, Peter Jost$^{1,2}$, Michael Woda$^{1}$, Philipp Merkeltach$^{1}$, Carl Schloöckmann$^{1}$, and Matthias Wuttig$^{1}$ — 1st Institute of Physics (IA), RWTH Aachen, 52056 Aachen, Germany; 2Department 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 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.

Disorder Induced Metal-Insulator Transition in Crystalline Phase Change Materials. Accepted for publication in Nature Mater.

Statistical analysis of contact resistance between P3HT and several electrode materials on flexible substrates — Arne Hendel, Miriam Hein, 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 challenges 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

Influence of nitrogen on optical properties of zinc oxide using Raman spectroscopy — Christian Reindl, Julian Benz, Thomas Sander, Stefan Lautenschläger, Sebastian Essermann, 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 dopant, ZnO: N layers produced by plasma-enhanced 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.

An EPR investigation of the nitrogen center in ZnO — Jan E. Stehr, Jan Philipps, Benedict Kramm, Angelika Foliy, Detlev M. Hofmann, and Bruno K. Meyer — Physikalisches Institut, Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, 35392 Gießen, Germany

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**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.
face is hydrogen free at high temperatures of T > 900°C in H2 ambient and monohydride terminated after cool down in H2.

**HL 44.75** Tue 18:00 P3

**Density-Functional Investigation of Gallium Phosphide-Silicon Interface**

— **Gabi Steinbach**, **Michael Schreiber**, **Shylle Gemming**1-2, **Henning Dössch**1, and **Thomas Hannappel**2 1Institut für Physik, Technische Universität Chemnitz, D-09107 Chemnitz, Germany 2Institute of Ion Beam Physics and Materials Research, HZ Dresden-Rossendorf, Postfach 51 01 19, D-01341 Dresden, 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 occurring 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 function for both interfaces are observed, revealing the high stability and the low remanent stresses at the GaP-Si interface. Extended studies continue 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 predetermination 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 predetermination. 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 predetermination. In addition, PL signatures for excitation above and below the ZnSe band gap are presented.
Investigation of morphological changes of SrTiO$_3$ surfaces induced by annealing and ion bombardment — Ralph Strohmeier, Juliane Seibt, Florian Hanzig, Tina Niestler, Mandy Kottsch, Hartmut Stöckler, 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 Strohmeier, Hartmut Stöckler, 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 electrical 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$_3$ — Nils Neumann$^1$, Kay Potzger$^2$, Hartmut Stöckler$^2$, Barbara Abendroth$^1$, Ralf Strohmeier$^1$, Robert Zieher$^1$, and Dirk C. Meyer$^1$ — TU Bergakademie Freiberg, Institut für Experimentelle Physik, Leipziger Straße 23, 09596 Freiberg

SrTiO$_3$ single crystal surfaces were 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 $\sim$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 Stöckler, Tilmann Leibsegang$^2$, Matthias Zschornak$^1$, Juliane Seibt$^1$, Florian Hanzig$^1$, and Dirk C. Meyer$^1$ — TU Bergakademie Freiberg, Institut für Experimentelle Physik, Leipziger Straße 23, 09596 Freiberg

— Forschungszentrum Dresden-Rossendorf, Bautzner Landstraße 128, 01328 Dresden, Germany

— Dresden-Rossendorf e.V., Institut für Ionenstrahlphysik und Materialforschung, Bautzner Landstraße 128, 01328 Dresden, Germany

— II. Physikalisches Institut, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

— Forschungszentrum Dresden-Rossendorf, Bautzner Landstr. 400, 01328 Dresden, Germany

Strontium titanate is an anodic 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 valence 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 Amann, Marc Brötzmann, Ulrich Vetter, and Hans Hofäss — 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 heterostructures, 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 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].

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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.


The study of Landé g-factor and effective mass of electrons in GaAs/AlGaAs quantum wells — Martin Etter, Michael Wiesner, Wolfgang-Michael Schulz, Robert Roßbach, Michael Jetter, and Peter Michler — Universität Stuttgart, Allmandring 3, 70569 Stuttgart, Germany

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 GaAs 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 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 performed 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.

Determination of the band offset for the heterostructure ZnO/Cu2O and ZnS/Cu2O via X-Ray Photoelectron Spectroscopy (XPS) — Benedict Kramm, Andreas Lauffer, Achim Kronenberger, Swen Graubern, Daniel Reppin, Alba Schreiber, Philipp Schurig, Angelika Polity, and Bruno K. Meyer — 1. Physikalisches Institut, 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 illumination spectra of the band offset of Cu2O/Cu2O or Cu2O/ZnO heterostructure 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

Photoluminescence studies of top-down Zn1−xMg2xO/ZnO quantum square samples with different dimensions — Martin Fischer¹, Markus Pichota¹, Torsten Henning¹, Alexej Chernikov², Carsten Bornemann³, Nikolaus Schlüters, and Rüdiger Schmidt-Grund¹ — Fachbereich Physik, Universität Leipzig, Marbg, Renthof 5, 35032 Marburg, Germany

Quantum structure samples with lateral lengths from 100 nm to 4 μm were prepared from PAMBE-grown Zn1−xMg2xO/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.

Spectroscopic ellipsometry for process control in PLD growth of ZnO-based nanostructures — Jan Zippel, Elena Hilmer, Markus Piechotka, Daniel Fischer, Renate Fischer-Che, Rüdiger Schmidt-Grund³, Michael Lorenz, and Marius Grundmann³ — Universität Leipzig, Institut für Experimentelle Physik II, Linnestr. 5, 04103 Leipzig — 1. Physikalisches Institut, Universität Gießen, Heinrich-Buff-Ring 16, 35392 Gießen, Germany

We present detailed measurements of the surface condition of typical substrates and the dynamics of growth processes in heterostructures. Process control is a vital part of modern thin film synthesis. We have used in situ spectroscopic ellipsometry (SE) to gain inside into the growth process of several oxides 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 several 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 crys-}

Cavity-photon mode dispersion in 1D confined optically anisotropic microcavities — Christian Sturm, Elena Hilmer, Rüdiger Schmidt-Grund, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Linnestr. 5, 04103 Leipzig — Fachbereich Physik, Universität Gießen, Heinrich-Buff-Ring 16, 35392 Gießen, Germany

Microcavities 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 (cavity modes) 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 microcavity. Thereby we found, that even for a uniaxial c-plane oriented cavity with a birefringence of 3% it is essential to take the anisotropy on the TE-TM splitting 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 microcavity
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/BaTiO₃ interface — Peter Schwinkendorf, Kerstin Brachwitz, Tammu 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 several problems left to be solved. In particular, the interface semiconductor/ferroelectric seems to be the major key to further progress.

The ZnO/BaTiO₃ (BTO) heterostructures were grown by pulsed laser deposition on SrRuO₃ (SRO) covered SrTiO₃ (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 ($g = 3.3 \times 10^{-6}$ S/m) serves as ohmic contact. Due to the high resistivity of the top layer of BaTiO₃ the interface is 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.


** HL 44.92 Tue 18:00 P3 **

** Growth induced structural defects in BaTiO₃:ZnO-heterostructures — Christian Kranert, Tammu 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 (BaTiO₃) and pyroelectric (ZnO) materials, respectively, in heterostructures results in new physical effects which can be used for modulators, sensors and memories. Their fabrication requires epiretal growth processes. We present investigations on the crystal structure of BaTiO₃:ZnO-heterostructures grown by pulsed laser deposition 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) BaTiO₃ layers.

We show that the orientation of BaTiO₃ 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 BaTiO₃ layers exhibit the assembly of a hexagonal impurity phase. Different rotation domains were observed in the top layer (BaTiO₃ on ZnO or vice versa) in agreement with a recent group-theoretical treatment [1].


** HL 44.93 Tue 18:00 P3 **

** Plasma oxidation of Ge(100)-surfaces characterized by MIES, UPS and XPS — Elihard Wegewitz, Sebastian Dahle, Oliver Höpff, Wolfgang Voß, Frank Endres, and Wolfgang Maus-Friedrichs — Institut für Energieforschung und Physikalische Technologie, Technische Universität Clausthal, Lehninstr. 4, 38678 Clausthal-Zellerfeld, Germany — Institut für Mechanische Verfahrenstechnik, Technische Universität Clausthal, Arnold-Sommerfeld-Str. 6, 38678 Clausthal-Zellerfeld, Germany — HAWK Göttingen, Fakultät Naturwissenschaften und Technik, Voss-Ossietzky-Str. 99, 37085 Göttingen, Germany **

Cleaning and passivation of Germanium surfaces is of tremendous technical importance. 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 29.76 kV decelerating voltage. After 20 h plasma treatment result in contamination free GeOₓ 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. Wierck — 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 microscopy. 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 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 Kronberger, Angelika Polity, and Bruno K. Meyer — I. Physikalisches Institut, Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, 35392 Gießen, Germany **

Cuprite (Cu₂O) and tenorite (CuO) are two well known phases of copper oxide. A metastable copper oxide, paracelsolomel (Cu₄O₃), is another phase of copper oxide which has been rarely studied. CuO is a p-type semiconductor which has many applications such as solar cells, sensors and lithium ion batteries. In this study CuO and Cu₄O₃ 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 Cu₄O₃ 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 Mettmann, Andreas Lauper, Daniel Reppin, Swen Graubner, Angelika Polity, Bruno K. Meyer, Sebastian Geburt, and Carsten Ronning **

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 to the fact that the chemical identity can be directly determined without considerations of ionisation state or binding energy. The quantification of SIMS data requires the usage of so called relative sensitivity factors (RSF) 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 the first time. Using it to determine impurities, 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 **

** Strukturundelektrische Eigenschaften von PLD-gezüchteten Zinkferrit-Dünnfilmen — Katja Mekner, Matthias Wagner, Rainer Schier, and Hans-Jürgen Tempel — Universität Leipzig, Semiconductor Physics Group, Institut für Experimentelle Physik II, Leipzig, Germany **

The quantification of SIMS data requires the usage of so called relative sensitivity factors (RSF). Finally, these RSFs have been used to investigate impurities in various Cu₂O layers.
Sputtering of ZnO by a modified Radio-Frequency Ion Thruster (RIT) as Ion-Beam-Sputter-Source — Mitin Becker, Angelika Polity, Darar 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.

Electrical and structural properties of Zn-Co-O thin films — Friedrich Schuen, Holger Hochmuth, Holger Von Wencs, Michael Lorenz, and Marius Grundmann — Universität Leipzig, Fakultät für Physik und Geowissenschaften, Institut für Experimentelle Physik II, Linnestr. 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 ZnM2O4 (M = Co, Rh, Ir) [1]. They can be fabricated near and at room temperature; for ZnRh2O4 [2] and ZnCo2O4 [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 (≈ 200°C) are polycrystalline and exhibit σ up to 185 cm2/Vs whereas room temperature fabrication reveals X-ray-amorphous films having σ = 6.8 S/cm.


Photoinduced absorption spectroscopy of poly(3-hexylthiophene):fullerene solar cells — Ralph Huber, Elizabeh von Hauff, and Jürgen Parisi — University of Oldenburg, Department of Physics, Energy and Semiconductor Research Laboratory, Carl-von-Ossietzky Str. 9-11, 28334 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 the excitation pulse to investigate the electronic and vibronic transitions in the excited state.
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 transmissive manner (probe beam). The change in absorption for different wavelengths can be used to identify excited states like excitons or free charge carriers. Muhsin and Modules

Lock-In Thermography Investigation of Polymer Solar Cells and Modules — ∙Maik Bareisklau, Roland Rösch, Burhan Muhisen, Marco Sierland, 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 quality 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.

Electric field induced excitation and charge transfer dissociation — ∙Sebastian Schwab, Julia Kern, Carsten Diebel, and Vladmir Dyakonov, 1,2 — Experimental Physics VI, Faculty of Physics and Astronomy, Julius-Maximilians-University of Würzburg, D-97074 Würzburg — 2ZAE 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 electron–hole pairmechanisms in PENTFT at different temperature ranges. Financial support by BMBF (project GREKOS) is gratefully acknowledged. [1] H. Klauk, et al., Nature 445 (2007) 745

Enhancement of the photocurrent in Diindenoperylene based organic photovoltaic cells — ∙Thermo Gerlich, Alexander Forbrig, David Cheyns, Paul Heremans, Carsten Diebel, and Vladmir Dyakonov, 1,2 — Experimental Physics VI, Physical Faculty, Julius-Maximilians University of Würzburg, D-97074 Würzburg — 1IMEC v.z.w., Kapeldreef 57, 3001 Leuven, Belgium — 2Bavarian 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. 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.

Characterization Of Pentacene-Based Organic Field-Effect Transistors With SAM-Functionalized Gates — ∙Nils Hauke Hansen, Sebastian Röding, and Jens Pflaum, 1,2 — Inst. Exp. Phys. VI, Julius-Maximilians-University, 97074 Würzburg — 2ZAE Bayern, 97074 Würzburg

In order to design low-voltage organic thin film transistors, ultrathin self-assembled monolayer (SAM) gate dielectrics have been proven of particular technological importance. In this work we investigate the bound on aluminomolybdate 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

Optical properties of pentacene layers on zinc oxide — ∙Nis Hauke Hansen, Sebastian Röding, and Jens Pflaum — ZAE Bayern, Zentrum für Anwendungsorientierte Mikro- und Nanoelektronik, Helmholtz-Zentrum München, München; 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-pentacene 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 is observed a thickness dependence of the exciton energies. This leads most likely to a tensioning of the thin films and a relaxation of the lattice constants, but also the angle between the molecules changes, while cooling them down.

**Single Molecule Current Sensors** — Maximilian Nothof, Steffen Höhla, Frieder Jelezko, Jens Pfalum, and Jörg Wrachtrup

In this study we present our results on nanometer scale current sensing using photoluminescence quenching of single fluorescent dye molecules. From X-ray diffraction and electron microscopy 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.

**Structural properties of thin films of organic charge transfer complexes** — Diana Nanová, Sebastian Beck, Milan Alt, and Michael Kröger

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 of the CT-compounds depends on the degree of charge transfer. Mixing two CT-complexes at different concentrations by sublimation and growth 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

**Time resolved Spectroscopy on different organic polymer/fullerene blends** — Berthold Jäckel, Björn Geseking, Carsten Deibel, and Vladimir Dyakonov

One main topic for highly efficient organic bulk-heterojunction solar cells is the spatial and energetic disorder on these dynamics were examined. 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 absorbance 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.

**Spectrally Resolved Transient Absorption in Polymer/Fullerene Blend Films** — Andreas Kämpfe, Julien Gorenflo, Carsten Deibel, and Vladimir Dyakonov

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 absorbance 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.

**Structural analysis of homoepitaxial grown surface structures on rubrene single crystals** — T. Schmeißer, R. J. Stöhr, J. Wrachtrup, and J. Pfalum

In this work we focus on the influence of the solution-processed bottom-contact pentacene and rubrene thin film transistors and rubrene/thin film transistors. The devices are 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 ambient atmosphere is considerable reduced (25% within 552 hours). The shift of the threshold voltage vs. time demonstrates that the absorption of H2O on the pentacene layer is the main reason for the reduced stability of devices stored under ambient conditions.

**Influence of silanization on the stability of rubrene single crystals** — Teodor Toader, Claudia Bock, and Ulrich Kunze

In this work we focus on the influence of the solution-processed bottom-contact pentacene and rubrene thin film transistors and rubrene/thin film transistors. The devices are 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 ambient atmosphere is considerable reduced (25% within 552 hours). The shift of the threshold voltage vs. time demonstrates that the absorption of H2O on the pentacene layer is the main reason for the reduced stability of devices stored under ambient conditions.
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

**Semiconductor Physics Division (HL)**

**Time:** Wednesday 10:15–13:30  
**Location:** FOE Anorg

**Photocative AFM-Measurements to prove the Meyer-Neldel rule in C60 films** — **Astrod Wachauer**, **Igor Brink**, **Markus Kratz**, **Muheeb Ullah**, **Helmut Sittich**, **Andrej Kadashchuk**, and **Christian Tischler** — 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 observed that the MNR for the temperature dependencies of the charge carrier mobility is fulfilled upon varying the charge carrier concentration in organic semiconductors [1]. In this study, we applied Photocative Atomic Force Microscopy (PC-AFM) in order to investigate the temperature dependence of the photocurrent in C60 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 C60 including almost nonconductive grains. Supported by Austrian Science Fund (FWF) NFN projects S9706-N20, S9707-N20 and P19636.

**Solution processed bulk heterojunction solar cells with molecularly doped active layers** — **Antonietta De Sio**, **Ali Veyssel Tunc**, **Elisabeth von Hauff**, **Felix Desclins**, **Enrico Da Cunha**, and **Jürgen Paris** — 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 polymeric poly[4,4′-(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 polymer devices increase with the doping concentration as a result of an enhancement of the field effect mobilities.

**Semiconductor Physics Division (HL)**

**Time:** Wednesday 10:15–13:30  
**Location:** FOE Anorg

**Investigation of ZnO interlayer and different substrates for dye-sensitized ZnO/polymer hybrid solar cells** — **Julia Waltermann**, **Kai-Michael Günther**, **Stefan Kontermann**, and **Wolfgang Schade** — 1 Clausthal University of Technology, EFZ, EnergieCampus, Am Stollen 19, 38640 Goslar — 2 Fraunhofer Heinrich-Hertz-Institute, EnergieCampus, Am Stollen 19, 38640 Goslar

Dye-sensitized solar cells composed of a 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 thick 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, PTO or aluminium doped zinc oxide (ZnO:Al)) are combined with ZnO layers prepared either by magnetron sputtering or by a sol-gel method. The samples are compared regarding surface topography, resistivity and possible build-up Schottky barriers.

**Semiconductor Physics Division (HL)**

**Time:** Wednesday 10:15–13:30  
**Location:** FOE Anorg

**Charge transfer state investigations in organic semiconductors** — **Oliver Schade**, **Eduard Preis**, and **Helmut Sitter** — 1 Physics VI, Faculty of Physics and Astronomy, Julius-Maximilians-Universität 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 Kästner1, Burhan Mursin1, Adam Getachew2, Christoph Ulbricht2, Özlem Usluer2, Daniel Ayuk Mbi Egbe1, and Harald Hoppe1,2 — Institute of Physics, Ilmenau University of Technology, Ilmenau, Germany — 2Linz 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=CH-Ph-CH-dCH-Ph-CH-dCH-)n have been studied. Linear and branched alkylo 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 structure with PCBM as acceptor.

HL 46.4 Wed 11:00 FOE Anorg Morphological aspects of the exciton transport in molecular thin films — A.K. Topczak1, T. Rollern2, and J. Pflaum1,3 — 1Inst. Exp. Phys. VI, Würzburg University, 97074 Würzburg — 23rd Phys. Inst., Stuttgart University, 70550 Stuttgart — 3ZAE 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 (6T), and tris-8-hydroxyquinolinate-aluminium (Alq3) 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 6T show a high EDL. For these films the necessity of taking interferences effects into account for a precise modelling became evident. In comparison, amorphous films of Alq3 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. Kurre, J. Pflaum, Appl. Phys. Lett. 92 (2008) 133506

HL 46.5 Wed 11:15 FOE Anorg Electronic Trap States in Methanofullerenes and their Influence on Organic Solar Cells — Ulrich Blakesley1,2, Sven Kurrle1, Dieter Neher1, Harald Hoppe1,2, Christoph Deibel3, and Vladimir Dyakonov1,2 — 1Experimental Physics VI, Physical Institute, Julius-Maximilians University of Würzburg, Am Hubland, D-97074 Würzburg — 2Bavarian 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. It has not been clear yet whether 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 this group of materials have not been comprehensively studied before.

We investigated the trap states of three commonly used fullerene derivatives, namely PC71BM, PC71BM and (z-bisPCBM), by thermally stimulated current measurements. Each of the studied methanofullerenes exhibits a broad trap distribution, whereby the PC71BM and bisPCBM reveal significantly deeper traps compared to PCBM. 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 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 illumination. 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 carriers in bulk heterojunction solar cells lead to free charge carriers in holes, 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 J.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 bi-molecular recombination of free carriers is strongly suppressed in phase-separated P3HT:PCBM 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 Gorenflo1, Matthias Gunz2, and Andreas Kampf2, — 1A.K. Topczak, 2Matthias Gunz, and Roland Rösch

The exciton diffusion length is a key criteria to optimized design of 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 illumination. Finally the local nature of this description enables important conclusions concerning the geometry dependent performance of thin film solar cells.
Jens Lohrmann, Carsten Deibel, and Vladimir Dyakonov — 1Experimental Physics VI, Julius-Maximilians University, D-97074 Würzburg — 2Bavarian 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 unavoidable 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 Mingeback**1, Carsten Deibel1, and Vladimir Dyakonov1,2 — 1Experimental Physics VI, Physical Institute, Julius-Maximilians-University of Würzburg, Am Hubland, D-97074 Würzburg — 2Bavarian Center for 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-C61 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 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).

**HL 46.11 Wed 13:00 FOE Anorg Charge Transport and Recombination Dynamics in Oxygen Exposed P3HT:PCBM Bulk Heterojunction Solar Cells**

— **Alexander Fobretig1, Andreas Baumann1, Julia Schaffernanz1, Carsten Deibel1, and Vladimir Dyakonov1,2** — 1Experimental Physics VI, Physical Institute, Julius-Maximilians-University of Würzburg, Am Hubland, D-97074 Würzburg — 2Bavarian Center 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-C61 butyric acid methyl ester (PCBM) bulk heterojunction solar cells was studied using the complementary measurement techniques of (photo-generated) 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 47: GaN on Si**

Time: Wednesday 10:15–11:30

**HL 47.1 Wed 10:15 POT 51 Kathodolumineszenzuntersuchungen an GaN auf Si(211)- und Si(311)-Substraten**

— **Mathias Möller**, Anja Dempe-wolf, Frank Bertram, Thomas Hempel, Jürgen Christen, Rohgaiyeh Ravash, Armin Dadgar und Alois Krost — Institut für Experimentelle Physik, Otto-von-Guericke-Universität Magdeburg, Deutschland

Mittels spektoral 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 quanten confinied staten effect (QCSE), welcher die Effizienz von optoelektronischen Bauelementen herabsetzt. Hierzu wurden systematisch geeignete hoch indizierter Si(h11)-Substrate benutzt, auf denen mittels MOVPE jeweils eine AIN-Keimschicht sowie eine AIGaN-Pufferschicht gewachsen wurden. Gefolgt von einer C-Achsen GaN-Schicht, welche durch eine AIN-Zwischenschicht unterbrochen sind. Ortsintegrale Spektren zeigen bei tiefen Temperaturen drei dominante Lumineszenzkanäle: das gebun-dene Exiziton (D2X), Donator-Akzeptor-Paarbande DAP sowie Basalflächenstepfellerlumineszenz BSF. Auf Si(211) ist die Stepfellerlumineszenz 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) ei-ne starke Inhomogenität im Vergleich zu Si(211) aufweist.

**HL 47.2 Wed 10:30 POT 51 Semi-polar GaN heteroepitaxy on high index Si-surfaces**


Due to the lack of GaN homosubstrates, the growth of GaN-based devices is usually performed on heterostructures 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 three-fold symmetry of Si(111) greatly promotes the c-axis oriented growth of GaN on this surface plane. A large spontaneous and piezoelectric polarization oriented along the c-axis exists in such hexagonal struc-ture 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 AIN seeding layer growth time play a significant role...
Spatially resolved cathodoluminescence spectroscopy of InGaN/GaN heterostructures on m-plane GaN grown on patterned Si (112) substrates — Christoph Karbaum, Frank Bertham, Sebastian Metzener, Jürgen Christen, Xianfeng Ni, Natalia Izyumskaya, Vitaliy Avrutin, Umit Özgür, and Hadis Moroko — Institute of Experimental Physics, Otto-von-Guericke-University Magdeburg, Germany — 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 (11-11) 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 SiO₂. The lateral and vertical epitaxial growth of GaN was initiated at the (11-11) Si sidewalls resulting in a partially coalesced m-plane surface. Finally, an InGaN layer capped with p-GaN was deposited. The GaN (D³X) emission observed from the c-wings 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 BSEPs on lifetimes of (D³X) and InGaN emissions will be discussed.

Monitoring the influence of interlayer thickness and Si doping on the stress behaviour of GaN grown on Si(111) — E. Fritze, J. Blassing, P. Drechsel, A. Dadgar, and A. Kroost — Institute of Experimental Physics, Otto-von-Guericke-University Magdeburg, Magdeburg, Germany — 2OSRAM Opto Semiconductors, Leibnizstraße 4, 99055 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 nm 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. Additionally 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 1·10¹⁸ cm⁻³ and 4·10¹⁸ cm⁻³ a wafer bow as low as 2.9 μm can be achieved using an optimized interlayer thickness.

Investigations of pn-junctions based on AlGaN / AlN structures for LEDs on Si(111) — Antje Rohrbeck, Hartmut Witte, Phanhee Sängkaew, Thomas Fuy, Armin Dadgar, Jürgen Christen, and Alois Krooss — Institute 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 mismatch 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 multi-layer 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 multi-layer 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.


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, SnO₂ 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 Ag₂O, PtO₂ and Au. A strong dependence of the dynamic properties on the gate material was observed. The usage of Ag₂O results in delayed response of the source-drain current even for frequencies below 1 kHz. For PtO₂ and Au absence of such an effect was observed up to 1 MHz. We attribute this difference to the diffusion of Ag into the channel material during device fabrication.

Covalent functionalization of ZnO nanowires — Andrea da Rosa, N. Moreira, and T. 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 two relevant mechanisms for surface stabilization: passivation of surface oxygen lone-pairs via dissociative chemisorption processes, electrostatic adsorbate-interactions 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.

Optical spin orientation by linearly polarized light in ZnO — Vera Klinkle, Christoph Schwarz, Christian Weier, Gernot Güntherodt, Matthias Althammer, Sebastian T.B. Goennenwein, Matthias Opel, Rudolf Gross, and Bernd Beschoten — Physikalisches Institut II A, RWTH Aachen University, D-52056 Aachen, 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 intentionally doped ZnO samples. For laser excitation energies far below the band gap, we can resonantly spin-polarize donor bound excitons with p-GaN/n-ZnO heterostructures.

Piezoelectric properties of ZnO-based microstructures — Christina A. Forbe, Irina Laubenstein, Marcel Ruth, Manuel H. W. Bader, Alexander M. Berkhemer, Mark R. Kaspers, Christian A. Bohschi, Rolf Moeller, and Cedric Meier — University of Paderborn, Experimental Physics & CeO²PP, Warburger Str. 100, 33108 Paderborn — 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 Zn1-xMgₓO-microstructures with different Mg concentrations in comparison to binary ZnO-microstructures. For these experiments Zn1-xMgxO-based microstructure devices have been fabricated on hydrothermally grown ZnO samples as well as on (Zn,Mg)O-eplayers 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
Semiconductor Physics Division (HL)

Optical Gain in Rolled-up Semiconductor/Metal Metamaterials

Detlef Heitmann, Matthias Klingbeil, Armin 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 magnetostriective material on a microscopic scale allows the creation of magnetoelectric (ME) composites with a very high ME effect. For magnetic fields, the 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 electrical properties and it will be shown how reliable conductivity measurements can give a hint on the quality of the obtained structures.

Electrical properties of 1D to 3D ZnO nanostructures synthesized by flame transport synthesis approach

Armin 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-organized 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 organized 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.

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.

Photonic Crystals and Metamaterials

HL 49.1 Wed 10:15 POT 251

Optical Gain in Rolled-up Semiconductor/Metal Metamaterials

Stephan Schafer, Markus Broell, Ricardo Costa, Matthias Klingbeil, Aune Koitmae, Wolfgang Hansen, Detlef Heitmann, and Stephan 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 photoluminescence by a Lorentz oscillator.

HL 49.2 Wed 10:30 POT 251

Calculation of Transmission through rolled-up three dimensional Metamaterials

Andreas Rottler, Stephan Schafer, Aune Koitmae, Matthias Klingbeil, Markus Broell, 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 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.

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 (TFF) 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. Purposefully 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 circuits (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 nanorings — Thomas Weiss1,2, Nikolay A. Gippius3,4, Sergey G. Tkhostov5, Gérard Granet6, Liwei Fu7, Richard Tauber7, and Harald Giessen1 — 1 Ith Physics Institute and Research Center Scope, University of Stuttgart, Stuttgart, Germany — 2LASEMA, University Blaise Pascal, Aubière, France — 3 A. M. Prokhorov General Physics Institute, Russian Academy of Sciences, Moscow, Russia

Nanorings have become one of the most important structures in modern nanoptics over the last few years. They can be used in different fields such as photonic circuits and nanophotonic devices. 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 nanorings 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

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/a-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 present the first fully integrated 3D photonic thin-film IRL device. This device is integrated 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 Wagner1, Lars Heerklotz2, and Frank Cichos2 — 1Molecular Nanophotonics, University of Leipzig, Germany — 2Photonic 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 distributed as compared to a homogeneous material and is described by the fractional local density of states (FLODoS). 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 FLODoS, 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 — Hoon Seng Lee1, Alexander Petrov2, Manfred Eich1, Roman Kubin2, Gerold Scheiderer3, Julien Bachmann3, and Korinelis Niehsch3 — 1Institut für Optische und Elektronische Materialien, TUHH, Hamburg, Deutschland — 2Institut für keramische Hochleistungswerkstoffe, TUHH, Hamburg, Deutschland — 3Institut für Angewandte Physik, Uni Hamburg, Hamburg, Deutschland

The study is undertaken to develop 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 benefit most from this study are ceramic thermal barrier coatings (TBC) and selective filters for thermopiles (TPV). Finite Integration Technique (FIT) simulations have shown that ytrria 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 wavelength range of 1-6 μm, 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 Kolle1, Peter Vukusic2, and Joanna Aizenberg1 — 1School of Engineering and Applied Sciences, Harvard University, 9 Oxford St, Cambridge, MA-02138, US — 2School 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 nanosstructures that provide outstanding, distinctive, dynamic and tailored coloration and high reflectivity. Various intriguing photonic structures have been identified on the wing scales of 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.
Invited Talk
HL 50.1 Wed 10:30 TRE Ma
Topological insulators and topological superconductors — •SUOCHENG 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 MÖLKENKAMP — 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 MIHRIN — 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.


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 fermions. In this talk, I shall 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 interaction-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 FELSNER1,2, STANISLAV CHADOV1, LUKAS MÜCHLER2, JÜRGEN KÜßLER2, SHOU CHENG ZHANG3, XIANGQING QI1, and HAI-JUN ZHANG3 —
1University Mainz — 2TU Darmstadt — 3Stanford 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 Heuser compounds show band inversion similar to that of HgTe. The new states in these zero-gap semiconductors (LaAuPb, LaPdBi, LnPbSb and LnPbBi) contain the rare-earth element Ln, which can realize additional properties ranging from superconductivity (for example LaPbBi) to magnetism (for example GdPbBi) and heavy fermion behaviour (for example YbPbBi).


Time: Wednesday 11:15–13:00

Invited Talk
HL 51.1 Wed 11:15 TRE Phy
Dynamical magnetic excitations of nanostructures from first-principles — •SAMIR LOUNIS1,2, ANTONIO CORSTA3, ROBERTO MUNIZ1, and DOUGLAS MILLS4 — 1Department of Physics and Astronomy, University of California Irvine, California, 92697 USA — 2Institut für Festkörperforschung and Institut for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — 3Instituto 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.

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Invited Talk
HL 51.2 Wed 11:30 TRE Phy
Magnetic order of LaVO_3/SrVO_3 superlattices — •COSIMA SCHUFERT1, ULRICH LÖPER2, UDOSCHWINGENSCHEL2, and ALLAN SHWINDENSCHULZ2 — 1Institut für Physik, Universität Augsburg, D-86135 Augsburg — 2Laboratoire CRISMAT, UMR CNRS-ENSICAEN(ISMRA) 6508, FR3095 Caen — 3KAUST, PCS3 Divi-
Pion, 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$_3$/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**

Florent Boucher, Mamata Biswal, Monique Body, and Christophe Legen — Institut des matériaux Jean Rouxel (IMN) - Université de Nantes, CNRS, 2 rue de la Houssinière, BP 32229, 44322 Nantes, France

Semiconductor Physics Division (HL) Wednesday

To clarify the magnetic and orbital order in these heterostructures, we established a linear relation between chemical shieldings ($\sigma$) and the calculated isotropic chemical shift ($\delta_{iso}$) 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 $\delta_{iso}$ values with the calculated isotropic chemical shieldings ($\sigma_{iso}$) is needed to interpret of NMR spectra. $^{19}$F $\sigma_{iso}$ values were calculated for alkali, alkaline earth and rare earth of column III B fluoride compounds using the GIPAW method implemented in the CASTEP software. Using DFT-PBE, we have established a linear relation between $^{19}$F calculated $\sigma_{iso}$ and experimental $\delta_{iso}$ 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 — **Andreas Schröng, 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 the realization of quantum ordered magnetic systems. 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. 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 linear ansaemal 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** and Peter M. Oppeneer — Department of Condensed Matter Physics, Charles University, Ke Karlovu 5, CZ-12116 Prague 2, Czech Republic

Here we concentrate on Elliott-Yafet spin relaxation due to electron-phonon scattering at 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).

**References:**


**HL 51.6** Wed 12:30 TRE Phy

Momentum Distribution and Renormalization Factor in Sodium and the Electron Gas — **Valerio Olevano** — Institute 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, it 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 measurement of the renormalization factor, one of the most important quantities in many-body theory, that we compare with GW and quantum Monte Carlo calculations. Both performed on sodium crystalline and on the homogeneous electron gas. Our calculated results are in good agreement with the experiment.

**References:**


**HL 51.7** Wed 12:45 TRE Phy

Construction of low energy Hamiltonians using maximally localized Wannier functions — **Roman Konowicz and Claude Edner** — 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 Hamilton 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 on effective Mn $\epsilon_l$ 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.

**References:**

Si-doped a-plane GaN samples with nominal doping levels up to $10^{20} \text{ cm}^{-3}$ were grown on r-plane substrate by metalorganic vapor phase epitaxy. Silane flow rates higher than those used for c-plane growth lead to the formation of non-polar, non-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 $10^4 \text{ cm}^{-2}$ [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] Wienke et al., Phys. Status Solidi B, 2010, 10.1002/pssb.201046372


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 $10^{20} \text{ cm}^{-3}$ 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.


InGaN quantum well based light emitters grown on (0001) GaN suffer from poor quantum efficiency 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 (1122) GaN layers were deposited by metalorganic vapour phase epitaxy on (1010) 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 (1122) orientation with a small fraction of (1013) oriented domains. With increasing nitridation layer thickness the (1013) phase is suppressed leading to a very smooth surface morphology (rms roughness < 4 nm). PL measurements show dominant basal plane stacking fault (BSF) I 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 (1122) reflection decreases to 1193 arcsec and 739 arcsec along [1100] and [1123] respectively with increasing nucleation temperature. Using high temperature nucleation smooth and homogeneous (1122) phase GaN layers have been obtained.


Polarisation of the spontaneous emission from nonpolar and semipolar InGaN quantum well structures was investigated using PL microscopy on semipolar and non-polar InGaN multiquantum wells grown by MOVPE on planar semipolar (1122) GaN directly grown on pre-patterned r-sapphire substrate by MOVPE. The optical properties of a 5-fold InGaN multiple quantum well (MQW) grown on planar semipolar (1122) GaN directly grown on pre-patterned r-sapphire substrate by MOVPE have been investigated using highly spatially and spectrally resolved cathodoluminescence (CL) microscopy. The sample was masked and structured via RIE generating grooves with c-plane-like sidewalls. The growth of GaN is initiated and striped pattern are formed along the sapphire a-direction. The integral spectrum of the GaN substructure exhibits a dominant (002) emission at 357.4 nm and a weak luminescence at about 361.7 nm related to basal plane stacking faults (BSFs). The DSP-CL was exclusively observed at the c-wings of the spectral profile. The 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-wings exhibits a homogeneous CL distribution without any DSP contribution. The luminescence of the InGaN MQW shows three different emission wavelengths at 425 nm, 445 nm and 470 nm according to surface morphology.


Indium incorporation in GaN quantum wells on various surface orientations was investigated using PL microscopy on semipolar and non-polar InGaN quantum well structures grown by MOVPE on bulk GaN substrates, (HVPE) GaN templates or foreign substrates. 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 GaN 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 (112-plane) is significantly larger which is assigned to a reduction of the strain-induced repulsive interaction between incorporated In atoms on the surface[1].


HL 53: Optical Properties I

Time: Wednesday 12:30–13:30

HL 53.1 Wed 12:30 POT 251
Microscopic theory of phonons in the semiconductor microcavity luminescence — Christian N. Böttger, Thomas Feldmann, 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 stated 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.

Many-body effects in phonon-sideband luminescence — Alexei Chernikov, Verena Bornwasser, Christoph N. Böttger, Thomas Feldmann, Sangam Chatterjee, Martin Künzel, Mackillo Kira, and Konstantin Kellner — Department of Physics and Material Sciences Center, Philipps-University, Renthof 5, D-35032 Marburg, Germany

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 semiconducting 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 53.4 Wed 13:15 POT 251
Quantum-optical correlations in dissipative quantum-dot systems — Martin Moote, Mackillo Kira, and Stephan W. Koch — Department of Physics and Material Sciences Center, Philipps-University Marburg, Renthof 5, D-35032 Marburg, Germany

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 polariton 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 → 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 54: Joint Session: Organic Semiconductors IV: Excitations and Charges

Time: Wednesday 14:00–17:00

Topical Talk

Topical Talk

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/Vs at 1 ps to its stationary value of about 10^{-9} cm^2/Vs 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-

light emission 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.


Light-Emitting Organic Memory — PETER O. KÖNNER, R. CLAYTON SHALLCROSS, VINCENT AUBERT, EDUARD MAIRACH, PHILIP ZACHARIAS, AND KLAUS MERERHOLZ — 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 dithienylethenes (XDTE) that can be optically switched between two energetically degenerate states by an external electric field. The XDTE molecules are isolated from the electrodes by a dielectric barrier, we can identify field induced effects responsible for the observed effects.

These results clarify the role of external electric field induced exciton-quenching on the luminescence efficiency of OLEDs and establish a bases for the understanding of the limiting processes in more complex devices.

Light-Emitting Organic Memory in a Series of CBP-Derivatives — SEBASTIAN HOFFMANN, MARTIN SCHRÖGEL, RODRIGO ALBUCQUEQUE, MICHAEL ROTHMANN, PETER STROHREICH, AND ANNA KÖHLER — Department of Physics, University of Bayreuth, 95440 Bayreuth — 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 to an increased charge transfer character of the intermolecular excited state for the more polar substituents. [1] S.T. Hoffmann et al., Phys. Rev. Lett. 105, (2010) 027404.

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 changes on the luminescence intensity in OLEDs based on 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. 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.

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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) (polythiophene (P3HT, PS)) composite can be greatly improved upon surface doping. Upon exposure to air and using oxidatively 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 cmV−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 α-S 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 Weil
— Heinrich-Damerow Institute for Physics and Science, Jacobs University Bremen, Campus Ring 1, 28759 Bremen
Regio-regular poly(3-ethylthiophene) (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 cm2/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.

HL 54.9 Wed 16:30 ZEU 222
The impact of polar bonds on electron transport through self-assembled monolayers —
●David A. Egger, Ferdinand Rissner1, Egbert Zojer1, and Georg Heimel2 —
1Institute of Solid State Physics, Graz University of Technology, Austria —
2Institut 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-ethynlenedithiols 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 Tobias P. I. Saragi —
Department of Mathematics and Science and Center for Interdisciplinary Nanoscience 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-Lorentzian 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

HL 55.1 Wed 14:30 FOE Anorg
Spectral and angle dependent emission of solar fluorescence collectors —
●Marcio Dyhr1, Katharina Baumgartner2, Reinhard Carus2, Paul-Tiburu Miclea3,4, and Stefan Schweizer3,5 —
1Centre for Innovation Competence StLi-nano, 2Martin Luther University of Halle-Wittenberg, Karl-Friedrich-von-Frisch-Str. 3, 06120 Halle (Saale) — 2Institut für Energieforschung 5 (Photovoltaics), Forschungszentrum Jülich GmbH, 52425 Jülich — 3Fraunhofer Center for Silicon Photovoltaics, Walter-Hübel-Str. 1, 06120 Halle (Saale) — 4Institute 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 Sm3+ 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 bonding composition of borates glasses consists of the network former boron oxide and metal oxides as network modifiers. The system can easily be doped with Sm3+ ions. However, the spectroscopic properties of Sm3+, 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
Light scattering by rough surfaces for increase of absorption

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 particulate scattering media. We have formulated analytically and described wave numbers of the topological surface contour \( k \) 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 diffuser. We have distinguished two regimes: i) \( k_s < k \), in which we apply a ray tracing approach with respect to Snellius’ Law for photon propagation at phase border between different media, and ii) \( k_s > k \), where the propagation of photons after scattering has been formulated on Huggens' 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 \( \beta \). In particular for the wave optical approach we find a "scattering function" that contains the contour function \( h(x,y) \) however that substantially departs from its puristic Fourier Transform.

Silver nanoparticles for enhanced light absorption in thin film amorphous silicon solar cells — Florian LÖKERMANN1, Frank HAMELMANN2, Helmut STEHRING2, and Ulrich HEINZMANN1 — Institute of Physics, Bielefeld University, 33615 Bielefeld, Germany — 1Malibu 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 wave-length 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 metal particles. In particular for the wave optical approach we find a "scattering function" that contains the contour function \( h(x,y) \) however that substantially departs from its puristic Fourier Transform.

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 an absorption coefficient of 0. In particular for the wave optical approach we find a "scattering function" that contains the contour function \( h(x,y) \) however that substantially departs from its puristic Fourier Transform.

Conformal Al doped ZnO on rough silicon surfaces — Martin OTTO1, Matthias KROLL2, Thomas KAISER2, Roland SALZER2, Paul T. MICLEA1, and Ralf B. WEHRSPRUNG1,3 — Martin-Luther-University Halle-Wittenberg, µMD Group - Institute of Physics, Heinrich Damerow Str. 4, 06120 Halle, Germany — 2Friedrich-Schiller-University Jena, Institute for Applied Physics, Max-Wien-Platz 1, 07743 Jena, Germany — 3Fraunhofer 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 · 10^{-5}Ωcm. An absorption enhancement of nearly a factor of 10 at a wavelength of 1150 nm compared to a simulated perfect ARC was observed.

ConformalCharacterisation of sputtered ZnO:Al TCO-layers on float glass produced by large ceramic and metallic targets — Sebastian WOSSNER1, Hartmut WITTE1, Fahri Uslu2, Jörg GÜNTHER2, Jürgen BLASING1, Martin BÄH2, and Alois KROST3 — 1Institut für Experimentelle Physik, Otto-von-Guericke-Universität Magdeburg — 2Euroglas 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:Al2O3 targets is one of the commonly used processes to produce ZnO-layers on float glass. Disadvantages are the fixed stoichiometric proportions and the high tem-perature required for the sputtering process.

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 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
Serial interconnection of thin film solar cells by laser ablation requires overlap and laser fluence for different photovoltaic materials used for semiconductor physics division (HL) Wednesday
Berlin, Germany
und Nanotechnologie für Photovoltaik Berlin, Schwarzschildstr. 3, 12489 Berlin, Germany
Numerical simulations for the efficiency improvement of hybrid dye-microcrystalline silicon pin-solar cells — ●SEVEN BURDORF,
GOTTFRIED HEINRICH BAUER, and RUDOLF BRÜGGEMANN — Институт
für Physik, Carl von Ossietzky Universität Oldenburg, Germany
Hybrid solar cells consisting of dye sensitizers incorporated in the
layer of microcrystalline silicon pin solar cell have been proposed and
even recently processed [1,2]. The dye sensitizer molecules are embed-
ded 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 trans-
port 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 efficiency improvement of
hybrid dye-microcrystalline solar cells compared to pure microcrystalline
solar cells by simulation. The results indicate that, under optimal con-
ditions, the efficiency can be improved by more than 20 % compared to
a pure microcrystalline silicon cell. The thickness reduction for the hy-
brid system can be as large as 50 % for the same efficiency. [1] T. Mayer,
U. Weiler, C. Kelling, D. Schlettwein, S. Makarov, D. Wöhrle, O. Ab-
dallah, M. Kunst and W. Jaegermann 2007 Solar Energy Materials and
Jaegermann, C. Kelling, 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 — ●BÖRN GEHERING1, BERTHOLD JACK1, CARSTEN DEHR1, and VLADIMIR DYAKONOV1,2 — 11Experimental Physics VI, Faculty of Physics and Astronomy, Julius- Maximalmians-University Würzburg, D-97074 Würzburg — 22Bavarian Centre for Applied Energy Research (ZAE Bayern), D-97074 Würzburg

Defect and charge transfer studies on hybrid solar cells with silicon nanocrystals — ●SABRINA NIESAM1, DANIEL HERRMANN2, WOLFGANG FABIAN1, NADINE EHRAH1, ANDRE STEGRE1, RUI PEBREIRA1, HARTMUT WUGGER5, MARTIN BRANDT2, EBERHARD RIEDE2, and MARTIN STUTTMANN3 — 3Walter Schottky Insti-
tut, Technische Universität München, 85748 Garching — 2Ludwig-
Maximilians-Universität München, 80538 München — 3University of Áviero, 3810-193 Áviero, Portugal — 4Institut für Verbrennung und Gasdynamik, Universität Duisburg-Essen, 47057 Duisburg

Hybrid inorganic nanoparticle-polymer solar cells are a promising al-
ternative 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

Invited Talk

Time: Wednesday 14:30-15:00

Location: POT 51

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 ma-
terial reorganization during the capping is observed, which determines mostly the quantum dot structure [1]. In the InAs/InGaAsP/InP sys-
tem the influence of the quaternary separation layers on the quantum
dash stacking and the strain field is demonstrated [2]. During sub-
monolayer InAs/GaAs growth quantum dot like structures form [3].
Express 3, 105602 (2010).
HL 57: ZnO: Optical Properties

Time: Wednesday 14:30–15:30
Location: 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, Slowa Schmidt, Martin Silles, 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.

Low-temperature dielectric tensor of MgZnO thin films and ZnO single crystals — •DAVID SCHUMACHER, RUDIGER SCHMIDT-GROGHD, HELENA HILMER, CHRIS STURM, HOLGER HOCHMUTH, MICHAEL LORENZ, and MARIUS GRUNDMANN — Universität Leipzig, Institut für Experimentelle Physik II, Limesstr. 5, Leipzig, Germany

We determined the temperature evolution of the spin-orbit interaction and crystal field splitting energies in a-plane MgZn1−xO (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 bandgap 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 was 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, Δ0 and Δf, 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 BECKER1,2, BERNHARD LAUMER1,2, FABIAN SCHUSTER1, MARTIN EICKHOF3,4, and DETLEV M. HOFMANN1,5,6 — 1 Physikalisches Institut, Justus-Liebig-Universität Giessen, Heinrich-Buff-Ring 16, D-35392 Giessen, 2 Walter Schottky Institut, Technische Universität München, Am Coulombwall 4, D-85748 Garching, 3 Institut für Physik, Technische Universität Ilmenau, 98693 Ilmenau, Germany, 4 Institute of Solid State Physics, Faculty of Science, University of Tokyo, Tokyo 113-8656, Japan, 5 Institute of Nanotechnology, Fraunhofer IAF, 76344 Freiburg, Germany, 6 Department of Physics and Material Sciences Center, Philipps-Universität Marburg, Renthof 5, D-35032 Marburg

ZnO quantum wells embedded in Zn(1−x)MgO 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

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.
Coherent optoelectronic control of a single exciton qubit


University of Paderborn, D-33095 Paderborn — Joint Quantum Institute, NIST & University of Maryland, Gaithersburg, MD USA

Due to their excellent coupling to light, excitons in semiconductor quantum dots (QDs) has been of major interest both for fundamental studies as well as for applications in the field of coherent optoelectronics. Novel 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 and potential-controlled pyramidal quantum dots have been shown to be highly indistinguishable, mutually indistinguishable photons from separate QDs have only recently been produced [1]. We use strain-induced InAs QDs excited by a common pulsed laser. One QD is embedded in a planar 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. Phase shifts of up to π 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, such as single photons, bunched photons and entangled photons, using semiconductor quantum dots (QDs) has been of major interest both for fundamental studies as well as for applications in the field of quantum information processing. Here we report progress in generating (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 photon-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**, **Anthony Bennett**, **Mark Stevenson**, **Cameron Salters**, **Raj Pathe**, **Ian Farrer**, **Christine Nicola**, and **David Ritchie**

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 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.
Semiconductor Physics Division (HL)

Wednesday

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 GÖPFERT1, LUKAS WORSCHECH1, STEPHAN LINGEMANN1, CHRISTIAN SCHNEIDER1, DAVID PRESS2, SVN HÖFLING3, and ALFRED FORCHL4. — 1Technische Physik, Physikalisches Institut, Universität Heidelberg, Philosophenweg 16, 69120 Heidelberg, Germany; 2Stanford 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.


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 MARQUARDT1, MARTIN GELLER1, ANDREAS BECKER1, BENJAMIN BAXEVANIS2, DANIELA FPANKUCHI2, ANDREAS D. WIECK3, DIRK REUTER4, and AXEL LORKE3. — 1Faculty of Physics and CE.NIDE, University of Duisburg-Essen, Germany; 2Institut für Theoretische Physik, Universität Hamburg, Hamburg, Germany; 3Chair 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.


HL 60.3 Wed 15:30 POT 251
Quantum dot memories based on antimony — •TOMAS NOWOZIN, ANNKA HÖGNER, ANDREAS MARENT, ANDREI SCHILWA, 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/SiO2-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 electron 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 KATSAROS1, NATALIA ARES1, PANAY OTIS SPATHIS2, MATTHIEU STOFFEL2, FRANK FROWNIE3, Massimo Mongillo1, VINCENzo BOUCHAR4, FRANCOIS LEFOCH3, ARMANDO RASTELLI2, OLIVER G. SCHMIDT2, and SIILVANO DE FRANCESCHI1. — 1CEA, INAC/SP5MS/LatEaQS, 17 Rue des Martyrs, 38054 Grenoble, France; 2IFW-Dresden, Institute for Integrative Nanosciences, Helmholtzstrasse 20, 01069 Dresden, Germany; 3CEA, LETI, MINATEC, F38054 Grenoble, France; 4Institut Neel, 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).


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 interference 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 lapes, 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.


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 100 or more particles. The discussion of the methodology will be illustrated by recent applications to atoms, molecules and extended systems. 

We use localized trial functions. We consider here the Finite Element method as a new approach to solve these Hartree-Fock equations. We will present numerical results about different electronic systems: such as different advantages and drawbacks involved by this strategy. We will discuss the methods of the optimization of the potential within the FLAPW method and how the problem of undetermined phases of the Green function of the single-particle Kohn-Sham equation and has been implemented within the 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.

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.

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. Blaha et al., Phys. Rev. B 82, 164148 (2010). [2] V. Blum et al., Comp. Phys. Comm. 180, 2175 (2009).

We 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, which introduces errors to the semi-local exchange-correlation functionals. 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).
Semiconductor Physics Division (HL) Wednesday

HL 62.1 Wed 15:15 POT 51
Temperature dependent microscopic energy relaxation in semipolar InGaN SQW imaged by nano-spectrally-time-resolved cathodoluminescence — Sebastian Metzner1, Frank Berthlam1, Jürgen Christen1, Thomas Wunderle2,3, Frank Lipski4, Stephan Schweiker5, and Ferdinand Scholz7 — 1Inst. of Exp. Physics, OvG-University Magdeburg — 2Inst. of Optoelectronics, Ulm University — 3Palo 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 SiO2 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, recombinination 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 Danhof1,2, Ulrich T. Schwarz1, Yojichi Kawakami3, and Akio Kaneta3 — 1Fraunhofer IAF, Tüllastr. 72, 79108 Freiburg, Germany — 2Institut für Mikrosystemtechnik, Georgs-Kühler-Allee 106, 79110 Freiburg, Germany — 3Kyoto University, Katsura Campus, Nishikyo-ku, Kyoto, 615-2112, 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 Mehltens1, Stephanie Bley1, Marco Schowalter1, Kathrin Sebald1, Mortiz Sevrey1, Jürgen Gutowsky1, Stephan S.A. Gerstl2, Pyung-Pa Choi3, Dirk Raabe2, Adrian Avramescu3, and Andreas Rosenauer1 — 1Institut für Festkörperphysik, Universität Bremen, Bremen — 2Max-Planck-Institut für Eisenforschung, GmbH, Düsseldorf — 3OSRAM 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 investigated an InGaN/GaN multi quantum well 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 $\mu$-photoluminescence measurements.

HL 62.4 Wed 16:00 POT 51
Liquid He Temperature Cathodoluminescence Spectroscopy in a Scanning Transmission Electron Microscope — Gordon Schmidt, Barbara Basteck, 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 (STEM (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 dI/dE field signal image 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 Pfeiffer, 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 homoeptaxial AIN layers in magnetic fields — Benjamin Neuschl1, Martin Feneberg1, Klaus Thonke1, Ramon Collazo2, and Zlatko Sitara2 — 1Institut für Quantenmaterie / Gruppe Halbleiterphysik, Universität Ulm, 89069 Ulm, Germany — 2Department of Materials Science and Engineering, North Carolina State University, Raleigh, North Carolina, USA
We present optical emission spectroscopy studies on high quality c-plane AIN 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.
Semiconductor Physics Division (HL) Wednesday

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$_x$Zn$_{1-x}$Se. — Daniel Mourad$^1$, Gerda Czycholl$^1$, Carsten Kruse$^2$, Sebastian Klempt$^2$, Reiner Retzlaff$^2$, Detlef Hommel$^2$, Maruca Garten$^3$, and Mikhail Anastassescu$^3$

1 Institute für Theoretische Physik, Universität Bremen — 2 Institut für Festkörperphysik, Universität Bremen — 3 Institut für Physikalische Chemie Ilie Margulescu, Rumanische Akademie

Compound semiconductor alloys of the type A$_x$B$_{1-x}$C$_y$find widespread applications as their electronic bulk band gap varies continuously with $x$, and therefore a tailoring 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$_x$Zn$_{1-x}$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$_x$Zn$_{1-x}$Se layers prepared by molecular beam epitaxy (MBE) and photoluminescence (PL) measurements on Cd$_x$Zn$_{1-x}$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. — Mortiz Seyfried, Kathrin Sebald, Anne 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 2.78nm and different center-to-center (CC) distances of the individual pillars were prepared out of planar monolithic VCSEL structures by focused-ion-beam etching. The structures were grown by molecular beam epitaxy containing either one CdSe/ZnSSe superlattices or CdSe/ZnSe wells and a GaAs barrier. The optical properties of the PMs were characterized by time-resolved photoluminescence (PL) and two-photon excited fluorescence (TPEF). The PL spectrum of the isolated QDs is fitted very well by a single Gaussian with a width of 120 meV. A reduction of the spectrum width by 10% at 15 K is observed for the PMs with a CC distance of the individual pillars. A reduction of the spectrum width by 20% at 15 K is observed for the PMs with a CC distance of 5 nm.

HL 63.3 Wed 16:15 POT 151
Long-lived electron spincoherence in ZnSe-based quantum wells. — Alexander Schwan$^1$, Evgeny A. Zhukov$^2$, Dmitry R. Yakovlev$^1$, and Manfred Bayer$^1$<sup>*</sup>

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$_{0.5}$Be$_{0.5}$MgSe quantum wells (QWs) characterized by type-I band alignment and binary QW material. The spin dephasing time $T_2^\text{S}$ 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 $T_2^\text{S}$ 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$^1$, Limi Chen$^1$, Wolfram Heimmrott$^1$, Sebastian Geburt$^1$, and Carsten Ronning$^2$

1 Dept. Phys., Philipps-University Marburg, Germany — 2 Institut of Solid State Physics, Friedrich-Schiller University, Germany

The energy transfer characteristics of Zn$_{1-x}$Mn$_x$S 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, because of the reduced dimensionality. To prove this modified Förster model Zn$_{1-x}$Mn$_x$S samples were prepared, which permitted 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 measured over more than 10 orders of magnitude. Different concentrations of Manganese from 4 $\cdot$ 10$^{-6}$ % to 4 % were incorporated by ion implantation into ZnS structures of different 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 treatments the concentration of killer centers could be controlled. The aim of this work was to prove the validity of the modified Förster model for a variety of Zn$_{1-x}$Mn$_x$S 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 Lehner$^{1,2}$, Jörg Kronenberg$^{1}$, Herbert Wolff$^1$, Thomas Wichert$^3$, und IOSDL-TEAM$^4$

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 ersten Fall war nach einseitiger Implantation von $^{111}$Ag in Te-reichen, 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 Diffusionszeit 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 einfach oder kompliziert strukturierten Cd-Atomen sind. Gethörzd durch das BMWF, Projekt 05 KKTTS1


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 Schrohr, Elke Wendler, and Werner Wiesch

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$^{10}$ions/cm$^2$.

In order to study a possible thermal origin of these effects, we irradiated...
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^{10}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

● Matthias J. Mühlauer, Christoph Brüne, Timo Wagner, Hartmut Buchmann, and Laurens W. Molenkamp — Physicalischches Institut (EP3), Universität Würzburg, 97074 Würzburg, Germany

Rubashin 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 planar HgCdTe is still a crucial dual to the quantum hall effect 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. Additionally we will show and discuss measurements on two coupled QPCs separated by a beam-splitter.


**HL 63.8 Wed 17:45 POT 151**

optical properties of ZnO-nanowire/CdSe-collodial-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 dot regions (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 CdSe QDs to render a tight and uniform attachment onto the surface. CdTe 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 Herrlitz, Eduard Laurov, 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-planes [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 30 meV. The effective mass of electrons in the conduction band of TiO_2 is found to be 17m_e.


**HL 63.10 Wed 18:15 POT 151**

Investigation on multibarrier Schottky contacts — Stefan Müller, Holger von Wensckes, Otwin Breitenstein, Jörg Lenzner, and Marius Grundmann — 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(V-I)characteristics of multi-barrier PdO_x/ZnO-Schottky contacts fabricated by reactive dc-sputtering. The ZnO nominally undoped thin films were grown by pulsed-laser deposition on a ZrO_2:Al buffer on a-Al_{2}O_{3}[1].

The V-I 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(\( A_0, 0.03A_0, 4 \times 10^{-3}A_0 \)). 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.

Mode-filtered electron injection into a waveguide interferometer — S.S. Buchholz, S.F. Fischer, U. Kunze, D. Reutten, and A.D. Wieck — Werkstoffe und Nanoelektronik — Angewandte Festkörperphysik, Ruhr-Universität Bochum

Injection of mode-filtered electrons into a phase-sensitive waveguide Aharonov-Bohm (AB) ring is studied for cylindrical nanowire heterostructures. Here, we study transport in an EWG interferometer (etched from a GaAs/AlGaAs heterostructure) in which a QPC is embedded in one of the waveguide modes. 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. 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, $n_1(t)$ 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 phase shift.

Anomalous structures in the conductance of Si/SiGe quantum wires — Jochen von Pock, Daniel Salloch, Gang Qiao, Ulrich Kunze, and Thomas Hackbart — Physik-Institut der Universität Zürich, Switzerland

The anomalous conductance plateau is located near $0.6/\pi$. Anomalous structures in the conductance of Si/SiGe quantum wires (QWRs) are observed as mode-filters in the lowest subband. 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, $n_1(t)$ shows a $2\Phi_0$ periodicity.

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Formation of p-Si/ZnO nanowire heterostructures for light emitting devices — Yaser Haj Heemid, Raphael Niepelt, Martin Gnauck, Frank Schmid, 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 over large 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 SiO2 [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.

**References**


**Time:** Wednesday 17:00–18:00  
**Location:** POT 51
Factors affecting the excitation process of Europium($\text{Eu}^{3+}$) ion in Europium-implanted AlGaN —  Jayanta Kumar

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 ($\lambda = 193\text{nm}$). 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.

**Performance Highlight**

**HL 66.1: Wednesday, 17:15 — GER 38**

Simulation of second harmonic generation from split ring resonators with the Discontinuous Galerkin Time Domain method — Evgeny 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 non-linear material models. 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 non-linear 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 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 SH peak is comparable to the values reported previously in the experiments [2] and FDTD simulations [3].


**HL 66.2: Wednesday, 17:30 — GER 38**

Analysis of optimization techniques for coherent optical control in nanostructures — Tobias Fankhäm, 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 functions like the flux transmission or spatio-temporal response; the algorithms’ convergence time and computational effort is analyzed.


**HL 66.3: Wednesday, 17:45 — GER 38**

Two state lasing from a quantum dot laser — Diana Kharchova, Kathy Lüdge, Niko Mazer, 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 and conditions for different device dimensions.


**HL 66.4: Wednesday, 18:00 — GER 38**

Analytical approach to modulation properties of quantum dot lasers — Kathy Lüdge1, Evgeny Viktorov2, Thomas Erneux2, and Eckehard Schöll1

1Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany
2Université Libre de Bruxelles, Optique Nonlinéaire Théorique, Campus Plaine, C.P. 231, 1050 Bruxelles, Belgium

We analyse 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.

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 sub-wavelength hole array on a square lattice in a semitransparent Au film, rotates the polarization state at oblique incidence, but this behavior 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.

A new assembly route to mesoscopic Bragg reflectors. 

**Stefan Guldin**, Matthias Kolle, Morgan Stefic, Richard Langford, Dominik Eder, Ulrich Wiesner, and Ullrich Steiner

**HL 66.6 Wed 18:30**  
**GER 38**

New transparent conductive metal based on polymer composite — Mehdi Keshavarz Hedayati, Mohammad Jamali, Thomas Strunkus, Vladimir Zaporozhchento, Franz Paepel, and Mady Elbarhri

Nanochemistry and Nanoeengineering, Institute for Materials Science, Faculty of Engineering, Christian-Albrechts-University of Kiel — 1Nanochemistry and Nanoeengineering, Institute for Materials Science, Faculty of Engineering, Christian-Albrechts-University of Kiel

— 2Helmholtz-Zentrum Geesthacht GmbH, Institute of Polymer Research, Nanotechnology 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 mesoscopic Bragg reflectors.

**Steven Duglin**, Matthias Kolle, Morgan Stefic, Richard Langford, Dominik Eder, Ulrich Wiesner, and Ullrich Steiner

**HL 66.8 Wed 19:00**  
**GER 38**

Launching Surface Plasmons by Carbon Nanotube Photoluminescence — Nicolai Hartmann, Johann Berthelot, Alexandre Bouhiller, and Achim Hartshuch

Chemie and CeNS, Ludwig-Maximilians-Universität München, Germany — 2Département 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.

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 67.5 Wed 19:00 FOE Anorg
Electrolyte-gated organic thin-film transistors for sensing applications — •Felix Buth, Deepu Kumar, Martin Stutzmann, and Jose 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 \( \mu \text{F/cm}^2 \) 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 \( \alpha \)-sexithiophene (\( \alpha \)-6T) 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 \( \alpha \)-6T/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 Veyssel Tunc1, Elizabeth von Hauff1, Ahmet Lutfi Ugur2, Ali Erdogmus2, and Jürgen Parisi1 —
1University of Oldenburg, Department of Physics, Energy and Solid State Research Laboratory (ESF) Carl-von-Ossietzky Str.9-11, 26129 Oldenburg, Germany — 2Yıldız Technical University, Department of Chemistry, Davutpasap 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′-dimethoxyoctyloxy)]-perylenedi-4,4′-phylene vinylene (MDMO-PPV) and in blends with different ratios of 1-(3-methoxy carbonyl) 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 PPy 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

Radiative recombination of \( \text{Cu}_2\text{ZnSnS}_4 \) thin films and single crystals — •Steffen Kretzschmar1, Justus Just2, Björn Schubert1, Susan Schorr1, Thomas Unold1, Serghie Levchenko2, Victor E. Tezlevan3, and Ernest Arushanov4 —
1Helmholtz Zentrum Berlin für Materialien und Energie, 14199 Berlin
2Institute of Applied Physics, Academy of Sciences of Moldova, Chisinau, MD 2028, Moldova
3University of Oldenburg, Department of Physics, Energy and Solid State Research Laboratory (ESF) Carl-von-Ossietzky Str.9-11, 26129 Oldenburg, Germany — 4Walter Schottky Institut, Technische Universität München, Garching, Germany

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 \( \text{Cu}_2\text{ZnSnS}_4 \) and 9.6% for \( \text{Cu}_2\text{ZnSn}(S,Se)_4 \) have been reported in the literature. So far there is little knowledge about the optical and electronic properties of these materials. In this work \( \text{Cu}_2\text{ZnSnS}_4 \) thin films grown by coevaporation and \( \text{Cu}_2\text{ZnSnS}_4 \) 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.

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$_x$Se$_{1-x}$Se$_8$ tie line, including the CuIn$_3$Se$_5$ and the CuIn$_2$Se$_3$ 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-In-Se$_8$ phase. With the resulting energy expression, CuIn$_3$Se$_5$ and CuIn$_2$Se$_3$ systems have been studied in the canonical ensemble. By analyzing the free energy landscape the transition between a low-temperature ordered and a high-temperature disordered CuIn$_2$Se$_3$ 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 $\mu$$_{Cu}$ and $\mu$$_{In}$. Plateau regions for the CuIn$_3$Se$_5$ and the CuIn$_2$Se$_3$ phases have been found and analyzed for different temperatures.

**LH 68.5 Thu 11:15 FOE Anorg Kathodolumineszenz-Mikroskopie von polykrystallinen Cu(In,Ga)Se$_2$ -Absorberschichten — **STEFAN RIBBE$^1$, THOMAS HEMPEL$^1$, FRANK BERTRAM$^1$, WOLFRAM WITTE$^2$, DIETRICH HARLE$^1$, and JÜRGEN CHRISTEN$^1$ — 1Institut für Experimentalphysik, Otto-von-Guericke-Universität Magdeburg, Deutschland — 2Zentrum für Sonnenenergie- und Wasserstoff-Forschung, Baden-Württemberg (ZSW), Stuttgart, Deutschland

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 spectroscopy — MATTHIAS MÜLLER$^1$, STEFAN RIBBE$^1$, THOMAS HEMPEL$^1$, FRANK BERTRAM$^1$, WOLFRAM WITTE$^2$, DIETRICH HARLE$^1$, and JÜRGEN CHRISTEN$^1$ — 1Institut für Experimentalphysik, Otto-von-Guericke-Universität Magdeburg, Germany — 2Zentrum 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 $\mu$m 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 grain size ($\bar{d}$ = 3 $\mu$m) structure of the untreated 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

**LH 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 UV conditions. ZnO deposition by Metal-Organic MBE leads to the formation of an ultra-thin intrinsic ZnSe buffer layer (1.2 $\mu$m 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.


HL 68.8 Thu 12:15 FOE Anorg
Band alignment of epitaxial ZnS on CuInS$_2$(001) and CuInS$_2$(112) — CARSTEN LEHMANN, FRANK KELLER, and CHRISTIAN PETTENKOFFER — 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 alignment 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].

HL 68.9 Thu 12:30 FOE Anorg
Spatially resolved photoluminescence studies on CuGaSe$_2$ and CuInSe$_2$ thin-films — CHRISTIAN GUTSCHE, Ruoqiang Cui, Kaja Eklke, and XPath KELLEHER — Christian Gutsche — Helmholtz-Zentrum Berlin, Berlin, Germany
Chalcopyrite absorbers such as CuIn$_{1-x}$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 $\leq 1 \mu m$ in a confocal cryostat setup. We compare the experimental observations of these two types of absorbers, CuInSe$_2$ with CuGaSe$_2$ respect to laterally resolved luminescence yields, local splitting of quasi-Fermi levels, local absorption coefficients and local pseudo band gaps, as well as 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, STEPHAN J. HESS, RUDOLF BREUGEMANN, MAX MEESSEN, WOLFRAM WITTE, DIMITRIOS HARISKO, and GOTTFRIED H. BAUER — Helmholtz-Zentrum Berlin, Berlin, Germany
Chalcopyrite absorbers exhibit spatial inhomogeneities in structural, optical and optoelectronic properties. We study the absorber thickness dependence 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 $\mu m$ 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. Photoluminescence 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 variable RTP processed CIGS$_2$ solar cells — JULIA RIEDEGER, JÖRG OHLAND, MARTIN NITTINGER, INGO RIEDEL, ROLAND MAINDL, SAOUSSEN MERDOS, and JOACHIM KLAES — Energy and Semiconductor Research Laboratory, Department of Physics, University of Oldenburg, 26111 Oldenburg, Germany
The open circuit voltage $V_{oc}$ of CuInS$_2$ solar cells was found to improve via incorporation of gallium. The Cu(In,Ga)$_2$S$_2$ absorber of the samples studied in this work 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)Se$_2$ Thin Film Solar Cells with Infrared Images Obtained with Lock-In Thermography — TORBEN KLINKERT, JÖRG OHLAND, ROBIN KNECHT, JÖRGEN PARISH, RAYMUND SCHÄFFLER, and BERNHARD DIMMELER — Thin Film Photovoltaics, Energy- and Semiconductor Research Laboratory, University of Oldenburg, D-26111 Oldenburg — Wührl 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)Se$_2$ 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.
Optical polarization of UV-A and UV-B (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 a 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.

Processing of III-nitride thin film light emitting diodes via wafer bonding and laser lift-off

We use this method to obtain further evidence that the droop is due 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.

HL 70.1 Thu 10:15 POT 151
Lasing and transport properties in a coupled dot-resonator system — •Perdrix, JIN, MICHAEL, MARTIN, JHAEGER 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 the 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 MARQUEZ-D 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 k · p model to provide a theoretical study of these nanostructures. Strain and polarisation potentials that modify the bulk electronic properties 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 zinclingate 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-order piezoelectric constants. This reduction of the piezoelectric potential allows for better electron-hole overlap and thus higher recombinations 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 — •ELEPHERIA KAVOUSANAKI 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 polarized photons to be emitted. \( |X⟩\) or \( |Y⟩\). The order in which the photons are emitted depends on which exciton, \( |X⟩\) or \( |Y⟩\), mediates the recombination (which-way). If the intermediate state is energetically degenerate, a coherent superposition of the two double-photon states is possible, \( (|X⟩|Y⟩ + |Y⟩|X⟩)/√2\). 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 70.5 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 polarized photons to be emitted. \( |X⟩\) or \( |Y⟩\). The order in which the photons are emitted depends on which exciton, \( |X⟩\) or \( |Y⟩\), mediates the recombination (which-way). If the intermediate state is energetically degenerate, a coherent superposition of the two double-photon states is possible, \( (|X⟩|Y⟩ + |Y⟩|X⟩)/√2\). 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 Bieexciton Binding Energies and Structural Properties of GaN/AlN Quantum Dots — •GERALD HÖNIG, CHRISTIAN KINDEL, MOMEM WINKELKEMPER, ANDREI SCHLIWA, SVEN ROOD, IRINA OSTAPOENKO, 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 bieexciton energy \( (E_{X} + E_{Y})\) by varying structural parameters [1] is of largest importance for QDs in microwavities, where the emission has to match the cavity-mode. The experimental observation of a sign change of the bieexciton binding energy \( (E_{X} + E_{Y})\) at \( E_{X} := E_{X} + E_{X}\), with \( E_{X} := \text{exciton energy} \) 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 \( 10^{5} \)) cause a spatial separation of the polarization and holes within nitride-based QDs, making a CI basis of renormalized HF states superior to single particle wave functions. We take a close look on different structural parameters influencing \( E_{X} \) as well as the quantity of correlation effects in GaN/AlN QDs. Both, positive and negative bieexciton binding energies are possible for respective QD structures. Funded by SFB 102.

Semiconductor Physics Division (HL)

Carrier multiplication in quantum dots: Quantum optical emission dynamics — Frank Jahnke1 1Institute for Theoretical Physics, University of Bremen, Germany 2National 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 their similar optical behavior 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.

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 as 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 faster with increasing carrier scattering.

Exciton fine structure splitting in self-assembled semiconductor QDs: Intrinsic and extrinsic effects — Ranber Gries, Kolja Schuh, Matthias Florian, and Frank Jahnke — Institute for Theoretical Physics, University of Bremen, Germany

Semiconductor quantum dots (QDs) are of considerable interest due to remarkable achievements in cavity quantum-electrodynamics. The discrete level structure of QDs and the similarity to atomic systems have 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.

Nonclassical light and stimulated emission in the strong coupling regime for single-quantum dot emitters — Christopher Gries, 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.

Microscopic description of the dynamics of luminescence and dephasing of semiconductor quantum dots — Heinrich A.M. Leymann1, Matthias Florian2, Jan Wiersig1, and Frank Jahnke1 1Institut für Theoretische Physik, Universität Magdeburg, 39016 Magdeburg 2Institut für Theoretische Physik, Universität Bremen, 28334 Bremen

Semiconductor quantum dots (QDs) are of considerable interest due to 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.
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. Plumhoff, Santosh Kumar, Roman Rezai, Eugenio Zallo, Andreas Herkelz, Kathrin Dörk, 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 into piezoelectric actuators via gold thermo-compensation bonding. Different diode-like-structures (n-i-p and n-i-i diodes) will be presented and the optical properties of embedded QDs 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 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. Schülein1, Florian Völck1, Florian Knall1, Dirk Reuter2, Andreas D. Wörn2, Tuan A. Truong3, Heejung Kim4, Pierre M. Petroff3, Achim Winnacker2, and Hubert J. Kreiner1** — 1Lerhrstuhl für Experimentalphysik I, 86159 Augsburg, Germany — 2Lerhrstuhl für Angewandte Festkörperphysik, 44780 Bochum, Germany — 3Materials 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 (~23 nm) confinement potential, in contrast to the wetting layer of QDs. Thus, the energy levels of the thin (~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 (X0 and X0 strongly 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 whole 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 — **runa a. ostapenko, christian kindel, Gerald Hönig, Sven roott, 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±0.2×10-29 C·m and 0.4±0.3×10-29 C·m. 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. Höning, 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**

**GaN quantum dots as optochemical transducers** — **Jörg Teubner1, Sebastian Koslowski2, Aparna Das2, Eva Monroy3, Philomela Komninou1, and Martin Kickhoff1** — 1 Physikalisches Institut, Justus-Liebig-Universität Gießen, Germany — 2CEA, CNRS, INAC/SP2M/NPSC, CEA-Grenoble, France — 3Department 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 Mezer, Christoph Kramer, Heinz Kaut, 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 the dot nuclei in a spin-light-emitting diode by analyzing the Overhauser shift. The built-in 15 min. break

**HL 71.6 Thu 11:45 POT 251**

Off-resonant generation of electronic spin coherence in InAs quantum dots — **Britt-Marie Meinert1, Alexander Schwan2, Stefan Spatzek3, Steffen Varwig1, Dmitri Yakovlev1, André Henriques2, and Manfred Bayer1** — 1 Experimentelle Physik 2, U...

Excitation energy was varied in an wide range up to 100 meV above the QDs resonances and even beyond the GaAs barrier 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 lose 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.

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 ellipticity 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.

Weuse a reflective all-optical pump-probe technique in order to characterize single single quantum dot molecules (QDMs), which are coupled by electron tunneling. By applying a bias voltage along the growth 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. Furthermore 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.
Structuring of Organic Conductors by Laser Ablation — Semiconductor Physics Division (HL) Thursday

Investigation of the origin of the memory effect in devices based on C60 — Philipp Sebastian, Alexander Zakhidov, Bojörn Lössem, 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 SiO2 layer on top of a indium tin (ITO) ground contact, followed by electron accepting C60 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 104 successfully applied write read erase 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 C60 and at the interface to the SiO2 layer.


Growth and morphology of aluminum contacts on P3HT films — Gunar Kaukel1,2, Robert Miser3, Eferdion Metwalli3, Volker Körstgens1, Kai Schlage2, Sébastien Couet3, Stephan V. Roth3, and Peter Möller-Buschbaum1 — TU München, Physik-Department, Lehrstuhl für Funktionelle Materialien, James-Francke-Straße 1, 85747 Garching — Martin-Luther-Universität Halle-Wittenberg, Institut für Physik, Fachgruppe Photovoltaik, Von-Delius-Platz 3, 06120 Halle — 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 homogenous 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 layer by the formation of an intermixing layer is revealed by X-ray reflectivity measurements.

Effect of high-k substrates on the photocurrent of organic semiconductor devices: Tailoring the Coulomb interaction — Miriam Engel1, Donald Lupascu2, Níves Rebelo de Moura2, and Roland Schmehl1 — 1Nanostrukturtechnik, Universität Duisburg-Essen, 47057 Duisburg — 2Institut 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-donor 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 IV 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.

Organic pin-Diodes with Adjustable Current-Voltage Performance Applicable at Ultra-High-Frequencies — Hans Klemann, Christoph Schünemann, Paul Pahner, Alexander A. Zakhidov, Bojörn Lössem, 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 (107) and since the diodes contain high mobility materials like pentacene and C60 we present high-frequency properties of these pin-diodes above 13.56MHz required for RFID-tags.


Photoinduced degradation process of Fir6 emitter molecules: a laser desorption/ionization time-of-flight mass spectrometry investigation — Níves Rebelo de Moura2, Ruben Seiferth1,2, Sebastian Scholz1, Bojörn Lössem2, and Karl Leo1 — 1Institut für Angewandte Photophysik, Technische Universität Dresden, George-Bähr-Str. 1, 01062 Dresden, Germany — 2Von Ardenne Anlagentechnik GmbH, Plattleite 19/29, 01324 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 life-
time of the blue phosphorescent emitters. For improving the lifetime of the OLEDs a deep understanding of the intrinsic chemical degrada-
tion is required. Our work is focused on the photoinduced degradation process of single layer of the Fir6 molecule used as blue phosphores-
cent emitter by laser desorption/ionization time-of-flight mass spec-
trometry (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)]+. The reaction between the Fir6 fragments and the Fir6 molecule itself resulting in the formation of [Fir6+(pyrazole)]+, and [Fir6-(pyrazole)+Ir(F2ppy)2]− could be observed as well. Additionally, the degradation processes of full pro-
cessed 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, WIERKE SARPEK, DAVID HARTMANN, and ALBRECHT WINNACKER — Université de Erlangen-Nuremberg, Department of Materials Science, Chair VI: Materials for Electronics and Energy Technology, Martensstr. 7, 91058 Erlangen, Germany — •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 electro-
chemical cells (LEC)s 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 forma-
tion 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 pur-
pose, an optimization of the device configuration and processing con-
ditions as well as the use of a proper driving mode can be helpful. We
show that the performance can be significantly enhanced due to mod-
fications in the stack configuration (e.g., interfaces, layer thickness,
cathode), processing conditions and by an adequate mode of opera-
tion without any losses in the device stability.

**HL 73.2 Thu 12:15 GER 38**

**OLEDs under high current densities – transient electrolu-
minescence turn-on dynamics and singlet-triplet quenching** — •DANIEL KAEMANN, HARTMUT FRÖH, 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 materi-
als with the advantages of solid state emitters. Even though various
optically pumped devices comprising different resonator types and ma-
terial 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,
been achieved yet. The high excitation density needed in the active
optically pumped devices comprising different resonator types and ma-
terials with the advantages of solid state emitters. Even though various
decade due to the promising combination of versatile organic materi-
al. Without any losses in the device stability.

**HL 73.3 Thu 12:30 GER 38**

**Investigation of the chemical and electronic structure of F16CoPc from Monolayer to thick films by photoemission spectroscopy** — •M. GROBOSCH and M. KNUPPER — IFW Dresden, D-01069 Dresden, Germany

We have grown F16CoPc 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 F16CoPc films. Within the first monolayers we could identify a
change transfer from the substrate on the F16CoPc molecules. Our
results indicate a clear difference in the valence band spectra for sub-
monolayer thin and several nm thick F16CoPc films. Furthermore,
for F16CoPc the ionization potential can be changed by the fluorination
of the molecules from 4.8 eV for CoPc to 6.5 eV for F16CoPc. The in-
vestigated heterointerface CoPc/F16CoPc can be characterized as fre-
from chemical reactions.

**HL 73.4 Thu 12:45 GER 38**

**Influence of sample geometry and contact metal on the characteristics of organic field-effect transistors** — •DOMINIK KLASS, CHRISTOPHER KIEL, JAN HARTL, and DORIS SCHLETTWEIN — Institute of Applied Physics, Justus-Liebig-University Giessen, Germany. email:schlettwein@uni-giessen.de

Thin films of F16PcCu 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
VDS. 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 bar-
rier, 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 mobil-
ity also for low values of VDS and consistent values with those from
typically evaluated large VDS 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** — •ELEK Nagy, DAVID STEINMETZ, CHRISTIAN HEPPE, JANINE RIECHRICH-MÖLLER, ROLAND ALBRECHT, JAN MEIER, MARTIN FISCHER, STEFAN GSELL, MATTHIAS SCHRECK, and CHRISTOPH BECHER — 1Universität des Saarlandes, FR 7.2 Experimentalphysik, D-66123 Saarbrücken — 2RUBION, Ruhr-Universität Bochum, D-44780 Bochum — 3Universität 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 photo-
stability. 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 sa-
turation, 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
c yogurt temperatures and perform 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

Johannes Zöllner, Dmitry Strekalov, Dominique Elsen, Ulrik L. Andersen, Andrea Aebello, Christoph Marquardt, and Gerd Leuchs — 1Max Planck Institute for the Science of Light, Institute for Optics, Information and Photonics, University Erlangen-Nuremberg, Erlangen, Germany — 2Jet Propulsion Laboratory, California Institute of Technology, Pasadena, USA — 3Department 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.


HL 74.3 Thu 11:15 HSZ 02 Studying Photon Number Distributions of (NV-) Single Photon Centres

Waldemar Schumm, Marco Gramaglia, Giorgio Brida, Ivo P. Degiovanni, Marco Genovesi, Helmut Hoffer, Stefan Kuck, Lapo Lolli, Matteo G.A. Paris, Silke Peters, Mauro Raiteri, Mark Rodenberger, Andreas Ruschhaupt, Emanuele Taralli, and Paolo Trains — 1Physikalisch-Technische Bundesanstalt, 38146 Braunschweig, Germany — 2Leibniz Universität Hannover, 30167 Hannover, Germany — 3Istituto Nazionale di Ricerca Metrologica INRIM, 10135 Torino, Italy — 4Università 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 vacancy 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 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 transition-edge sensor (TES). The data from 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, Laura Kipfstuhl, Christian Hepp, Martin Fischer, Stefan Gresl, Matthias Schrecker, and Christoph Beecher — 1Universität des Saarlandes, Fachrichtung 7.2 (Experimentalphysik), Campus E2.6, 66123 Saarbrücken — 2Universität 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 color 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 freestanding diamond solid-state devices for optical quantum-information-pattern them by focused 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 — 1Institute 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 photon 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 $g \approx 150 \mu eV$. 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 polarization 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 Walters, Andreas W. Schell, Günther Kwees, Nils Nüsske, Max Schoenberg, Bernd Löchel, Michael Barth, and Oliver Benson — 1Nano-Optics, Institute of Physics, Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin — 2Operator 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 quantum photonic technology. We present a novel scheme to address 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-centre 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 Nanooptics

Günther Kwees, 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 nanodonna. The NV centres were systematically rearranged through AFM nanomanipulation around the
Quantum key distribution using electrically triggered quantum dot-micropillar single photon sources — *Tobias Heinzel*, Markus Raub, Christian Schneider, Martin Fürst, Sebastian Nauerth, Matthias Lerner, Henning Weier, Stephan Reitzenstein, Sven Höfling, Martin Kamp, Harald Weinfurter, and Alfred Forchel — Technische Physik and Wilhelm Conrad Röntgen Research Center for Complex Material Systems, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany; Lehrstuhl für Physik, Ludwig-Maximilians-Universität, 80799 Munich, Germany — quitools GmbH, 80539 Munich, Germany — 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. In practice, the lack of efficient single photon sources has 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.

**Topical Talk**

**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

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$_2$ZnSn(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 materials for more efficient photovoltaic energy conversion.

**HL 75.2 Thu 11:45 TRE Phy**

**What is the $G^0W^0$ band gap of ZnO?** — Martin Stanovsky, Gabriel Antonius, David Waroquiers, Anna Miglio, Hemant Dixit, Patrick Rinke, Hong Jiang, Matteo Giantomassi, Xavier Gonze, Michel Côté, and Gian-Marco Rigat

— 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 Physica, 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**


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 PdS$_2$ [7].

HL 75.4 Thu 12:15 TRE Phy

Ab initio calculations of electronic excitations: Collapsing spectral sums

Arian Berger1,2, Lucia Rening1,2, and Francesco Sottile1,2 — 1Laboratoire des Solides Irradiés, École Polytechnique, CNRS, CEA-DIRM, 9128 Palaiseau, France — 2European 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 Rinke1, Hong Jiang1, Matthias Scheffler1, Andreas Greuel2, Michael Rohlfing3, Anderson Janotti1, Emmanuel Koppakis1, and Chris G. Van de Walle1 — 1Fritz-Haber-Institut der MPG, Berlin — 2Université Osnabrück, Osnabrück — 3University 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 TiO2 as an example to illustrate some of the problems. Many-body perturbation theory in the G0W0 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 theionic contribution to the dielectric function, which can be substantial in oxides, in the G0W0 calculations and to incorporate both effects consistently into Bethe-Salpeter calculations. Another aspect to consider is the role of electron correlations. [1] Y. Tzukua et al., J. Phys. Soc. Jpn. 63, 347 (1994). [2] J. Pascual et al., Phys. Rev. B 18, 5606 (1978).

HL 76: Nitride-based Green Lasers

Time: Thursday 11:45–13:15

Location: POT 51

Dynamics of (AlIn)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 (AlIn)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 electro-luminescence 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.

The loss mechanisms in green-emitting laser diodes — Andreas Kruse1, Moritz Brendel1, Uwe Rossow1, Hyongju Chauveau2, Jean-Yves Dubou2, and Andreas Hangleiter1 — 1Institut für Angewandte Physik, TU Braunschweig — 2CHRÉA-CNRS, Valbonne, France

While GaN 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.

Growth and characterization of AlInN for cladding layers in long wavelength GaN based laser structures — Ernst Ronald Buss1, Heiko Brehmers1, Uwe Rossow1, Egidijus Sakalauskas2, Rüdiger Goldmann3, and Andreas Hangleiter1 — 1Institute of Applied Physics, TU Braunschweig, Mendelssohnstrasse 2, Braunschweig — 2Institute of Physics, TU Ilmenau, Weimarer Straße 32, Ilmenau — 3Institute of Experimental Physics, Otto-von-Guericke-University Magdeburg, Universitätstrasse 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 AlGaN 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 x1n ≈ 0.179 show pseudomorphic growth and lattice matching for 845°C and 50μbar. 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 GaN/GaN Laser Diode Structures — LAKES HOFFMANN1, HEIKO BREMMER1, HOLGER JÖRNS1, UWE ROSOW1, JOHANNES THALMAIR1, JOSEF ZWECK2, MARCO SCHOWALTER3, ANDREAS ROSENRAUER1, and ANDREAS HANGLEITER3 — 1TU Braunschweig, Institute of Applied Physics, Braunschweig, Germany — 2Universität Regensburg, Institut für Experimentelle und Angewandte Physik, Regensburg, Germany — 3Universität 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 annealation. 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 LEUTRE1, KAMRAN FORGHANI1, FRANK LIPSKI1, FERDINAND SCHOLZ2, INGO TISCHEN2, BENJAMIN NRUȘCHIL2, and KLAUS THONK2 — 1Institut für Optoelektronik, Universität Ulm — 2Institut 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 [1122] facets and GaN stripes with {1011} 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 of AlGaN substrates is 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 SiO2 and SiN2 masks. The influence of mask geometries (stripes | m and Λ 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 DARTSCH1, CHRISTIAN TISSAREK1, STEPHAN FIGGEL1, TIMO ASCHENBRENNER1, CARSTEN KRÜS1, MARCO SCHOWALTER2, ANDREAS ROSENRAUER1, and DIETLEF HOHMEL1 — 1University of Bremen, Institute of Solid State Physics - Semiconductor Epitaxy — 2University of Bremen, Institute of Solid State Physics - Electron Microscopy

InGaN quantum dots (QDs) and their implementation into the micro cavity of a vertically 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 hybrid 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 5 Å GaN cavity surrounded by a 40 fold bottom- and a 10 fold GaN/AlInN top-DBR. Electroluminescence of the InGaN QDs was achieved 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

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, BENEDICT GHUREK1, 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 (OTFT) 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-Motters model (VM) of the charge carrier density dependent mobility $\mu = \mu_0(V_{GS} - V_{TH})^{\eta}$, where the parameter $\eta$ 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 GRAAF1, FRANZISKA LÜTTICH1, DANIEL LEHMANN2, DIETRICH R.T. ZAHN2, and CHRISTIAN VON BORCZYKOWSKI1 — 1Optische Spektroskopie und Molekülphysik, Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz, 2Halbleiterphysik, 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/insulator) 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 KERRER, 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 magnitude 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 held 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.

**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 transistor 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.


**Electronic properties of spiro-compounds: A combined photoelectron spectroscopy and energy-loss spectroscopy study**

• B. Mahs1, M. Groboshi2, T. Saragi1, J. Salbeck2, and M. Knupper3. — IFW Dresden, Helmholtzstrasse 20, 01069 Dresden, Germany

1Macromolecular Chemistry and Molecular Materials, Institute of Chemistry, Department of Science and Center for Interdisciplinary Nanostructure Science and Technology (CINaST), 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.

**Dye directed changes in ZnO matrices in organic/inorganic photovoltaic systems**

• Harald Graas1, Franziska Lütthi2, Mirko Kirch1, Christian Dunkel2, and Torsten Oechermann2. — 1Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz

2Institut 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 adsorb 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 observable.
Energy level alignment at polymer/PCBM heterojunctions under operating conditions in an organic photovoltaic cell structure — JOHANNES FRISCH1, ANDREAS WILKE1, PATRICK AMSELEM1, JENS NIEDERHAUSEN1, ANTRJE VOLLMER2, and NORBERT KOCHE3 — 1Humboldt-Universität zu Berlin, Institut für Physik, Brook-Taylor-Str. 6, D-12489 Berlin, Germany — 2Helmholtz-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) (P3HT)/PCBM) heterojunctions using 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 model calculations. 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.

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.

improvement of the CdSe/P3HT solar cells efficiency due to surface modification of the CdSe nanoparticles by alkylamine treatments — NIKOLOV RABDYCHEV, IRINA LOCTEV, ROGER BOSWORTH, JOHANNA BEVANN-OLESKIV, and JÜRGEN VARNAR — 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 process. 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. A study of the solar cells (P3HT:PCBM) with 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.
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 N2 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 exhibits a nearly uniform absorptivity beyond 90% in the whole visible to near-infrared spectral region. This is due 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 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. The structuring leads to the formation of a p-n junction which is the origin of the high absorption in the near infrared. Furthermore, sulfur acts as a donor in silicon. Hence, microstructuring of p-doped silicon in SF6 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 Messer**, Pawel Ziolkowski, Niels Petersmann, Gabi Schiering, Niels Benson, Hartmut Wieggers, and Roland Schmehl — Universität Duisburg-Essen, Nanostrukturtechnik, 47057-Duisburg — DLR (German Aerospace Center), Institut of Materials Research, 51147-Köln — Universität Duisburg-Essen, KIT Institut für Nanotechnik, 47057-Duisburg — DLR (German Aerospace Center), Institut of Materials Research, 51147-Köln

To reduce costs per watt of commercial photovoltaics (PVs) silicon nanoparticles are considered as an interesting alternative to conventional PV films. To proof the principle concept a pn-junction is created by spark plasma sintering of highly p- and n-doped (∼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 photoelectric effect: Ta kz: 1 nozp.

**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 — Helmholz-Zentrum Berlin, Kekuléstr. 5, 12489 Berlin

To gain a better insight into the efficiency-limiting processes in polycrystalline silicon (pol-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 simulation of the model has been achieved through simultaneously fitting the measured dark and light J-V curves of twelve poly-Si thin film minidummies with dissimilar thickness and absorber doping concentration. Effective defect density, capture cross section products of 10...100 cm^{-3} have been determined in the poly-Si absorber by this procedure. Transient photocurrent and resistance decay measurements of the poly-Si absorbers have also been conducted in the low injection regime (∼4.5·10^{-14} cm^{-2}). High lifetimes of 100µs 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**, Jan P. Richters, Karsten von Maydell, and Carsten Agent — EWF 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 carrier 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 Gutfried 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**, Uli...
Scanning Spreading Resistance Microscopy for Characterization of Laser Doped Selective Emitter Structures in Solar Cells — Stefan Doering¹, Stefan Jakusch¹, Thomas Mikolajick², Jens Krause², Rico Boheim³, and Marc Petri¹

1NaMLab gGmbH, Dresden, Germany — 2TU Dresden, Dresden, Germany — 3Roth & 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 dimension 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 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.

Comparison of the annealing treatments of PVD and ALD Al₂O₃ passivated silicon for solar cell applications — Frank Brenner¹, Maria Tarasova², Steve Kunze³, Stefan Jakusch¹, and Thomas Mikolajick¹

1Lehrstuhl für Nanoelektronische Materialien, TU Dresden, Germany — 2Institut 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 Al₂O₃ 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 (N₂/H₂) was preferable to nitrogen. Moderate temperatures decreased the density of interface states, increased the density of fixed charges and, therefore, decreased the carrier lifetime. A high temperature treatment degraded the passivation layers significantly. Al₂O₃ 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.

Novel Green Laser Diodes

Time: Thursday 14:30–17:15

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, Ainan, 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
Invited Talk
HL 80.2 Thu 15:00 POT 51
Room-temperature CW operation of BeZnCdSe green laser diode — Hitachi Central Research Laboratory, Kokubunji-shi, Tokyo, Japan — National Institute of Advanced Industrial Science and Technology, 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 laser displays. Although several approaches using III-nitride-based semiconductors and their successful laser operations with wavelengths of over 500 nm have already been reported, their threshold currents still increase as their lasing wavelengths approach 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 that a 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 sili-con substrate — Aichi Institute of Technology, Yakuza, Toyota 470-0392, Japan

Growth and properties of semi-polar and non-polar GaN on Si substrate were investigated. In 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. — Hitachi Central Research Laboratory, Kokubunji-shi, Tokyo, Japan — National Institute of Advanced Industrial Science and Technology, Tsukuba-shi, Ibaraki, Japan

Semipolar GaN substrates enable the formation of dislocation-free InGaN quantum wells (QWs). Reduction of these dislocations is critical for the achievement of high-performance laser diodes in the green spectral region. Here, we discuss the advantages of using semipolar orientations for InGaN QW laser diodes. 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 therefore 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,Ga)N laser diodes — Institut für Experimentelle und Angewandte Physik, Universität Regensburg, 93040 Regensburg, Germany

To achieve lasing in the green spectral range 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 homogeneously broadened photoluminescence spectra with 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, spontaneous emission is mainly determined by dark spots on the high Indium content surfaces. 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 semi-polar 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

HL 81.1 Thu 14:30 POT 151
Acoustic phonons and spin coherence in graphene nanoribbons — 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 coupling to nuclear spins and the lattice and the relaxation time T₁ 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 q²-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.


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 — University of Regensburg, 93040 Regensburg, Germany

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.

Semiconductor Physics Division (HL) Thursday

∙

Spin Transport and Spin Precession in Bilayer Graphene with Transparent and Tunneling Ferromagnetic Contacts —

Bastian Birnker, 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 homogeneous tunnel barrier. The L-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 81.3 Thu 15:00 POT 151 Spin Transport and Spin Precession in Bilayer Graphene with Transparent and Tunneling Ferromagnetic Contacts —


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. Unlike 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 SiO2 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.


HL 81.4 Thu 15:15 POT 151 Dynamic Hall effect driven by circularly polarized light in graphene —


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. Unlike 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 SiO2 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.


HL 81.5 Thu 15:30 POT 151 Magnetotransport property of multigraphene in pulsed magnetic fields up to 62 T —

José Luis Barzola Quiquia1, Humberto Peredo1, Rolf J. Haug2, and Rolf J. Haug2 — Institut für Festkörperphysik, Leibniz Universität Hannover, D-30167 Hannover, Germany

We analyse the electronic properties of a monolayer graphene ring. Graphene is obtained by micromechanical cleavage of natural graphite and is placed on a silicon substrate with a 285 nm 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 280 nm. 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.

HL 81.8 Thu 16:30 POT 151 Investigating Aharonov-Bohm oscillations in a monolayer graphene ring structure —

Dmitri Shironov, Henrik Schmidt, and Rolf J. Haug — Institut für Festkörperphysik, Leibniz Universität Hannover, D-30167 Hannover, 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.

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.

Graphene solution-gated field effect transistor arrays for sensing applications — ●Lucas H. Hess, Pardis Ratsami, Max Seifert, Moritz Haup, Marcus Danneker, Ian D. Sharp, Martin Stutzmann, and Jose A. Garreiro — 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, microscopical graphene SGFET arrays are fabricated on large-scale graphene samples and characterized in aqueous environments. Both, in the electron and hole regime, the measured conductance data are significantly higher than in insulator-based devices based on silicon or silicon nitride transistors. The low-frequency noise of graphene SGFETs is investigated, revealing an effective gate noise of tens of $\mu V$, 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.

Polymer Brushes on Graphene — ●Max Seifert1,2, Mariin Starnacker1,2, Alexander Gigler3, Ning Zhang2, Frank Deubel2, Candy Xuan Lim4, Kiang Loh4, José Garrido5, Rainer Jordan2,3, Martin Stutzmann1, and Ian Sharp1,2,3,4 — 1Walter Schottky Institut, TU München, Germany — 2Wacker-Lehrstuhl für Makromolekulare Chemie, TU München, Germany — 3CeNS and Department of Earth and Environmental Sciences, LMU München, Germany — 4Department of Chemistry, National University of Singapore, Singapore — 5Professors 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 from the substrate. Photoreactive 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.

Interaction of intersubband transitions and ponderomotive response 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 500119, 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 ultrafast broad-band THz spectroscopy. The THz radiation is generated by phase-matched optical rectification of fs near-infrared pulses in 50-µm-thick GaS 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 phase shift 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.


Ultrafast Dynamics of ZnO and ZnO-BaTiO3 thin films — ●Sinhgdatanu Acharya1, Sumedha Chouthe1, Tasmo Böntgen2, Rüdiger Schmedt-Grund2, Marius Grundmann3, and Gerhard Seifert1 — 1Institute of Physics, Martin-Luther-University, Halle-Wittenberg, Von-Danckelmann Platz 3, D-06120, Halle, Germany — 2Institute for Experimental Physics-II, University of Leipzig, Linnesträße 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 TiS laser pulses (150fs, 400nm) were used as pump, induced transmission changes were probed by supersonic continuum (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 an abrupt drop of the radiative state population and consequent 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 generate interference of transmitted THz radiation 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.

Time-resolved photoluminescence from GaAs/AlGaAs multiple quantum wells quenched by pulsed mid-infrared radiation — ●Sabine Zysell, Harald Schneider, Stephan Winnehl, 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.

Department of Chemistry, National University of Singapore, Singapore — ●Elisabeth Bothschafter1,2, Alexander Paarmann3, Nicholas Karpowicz2, Reinhard Kienberger1,2,3, Ralph Ernstorfer1,2,3,4

Coherent Lattice Vibrations in TiO2 — ●Elisabeth Bothschafter1,2, Alexander Paarmann3, Nicholas Karpowicz2, Reinhard Kienberger1,2,3,4

Coherent Lattice Vibrations in TiO2

Thursday

HL 81.10 Thu 17:00 POT 151

Polymer Brushes on Graphene — ●Max Seifert1,2, Mariin Starnacker1,2, Alexander Gigler3, Ning Zhang2, Frank Deubel2, Candy Xuan Lim4, Kiang Loh4, José Garrido5, Rainer Jordan2,3, Martin Stutzmann1, and Ian Sharp1,2,3,4 — 1Walter Schottky Institut, TU München, Germany — 2Wacker-Lehrstuhl für Makromolekulare Chemie, TU München, Germany — 3CeNS and Department of Earth and Environmental Sciences, LMU München, Germany — 4Department of Chemistry, National University of Singapore, Singapore — 5Professors für Makromolekulare Chemie, Department Chemie, TU Dresden, Germany

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Ultrafast Phenomena

Location: POT 251

Time: Thursday 14:30-17:15

Interaction of intersubband transitions and ponderomotive response 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 500119, 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 ultrafast broad-band THz spectroscopy. The THz radiation is generated by phase-matched optical rectification of fs near-infrared pulses in 50-µm-thick GaS 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 phase shift 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.

and Ferenc Krausz 2,4 — 1Fakultät für Physik, TUM, Garching — 2Max-Planck-Institut für Quantenoptik, Garching — 3Fritz-Haber-Institut der MPG, Berlin — 4Department 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]). 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$_2^-$ states whereas the conduction band has mainly Ti$_3^-$ character [3]. We assume that the abrupt change in the potential energy surface upon excitation occurs the observed coherent lattice oscillation.


HL 82.5 Thu 15:30 POT 251

Modulation of photoluminescence kinetics of InGaAs quantum dots embedded into a microcavity using picosecond acoustics — C. Breugmann 1, T. Bergherr 2, A.V. Scherbakov 2, M. Bombeck 2, S. Höfling 1, C. Schneider 1, A. Forchel 1, A.V. Akimov 2, D.R. Yakovlev 1,2, and M. Bayer 1

1Institut der MPG, Berlin — 2Max-Planck-Institut für Quantenoptik, Garching

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$_{0.33}$Ga$_{0.67}$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 variable 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 $\sim 100$ ps.

15 min. break

HL 82.6 Thu 16:00 POT 251

Extreme Nonlinear Optics in Semiconductors with Shaped Laser Pulses — Matthias Reichelt 1, Andreas Walther 1, and Torsten Meier 1 — 1Institut für Physik und CeOPP, 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 kinetics of quantum dots (QDs) embedded into a microcavity (MC). The emitted radiation spectrum. [1] We show that the pattern of the


HL 82.7 Thu 16:15 POT 251

Coulomb-induced relaxation dynamics in single-walled carbon nanotubes — Erik Verdenhalven, Andreas Knorr, and Ermin Malic — 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

Microscopic calculation of non-linear polarization spectra of light-harvesting complexes — Mario Schottl 1, Marten Richter 1, Thomas Renger 1, and Andreas Knorr 1 — Institut für Theoretische Physik, Technische Universität Berlin, Germany — 2Institut 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.


HL 82.9 Thu 16:45 POT 251

First principles of phonon squeezing in silicon — Tobias Zierl, Eruwe 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 7 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 — Michal Pochwala, Huynh Than Duc, Jens Förster, 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/Al$_x$Ga$_{1-x}$As. 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.


**HL 83.1** Thu 15:00 TRE Phy

Excited States from GW: the role of self-consistency

- Fabio Caruso\(^1\), Xinguo Ren\(^2\), Patrick Rinke\(^3\), Angel Rubio\(^4,5\), and Matthias Scheffler\(^1\)

\(^1\)Fachbereich Physik, Universität Osnabrück, Germany
\(^2\)Universidad del País 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 ($G_W$). 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 FHIAIMS [http://www1.hu-berlin.de/mpg.de/amos]. The self-consistent treatment corrects several pathologies of the $G_W$ 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 underestimate the charge-transfer energy. This error can be traced back to the wrong description of the HOMOLUMO gap and its evolution with intermolecular distance. This error is captured 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+$\Gamma_0$W approach

- Michael Rohlffing - 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 described 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$(111)-(2 \times 1)$ surface, the SiH$_4$ molecule, an argon-alumina interface, and liquid argon.


**HL 83.3** Thu 15:30 TRE Phy

First-principles study of (GW+PAW) on new phosphors for white LED

- Bruno Berthand\(^1,2\), Masayoshi Mikami\(^3\), Martin Stanekovski\(^1\), and Xavier Gonze\(^4\)

\(^1\)European theoretical spectroscopy facility (ETSF), Université Catholique de Louvain, Louvain-la-Neuve, Belgium
\(^2\)CERDECAM, Institut Supérieur Industriel d’Electronique, Bruxelles, Belgium
\(^3\)Mitsubishi Chemical Group Company, 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$_2$Si$_2$O$_5$N$_2$Eu developed at the Mitsubishi Chemical Group (S&T) Research Center, and the other is a bluish green phosphor Ba$_5$Si$_4$O$_{12}$N$_2$Eu that exhibits little luminescence at room temperature. Our results rely on many body perturbation approach (GW+PAW) applied to the two hosts : Ba$_5$Si$_4$O$_{12}$N$_2$ and Ba$_5$Si$_4$O$_{12}$N$_2$. The calculation shows a slightly narrower energy gap for Ba$_5$Si$_4$O$_{12}$N$_2$Eu. The approach uses full excited states, many configurations 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 in paramagnetic battery materials

- Yuehsing Zhang\(^1\), Florent Boucher\(^1\), Aurele Castets\(^2\), Dany Carlier\(^2\), and Michel Ménétrier\(^2\)

\(^1\)IM, Nantes, France
\(^2\)ICMCB, Pessac, France

Solid state NMR in materials for lithium-ion batteries is considerably more difficult in paramagnetic systems than in other types of materials due to the partial cancellation of the magnetic moment associated with the Fermi contact term.

We have used theoretical calculations based on Density-Functional Perturbation Theory, leading to a dramatic decrease of calculation times. 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 approach (GW+PAW) applied to the two hosts : Ba$_5$Si$_4$O$_{12}$N$_2$Eu and Ba$_5$Si$_4$O$_{12}$N$_2$ and found that it partially cancels the standard main contribution was given by the Fermi contact term 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 shift 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 compared to the experimental ones. Adding orbital potential “U” or exact exchange on transition 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 transition metal and oxygen ions. This means that appropriate exchange correlation potential for transition metals and oxygen ions is really crucial to calculate the contact shift of lithium ion.

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 Boulangier\(^1,2\), Michel Cote\(^2\), and Xavier Gonze\(^4\)

\(^1\)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 respect to atomic displacements. We have studied the importance of this extra term for diatomic molecules and found that it partially cancels the standard contribution. A deeper analysis with Eu-doped models sheds new light onto 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 cannot 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\(^1\), Dominik Biffart\(^2\), and Paul Boulanger\(^2\)

\(^1\)Institut de Chimie des Matériaux de Carbone, France
\(^2\)Fachbereich 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 quasi-particle 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.

**Topical Talk**

**Title:** Insights in the T-matrix formalism

**Authors:** Pina Romaniello, Ali Alavi, Stefano Pittalis, and Lucia Reining

**Abstract:**

In many-body perturbation theory the self-energy \( \Sigma \) 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 \( \Gamma \) 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].


**References:**


**Localisation:** TRE Phy, Location: TRE Phy

**Time:** Thursday 17:45–19:15

**Location:** TRE Phy

**Topical Talk**

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**Authors:** Pina Romaniello, Ali Alavi, Stefano Pittalis, and Lucia Reining

**Abstract:**

In many-body perturbation theory the self-energy \( \Sigma = GW \) 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 \( \Gamma \) 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].


**References:**

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.


Time: Thursday 18:00–21:00
Location: P4

HL 85: Poster Session II

HL 85.1 Thu 18:00 P4
Quasiparticle wave functions in alloys — Alexander Möller, Marko Stößzel, Gabriele Benndorf, and Marius Grundmann — Universität Leipzig, Institut für Exp. Physik II, Abteilung Halbleiterphysik, Linnestr. 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 — Ross Cherian and Gabriel Bester — Max-Planck-Institut für Festkörperforschung, Heisenbergstraβe 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 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 Blanc, 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 photonic-phonon 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-phonon bound states can be excited. Furthermore, we analyze functional elements which are important for possible experimental realizations.


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 of Technology (KIT), 76128 Karlsruhe, Germany

1—Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany
2—Free 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.

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 threelfold structure in the first Brillouin-zone of the fcc-lattice.

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 found for a system of two coupled two-dimensional high-Q nanocavities [2] with an embedded quantum dot.


Crossed Photonic Crystal Waveguides for Quantum Dots Signal Detection — XiHong Song, Torsten Meier, and Jens Förstner — Department of Physics and CeOPP, Warburger Str. 100, D-33008 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.


Tunable Transmission in Rolled-Up Three Dimensional Metamaterials — Anne Kottmeyer, Stephan Schwager, Matthias Klingbeil, Markus Broeell, Jochen Kerßlentz, Ricardo Costa, Andrea Stemmmer, Yulvia Stark, Detlef Heitmann, and Stefan Mändach — 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 fiber 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 characterististic modulation of the transmission through the tube walls.

We gratefully acknowledge support by the DFG through GRK 1286.


Numerical Simulation of Exciton Dynamics at Ultralow Temperature — Sunipa Som1 and Heinrich Stolze2 — Institut für Physik, Universität Rostock, Rostock, Germany — 2Institut 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 the 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 ultralow 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 the temperature varies with time. 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.


Magneto-Optical Ellipsometry of Ferromagnetic Thin Films — Tobias Herzog, Tannönt Bökteng, Rüdiger Schmidt-Gundt, Michael Lorenz, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Linnestr. 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 magentite thin films as model systems. The method proved to be a reliable tool to measure important optical properties and magneto-optical effects simultaneously.

Optical properties of crystalline and amorphous TiO2 modifications — Marc Landmann1, Thomas Köhler2, Eva Raubs2, Thomas Frauenheim2, and Wolf Gero Schmidt4 — 1Lehrstuhl für Theoretische Physik, Universität Paderborn, Germany — 2Bremen 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 transistors [1]. TiO2 also offers hysteresis 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.

Semiconductor Physics Division (HL) Thursday

HL 85.12 Thu 18:00 P4
Investigation of the effect of plasmonic metal nanostructures on nanocrystalline TiO$_2$:Eu$^{3+}$ nanoparticles — CARITI BENEL$^1$, BARAT KURIANJAN$^1$, ULRICH HERR$^2$, MANUEL GONCALVES$^2$, OTTHMAR MARTZ$^3$, JANNES HONEBERGER$^2$, and PAUL LEIDLER$^2$$^1$ Inst. of Experimental Physics, 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 concentrations 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 $D_{0}$-$F_{2}$ 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 nanoparticle 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 RENGE — Technische Universität Ilmenau, 98683 Ilmenau, Germany

Localizations 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 second harmonic generation (SHG) were found.

[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 HANNENWALD, and FRIEDHELM BECHSTEDE — Institut für Festkörpertheorie und -optik und 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.

Optical properties of as-grown and ion implanted Cu2O thin films — CHRISTIAN MÜLLER$^1$, SEBASTIAN GEHRUT$^1$, ANDREAS LAUFER$^2$, BRUNO K. MEYER$^2$, and CARSTEN RONNING$^2$ — Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — $^2$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 films on glass substrates were patterned using 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 donor/acceptor behavior. Ion implanted samples were examined to discover extrinsic donor- and acceptor species and optical active impurities.


HL 85.15 Thu 18:00 P4
Photoluminescence of Ga(AsBi) — NILS ROSEMAN$^1$, ALEXEI

New results on the spatial distribution of the electric near-field and the squared intensity of the crystal quality as well as an increase in composition fluctuation.

HL 85.16 Thu 18:00 P4
UV photoluminescence spectroscopy of AlGaN alloys with different Al-contents — CHRISTOPH REICH, JESSICA SCHLEGEL, STELLMAN, URI GVOGT, and MICHAEL KREISLI — Technische Universität Berlin, Institut für Festkörperphysik, Hardenbergstr. 36, 10623 Berlin, Germany

AlGaN alloys are very promising 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 performed optical spectroscopy of GaN 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, SEBASTIAN IMHOP$^1$, ALEXEI CHIRKIN2, MARTIN KOCH$^3$, NICO S. KÖSTER$^3$, KOLJA KOLATA$^3$, SANGAM CHATTERJEE$^3$, STEFAN W. KOCH$^3$, XIANFENG LU$^3$, SHANE R. JOHNSON$^3$, DANIEL A. BEATON$^3$, THOMAS TIEDEM$^3$, OLEG RUBET$^3$, and ANGELA THILHARDO$^3$ — $^1$Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz, Germany — $^2$Fachbereich Physik, Phillips-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 BC, 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 ranges. 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
Semiconductor Physics Division (HL) Thursday

devices, we subsequently embed the nanowires in an insulator (SiO
Müller based nanowires. To this end, p-Si(111) substrates with a top layer of
Small bandgap semiconducting nanowires allow fabricating nanoscale
disorder. A model is introduced to account for both cluster localization and alloy
ments we analyze the data using a Monte Carlo approach. A two-scale
disorder-related features are observed. To better quantify the experi-
tions to experimental results. We find almost perfect agreements for a
x-ray reflections of such optically excited SLs and compare the predic-
tural dynamics initiated by an optical pump pulse and thereby gain
observation of transient rocking curves we can deduce the struc-
ton superlattices (SL) in which photoexcited coherent acoustic phonons
mapping of linear and non-linear phenomena and different samples.

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
are observed.

The propagation of optical pulses through quantum dot media is in-
vestigated. We concentrate on solitary solutions in the conservative
and the gradual transition to the dissipative regime. The influence of
pumping and pumping with cosine temporal form is studied. We intro-
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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 MATTHIAS 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 SO following each n unit cells of (LaSr)\(_n\)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 → ∞) and layered (n = 2, n = 3) SrO(Lao.65Sr0.35MnO)\(_3\) for temperatures above and below the ferromagnetic transition. Fast electronic heating, coupled to electron-phonon coupling and a slow transfer of energy into the lattice structure with strongly anisotropic properties such as a reduction of the excitonic bound state lifetimes 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 SDTs are extracted. 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, and MATTHIAS 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 μJ/cm\(^2\)). To reach a sensitivity on the order of ∆R/\(R_0\) = 10\(^{-7}\), 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 of weakly excited oxide superlattices which exhibit modulations due to the creation 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 SDTs are extracted. We discuss transient spectral changes and the build-up of zone-folded coherent acoustic phonons in the layered samples.

**HL 85.27 Thu 18:00 P4**

Photocurrents in Semiconductor Carbon Nanotubes with Spin-Orbit Interaction ⋅ HONG LIU\(^1,2\), HYUNH THANH DUC\(^1,3\), STEFAN SCHUMACHER\(^3\), and TORSTEN MEIER\(^3\) — 1Department Physik and CeOPP, Universität Paderborn, D-33098 Paderborn, Germany — 2Physics Department, Nanjing Normal University, Nanjing 210067, 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 linear optical response using multi-band self-energy and multi-band vector 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 observations on single-color injection of photocurrents in semiconductor quantum dot structures\([2]\).


**HL 85.28 Thu 18:00 P4**

Analysis of Multidimensional Fourier Transform Spectroscopy for Semiconductors with a Phenomenological Level Model ⋅ CHRISTIAN WIEBELEB, MATTHIAS REICHEL, 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 model is extended to three-dimensional Fourier transform spectroscopy \([3]\) to investigate a recent experiment. \([4]\).


**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 REICHEL, 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\([2]\).


**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 — 1: GRIEBECK\(^1\), V. LEICHEIN\(^1\), I. CARESS\(^1\), M. GLAZOV\(^3\), T. RENCK\(^1\), D. SCHUH\(^1\), W. WEGSCHIEDEL\(^1,2\), and C. SCHÜLLER\(^1\) — 1Institut für Experimentelle und Angewandte Physik, Universität Regensburg, 93040 Regensburg, Germany — 2present adress: ETH Zürich, 8093 Zürich, Switzerland — 3A.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 negligible 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 8-folded 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 a two-dimensional electron systems: dependence on temperature and quantum well width — 1: MICHAEL GRIEBECK, DOMINIK WALLER, GERD PLECHINGER, ELISABETH LEIHERDEN, TOBIAS KORN, DIETER SCHUH, WERNER WEGSCHIEDEL\(^1,2\), and CHRISTIAN SCHÜLLER — 1Institut für Experimentelle und Angewandte Physik, Universität Regensburg, 93040 Regensburg, Germany — 2present adress: Laboratorium für Festkörper-physik, 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 PAPENKORST, TILMANN KUHN, and VOLLRATH MARTIN AXT
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 measured effects in a solid state system. 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 amplification due to the coupling of an electronic quantum beat to the LO phonon frequency is observed. 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, TILMANN KUHN, and VOLLRATH MARTIN AXT
1 Institut für Festkörpertheorie, Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany — 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 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 calculated 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, DANIEL BUCHGOLZ, and PETER SCHMELCHER
1 Zentrum für Optische Quantentechnologien, Universität Hamburg, Germany — 2 Theoretische Physik, 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 controlled 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 — ARKADIUSZ GANZCZARYK, MARTIN GELLER, AXEL LORKE, DIRK REUTER, and ANDREAS D. WIECK
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 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].


HL 85.36 Thu 18:00 P4 Boltzmann equation approach to rectification at a potential step — STEPHEN ROJEC, DANIEL URBAN, FRED HUCHT, and JÜRGEN KÖNG — 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 negative injection bias effect as a function of the determined transverse voltage for the measurements in Ref. [1, 2].


HL 85.37 Thu 18:00 P4 Transport properties of ferromagnet-semiconductor hybrids — LAKHMYRI RAVINDRA, RASMUS BALLMER, SVEN BUCHHOLZ, SASKIA F. FISCHER, ULRICH KUNZEL, ARNE LUDWIG, DIRK REUTER, and ANDREAS WIECK — Werkstoffe und Nanoelektronik, Ruhr-Universität Bochum, D-44780 Bochum, Germany — 1 Neue Materialien, Humboldt Universität zu Berlin, D-12489 Berlin, Germany — 2 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 semi-
conductor could be controlled by the ferromagnetic element [1]. Our
devices consist of GaAS/AlGaAs heterostructure field effect transis-
tor (HFET) with a ferromagnetic Permalloy (Py) nanomage only 35
nm apart from the GaAs channel. The nanostructuring is done with elec-
tron beam lithography and the GaAs channel is patterned by shal-
low 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 mag-
netic field applied in the longitudinal direction which is due to the
magnetic fringing fields emanating from the Py gate.


HL 85.38 Thu 18:00 P4
Concept of a ballistic transfer device in a GaAs/AlGaAs
4-terminal structure using electron refraction — (Michael
Szelenz, Daniel Salloch, Ulrich Kunze, Dirk Reuter, and
Andreas Wieck) 4-Lehrstuhl fuer Werkstoffe und Nanoelektronik,
Ruhr-Universitaet Bochum — 2-Lehrstuhl fuer angewandte Festkor-
physik, Ruhr-Universitaet Bochum

We present a concept of a ballistic four-terminal device based on elec-
tron beam lithography and 1D nanostructures. The conceptual device
consists of a straight arm (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 1.2 · 10^6 cm²/Vs and 2.4 · 10^6 cm²/Vs, respectively. The
device, running 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 nanoscale electron
beam lithography with time-saving UV-lithography. The resist pat-
ttern 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 or more often at the stem's
boundaries and finally hit one of the opposite branches.


HL 85.39 Thu 18:00 P4
Preparation of quantum transport in GaAs/AlGaAs
core/shell nanowires — (Parc Halzentmann, Stephan Wirthe,
Christian Blomers, Karl Weis, Kamil Sladek, Andreas Penz,
Hilde Hardtdegen, Stefan Trenklenkamp, Thomas Schapers,
and Detlef Grützmacher) — Institut fuer Bio- und Nanosys-
temes (IBN-1), Forschungszentrum Julichen, 52425 Julichen, 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 im-
proved 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 in-
trinsic AlGaAs layer, an n-doped AlGaAs layer, an intrinsic AlGaAs
layer and finally a thin GaAs cap layer. For electrical characteriza-
tion the wires were removed mechanically from the original substrate
and subsequently placed on a prepatterned SiO₂-covered Si (100) sub-
strate. Each wire was contacted individually with Au/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 ther-
onelectric transport in laterally microstructured ZnO-based
nanostructures — (Steve P. Hettel, Cornelia Eickhoff, Bruno K.
Meyer, and Peter J. Klar) — Physikalisches
Institut, Justus-Liebig-Universitaet Gießen, Heimrich-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 ex-
ternal 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 heat material.
As the current must flow through the interfaces, all surface pa-
rer layers 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 per-
fomed 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.

Electrical transport properties of TiO₂ single nanotubes —
(Tuhin Subhra Maiti, Jose Quejila, Winfried Böhm, Pablo Esqu
di, Tobias Ruff, and Patrik Schmuk) — Division of Superconductivity
and Magnetism, Institute for Experimental
Physics II, University of Leipzig — 1Department of Materials
Science and Engineering, University of Erlangen Nuremberg

In the present work we investigate the electrical conductivity of single
TiO₂ nanotubes. TiO₂ nanotubes were synthesized by anodization of Ti in
fluoride containing electrolytes. For the characterization of the
electrical properties of the nanotubes an atomic force microscope
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 10^-2 Ωcm. Furthermore, we
explored the effects of atmospheric conditions and light irradiation on
conductivity of single TiO₂ nanotubes.

Temperature dependent transport measurements in quasi-
freestanding graphene on SiC(0001) — (Epaminondas
Karakassidis, Sonja Weingart, Claudia Bock, Ulrich
Kunze, Florian Speck, and Thomas Seyller) — Werkstoffe
und Nanoelektronik, Ruhr-Universitat Bochum — 2Technische 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√3×√3)R30°
reconstruction into graphene via hydrogen intercalation [1]. The
hole concentration of 6 · 10¹² cm⁻² and a mobility of
1900 cm²(Vs)⁻¹ are derived from Hall effect measurements at 2D
structures. These values are constant in a temperature range of
1.4 K ≤ T ≤ 300 K and correspond to a constant mean free path of
l ≈ 50 nm. At T = 1.4 K the bend resistance characteristic of the
1D orthogonal cross junction (w = 50 nm) shows magnetic field de-
pendent negative peaks indicating ballistic transport. As temperature
is increased to T = 50 K a transition from the ballistic into the dif-
fusive transport regime is observed. These results demonstrate that
additional scattering in 1D systems plays an important role.

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which can be tested experimentally by simultaneous transport and lo-
gitudinal and transverse resistance and the disorder distribution,
sults demonstrate a microscopic connection between the macroscopic
components, and provides a small dissipative conductance. Our re-
We show, using diagrammatic methods within a local conductivity
input wire the separation of spin-up and spin-down electrons in this
the center wire that connects the two filter stages, the spin precession
Hall effect. In-plane fields normal to the direction of the electrons' mo-
spin-filter cascades [1]. The transport measurements are conducted at

Room-temperature nanosecond spin-lifetimes in bulk cu-

Thermally activated Transport in Quantum Hall Systems
— · MARKUS GOLLA, MAADI SALMAN, FATHI
— · Institut für Angewandte Physik und Zentrum für Mikrostrukturforschung, Leibniz Universität Hannover, D-31061 Hannover, Germany

We have the Photoleitun gen the T H2-Spektralbereich an Graphen-

Dielectric Film of the Field Effect Transistors
First Principles Investigation of La incorporation in high-

silic on pin solar cells investigated by multi-frequency EMDR
— · CHRISTOPH MEIREN, CHRISTIAN TEUTLOFF, JAN BEHRENS, MATTHIAS FEHN, ALEXANDER SCHNEGG, KLAUS LIPS, ROBERT BITTL — · Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — · Institut für Silizium-Photonik, Helmholtz-Zentrum Berlin für Materialien und Energie, Kekulestr. 5, 12489 Berlin, Germany

electrically detected magnetic resonance (EDMR) can be used to in-
vestigate paramagnetic centres influencing charge transport in semi-
conductors even at concentrations well below the sensitivity threshold
of conventional electron paramagnetic resonance (EPR). This tech-
nique measures conductivity changes in the sample that occur when
spin transitions cause an enhancement or a quenching of currents. EMDR was e.g. successfully employed to microcrystalline Si pin solar

Low-temperature processed Schottky-gated field-effect transistors based on amorphous oxide channel material
— · MILES LORENZ, MICHAEL BECKER, GIANCARLO VON WENCSTERN, MARCUS GRUNDMANN, PEDRO BARQUINHA, ELVIRA FORTUNATO, RODRIGO MARTINS — · Universität Leipzig, Fakultät für Physik und Geowissenschaften, Institut für Experimentelle Physik II, Linnestr. 5, 04103 Leipzig — · CENMAT/IN3, Departamento de Ciencia 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 stand-
ard photolithography using lift-off technique and metalization of the electrodes was accomplished by dc-magnetron sputtering. The best
devices exhibit a threshold swing of 8 – 90 mV/decade and gate

First Principles Investigation of La incorporation in high-k
Dielectric Film of the Field Effect Transistors — · EBRAHIM NADIMI, ROLF ÖTTRING, PHILIPP FLEINZ, MARTIN TRENTZSCHE, TORBEN KEDEM, RICK CARTER, CHRISTIAN RADEHUS, and MICHAEL SCHREIBER — · Institut für Physik, Technische Universität Chemnitz — · GWT TU Dresden GmbH, Geschäftsstelle Chemnitz — · Global Foundries, Dresden
Semiconductor Physics Division (HL)

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. 01M3183A. 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 Bi2Te3, were obtained by a heating procedure. Depending on thickness ratio \( p = d_{\text{BiTe}}/d_{\text{Pb}} \), where the thicknesses of \( d_{\text{BiTe}} \) and \( d_{\text{Pb}} \) are the thicknesses of Bi2Te3 and Pb, respectively, the thermoelectric was up to \( \Delta S \approx 200 \mu \text{K} \) 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 — ●Nielz Mayer, Kathy Lüdge, and Eckhard Schöll — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin
Optoelectronic devices based on semiconductor quantum dot structures promise candidates for future high speed telecom applications with low operation currents, high temperature stability, low chip 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 an InGaAs/PbSe 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.


HL 85.54 Thu 18:00 P4 Influence of interface roughness on relaxation rates and optical gain in a quantum cascade laser — ●Milan Żeleźni, Vítomir Milanović, Jelena Radovanović, and Igor Stanković — Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia — 2Faculty of Electrical Engineering, University of Belgrade, Bela, kralja Aleksandara 73, 11020 Belgrade, Serbia
We present a model for calculating the optical gain in a midinfrared QCLs based on the carrier cascade laser in a thermal field, based on solving the set of rate equations that describe the carrier density in each level, accounting for the optical-photon 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 magnetic field. Numerical results are presented for the structure designed to emit at 11.4 μm, 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/AIGaInP 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 Funktionele 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/AIGaInP quantum dot lasers with different length at different operating parameters, which are pulse width, frequency chirp and temperature. We observed operation at room temperature with a relatively low threshold current density of 792 A/cm² 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 Gilberg, Vitalij Ivanov, and Johann Peter Reitmaier — 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 QDesh active materials. In this work the conditions for trials. In thin of InAs QD lasers and QDesh on the quantum InAgAAs 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 QDesh growth modes. A formation of rather round-shaped dots was observed under Ar2 atmosphere. These new type of QD layers exhibited a significantly reduced height distribution, which reduces the homogeneous 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 InGaAAs 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 compared InP based QD laser. We attribute this stronger 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 Haup1,2, Michael Furitsch1, Hans Lindberg1, Ines Pietzonka1, Uwe Strauss2, and Gerd Bacher2 — Osram Opto Semiconductors GmbH, Leibnitzstrasse 4, 93055 Regensburg, Germany — 1TUM Universität-Duisburg-Essen (RP2) structure with 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
Biofunctionalization of ZnO nanowires for DNA sensory applications — Bettina Rudolph1, Bettina Rudolph2, Wolfgang Fritzsch1, and Carsten Ronning1 — 1Institute of Solid State Physics, University of Jena, Max-Wien-Platz 1, D-07743 Jena — 2Institut für Photonic Technologien e.V., Albert-Einstein-Straße 9, D-07745 Jena

In recent years, DNA detection 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 biosensors 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 for DNA sensor evaluations.[1]  


Preparation and immobilization of noble metal nanoparticles for plasmonic solar cells — Ruoli Wang1,2, Martin Pitzer1,2, Dongzhui Hu1,2, Daniel M. Schaadt1,2, and Liljana Fruk2 — 1Institut für Angewandte Physik, Karlsruhe Institut für Technologie (KIT),76131 Karlsruhe — 2DFG-Zentrum für Funktionelle Nanostruk (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. Polyl 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 particularly focus on the use of nanocubes and nanospheres for solar cell device development. We have extended the nanoparticle preparation, a new method to immobilize nanoparticles 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.

Semiconductor-Insulator-Semiconductor solar cells on wet-chemically etched silicon nanowire carpets using different tunnel barrier materials — Martin Schreivogel1, Bojan Hoffmann2, Gerald Brändl2, Martin Schreivogel1, Bojan Hoffmann2, and Gottfried Christiansen1,2 — 1Institut für Photonic Technologien, Jena — 2Max-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 resulting 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.

Spatially resolved photoluminescence and AFM measurements on Cu(In,Ga)Se2-based thin film absorbers prepared with different throughput speeds — Max Menzen1, Oliver Neumann1,2, Dominik Zutz1, Christoph John1, Ingo Riedel1, and Jürgen Parisi — Thin Film Photovoltaics, Energy and Semiconductor Research Laboratory, University of Oldenburg, D-26111 Oldenburg

CIGS-based thin film solar cells are of high interest due to good electrical properties and low material consumption. Traditional thin-film solar 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. Polyl 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 particularly focus on the use of nanocubes and nanospheres for solar cell device development. We have extended the nanoparticle preparation, a new method to immobilize nanoparticles 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.

Chalcopyrite thin film solar cells made of the compound semiconductor Cu(In,Ga)(S,Sep2 thin film solar cells — Martin Knipper1, Robert Möller2, and Martin Schreivogel1 — 1Institut für Physik, Carl von Ossietzky Universität Oldenburg, Germany — 2Zentrum 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 AM1.5G determined surface roughness on CIGS thin-film solar cells 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 increasing 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. We study the behavior and interdependence of quantities such as photoluminescence (PL) yield, quasi-Fermi level splitting and AM1.5G determined surface roughness on CIGS thin-film solar cells 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 increasing absorber thickness. These results are compared to those on samples thinned by bromine-methanol etching.

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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	extsubscript{2} solar cells by voltage dependent electroluminescence — Felix Daumer	extsuperscript{1,2,} Christian Schett	extsuperscript{1}, Stefan Puttnins	extsuperscript{1,2}, Andreas Rahn	extsuperscript{1}, and Marius Grundmann	extsuperscript{2} — Solaron AG, Ostende 5, 04288 Leipzig, Germany — Institut für Experimentelle Physik II, Universität Leipzig, Linnestr. 5, 04103 Leipzig, Germany

Cu(In,Ga)Se	extsubscript{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 is 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 we will show 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 CuInSe	extsubscript{2} — Janos Kiss, Thomas Grubh, and Claudia Felsers — 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	extsubscript{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 film is deposited as buffer layer. Despite the exhaustive experimental and theoretical research, the atomic and electronic structure of the CIS-CIS 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 CuInSe	extsubscript{2} via performing density functional theory (DFT) calculations on large supercells. We found that bulk CuInSe	extsubscript{2} 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 CuInSe	extsubscript{2}.

HL 85.66 Thu 18:00  P4
Preparation and characterization of Bi	extsubscript{2}S	extsubscript{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	extsubscript{2}S	extsubscript{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	extsubscript{2}S	extsubscript{3} was additionally deposited on epitaxial LaAlO	extsubscript{3} and SrTiO	extsubscript{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 Szabo, 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 (n=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-handgap compounds InGaAsP (0.13 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 Asmus, Rüdiger Schott, and Andreas D. Wiek — Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum

In the last years a great number of alternative and regenerative energy sources becomes more and more important. Solar energy is one of the most promising energy sources for future energy production. The different semiconductor band gaps lead to different emission spectra of solar cells. Thus, the optimization of the solar cell properties is the main focus of research.

This work presents the development and production of a GaAs-based micro-photovoltaic cells with a focus on the material characterization and the optimization of the cell performance. The cells are produced by a typical three step process: first the MBE growth of the GaAs layers, second the wet chemical etching and finally the contact deposition. The characterization of the cell properties is done by電流—电压特性 measurements, the J-V curves allow the determination of the efficiency of the cells. Additionally dark lock-in thermography was used to investigate the uniformity of the cell technology and to detect local defects.

HL 85.69 Thu 18:00  P4
Electroluminescence of Thin Film Silicon Solar Cells — Viola Mönkedölken, Matthias Niederhörger, Helmut Stien, and Ulrich Heinemann — Fraunhofer-Institut für Mikrostrukturphysik, Bielefeld University — 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-modules 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) provides a large DLIT signal, due to the high temperature caused by the increased current. In contrast EL shows effects of the semiconductor material. Shunts are caused by defects in the thin film structure or 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 (λe<λs<λl). Using adequate filters this behavior leads to the analysis of the individual diodes of tandem modules.

In general EL and DLIT show a similar behavior, 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 and Stephan L. Schweizer — Fraunhofer Institute for Microstructure Physics — Martin-Luther-Universität Halle-Wittenberg — Wittenberg — Max-Planck Institute for Metals Research
Metal-assisted Chemical Etching (MaCE) has been proved as a cost-effective route to create silicon nanostructures. In this study, MaCE was employed to texture 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 junctions to achieve more efficient mc-Si solar cell.

Semi-coherent optical modelling of thin film silicon solar cells

Metal-assisted Chemical Etching (MaCE) has been proved as a cost-effective route to create silicon nanostructures. In this study, MaCE was employed to texture 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 junctions to achieve more efficient mc-Si solar cell.

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 modeling with Sentaurus TCAD based on one-dimensional semi-coherent optical model by Janze 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 experimental data. In order to describe the scattering effects at rough interfaces the intensities of the diffuse light are scaled with angular distribution functions. These measurements are obtained from angle resolved scattering experiments. The optical model will be verified by experimental data and compared to the Raytracing 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.


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 simulation approach

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 re-crystallization time and low laser power which limits the a-Si deposition rate. 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.

Transmission Electron Microscopy for thin film solar cells

Transmission Electron Microscopy (TEM) is a powerful tool for investigating the microstructure of thin film solar cells. It allows for a detailed analysis of the material properties and interfaces. In this study, TEM was used to characterize the microstructure of a-Si:H solar cells with different deposition conditions. The TEM images revealed a clear correlation between the microstructure and the electrical properties of the cells. This work is supported by the German Federal Ministry for Education and Research (BMBF).
Lasing in ZnO and CdS Nanowires — Andreas Thielmann, Sebastian Gebrüg, Michael Kozlik, Julian Küchen, 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 morphology. 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.


Lasing in ZnO and CdS Nanowires — Andreas Thielmann, Sebastian Gebrüg, Michael Kozlik, Julian Küchen, Christian Borschel, and Carsten Ronning — Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena

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Low temperature Coulomb anomaly in CMOS compatible silicon quantum dots — Steffen Jauwersena, Mayank Mandal, Dharmraj Kotkerapatib, David Wharamc, Dieter Kern, Marc Sanquerd, and Maud Vinetd — 1Eberhard Karls Universität, Tübingen — 2CEA INAC, Grenoble, France — 3CEA 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 a crucial role. Furthermore fluctuations in the number of dopants in the active region of transistors is 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 sourcedrain 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 $dV_d/dV_g > 1$. 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.


InGaN/GaN nanowire (NW) heterostructures grown by molecular beam epitaxy were compared in this study to 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 an InGaN/GaN nanowire show a wurzite structure of the GaN core and the epilayer 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.

Influence of the nanowire interdistance on growth conditions and crystal structure of self-catalyzed GaAs nanowires grown via MBE — Joachim Humbmann, Benedikt Bauer, Andreas Rudolph, Anna Fontcuberta i Morral, Dieter Schuh —

Dopant-induced morphology evolution of silicon via wet chemical etching — Guogong Yuan, and Saskia F. Fischer

In low dopant concentration silicon the etching process proceeds along 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 phase. The morphol-
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. For this purpose, we applied the Laser Direct Etching (LDE) technique to a SiO$_2$ substrate. 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 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.

Towards site controlled growth of InAs quantum dots on patterned GaAs by microsphere photolithography — •UliRcH RENgSTL, ElIsABEth KOROKnAY, RoBERT RoBnASSch, MiCHAEl JET-TEr, and PETER MICHLER — Institut für Halbleiteroptik und Funk- tionelle Grenzflächen, Universität Stuttgart, Almandring 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 prepatternning a large surface uses microsphere photolithography [1]. For partial exposure of UV-sensitive photoresist, we use a hexagonal close-packed micro- sphere monolayer as an array of microlenses to focus UV-light. We obtained structures with controllable diameters of 300 to 700 nm on 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 prepatternning also leads to an increased accumulation of deposited InAs inside the holes, which supports island formation within the QD ensemble. 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 · 10^{20} 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 cm²/V·s in optical spectroscopy (which is comparable to bulk ITO) to 0.4 cm²/V·s in Hall measurements. This suggests that the mobility for electrical transport in nanoporous ITO films is strongly suppressed by scattering at interparticle boundaries.


Electronic properties of GaN nanowires with different doping concentrations — •MARKUS SChAEFFER, PASCAL HILLE, FLoRIA n FURTMAyR, and MARTIN ECKHOFF — 1 Physikalisches Institut, Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, D-35392 Gießen, Germany — 2 Walter Schottky Institut, Technische Universität München, 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 of plasma-assisted metalorganic vapor phase epitaxy. Using electron microscopy and electron beam lithography. The NWs were aligned by dielectrophoretic manipulation, which allows 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.


Atomistic tight binding models of semiconductor quantum dots — •ÉLISABETH GOLDMANN and FRANK JAHRNKE — Institut für The- oretische 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 sp²s* 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 · 10^5 atoms.

With this ETB model we investigate the electron and hole wave functions and confinement energies of semiconductor nanowire structures such as spherical- and pyramidal-shaped self-assembled InAs quantum dots in a InGaAs 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.


X-ray characterization of Au-free grown GaAs nanowires on Si — •ANDREAS BEERMANN, STEEPEnn BiERMAUnS, AN- TON DAVIDYCO, Lutz GEBHHAR, and UliRCh FRIEChS — 1Universität Siegen, Festkörperphysik, Germany — 2Paul-Drude-Institut für Festkörperproulektronik, 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 growth 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 separa-
rately. Using asymmetric x-ray diffraction on particular zinc-blende (ZB) and wurzite (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 ZB 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.

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**Coupled Quantum Dots for Thermopower Measurements**

- Holger Thierschmann, Lüd Maier, Johannes Knorr, Matthias Mühlbauer, Hartmut Bußmann, 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 thermo-electric 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, thermo-electric 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 thermo-electric properties of two coupled quantum dots. To fill this gap, we designed samples that enable us to perform conductance measurements as well as thermo-electric 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.


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**Electroluminescence from silicon nanoparticles**

- Jens Thies	extsuperscript{1}, Martin Geller	extsuperscript{2}, Axel Lohse	extsuperscript{2}, Hartmut Wiggers	extsuperscript{2}, and Cedrik Meier	extsuperscript{2}
  - 1Fakultät für Physik und Chemie, Universität Duisburg-Essen  
  - 2Physikalisches Institut (EP3), Universität Würzburg, Germany

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 Si as the precursor. The nanoparticles were dispersed in 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	extsuperscript{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.


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**Engineering self-assembled SiGe islands for robust electron confinement in Si**

- Roman O. Rezayi	extsuperscript{1,2}, Suwitt Kiravittaya	extsuperscript{1}, Vladimir M. Fomin	extsuperscript{1}, Armando Rastelli	extsuperscript{2}, and Oliver G. Schmidt	extsuperscript{1}
  - 1Institute for Integrative Nanosciences, IFW-Dresden, D-01069 Dresden, Germany  
  - 2Laboratory 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 nonmonotonic 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 po-
obtained from the transport measurements. 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 nanorodically undoped channels of different widths and thicknesses and various gate lengths, fabricated in the FP7 project AF$\xi$ID with a CMOS compatible process, have been investigated. In this case the Coulomb island may be formed by a single band 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 have dopant volumes of the order of 10$^{10}$ atoms cm$^{-3}$, and a silicon core channel of 8 nm in diameter and 2 nm in thickness. 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.

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 indicate a competition 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 magnetic field. 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.

We report on electronic transport in triple quantum dots in series created from CEA LETI, Grenoble, France — 3CEA INAC, Grenoble, France — 3CEA LETI, Grenoble, France

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 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 its low direct bandgap. At low temperature, magnetic transport measurements were carried out in order to observe electron interference effects.

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 is an InAs quantum dot 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.


We performed magnetotransport measurements on individually contacted GaAs/(Ga,Mn)As nanowires at low temperatures. The core-shell nanowires were grown by MOVPE at a 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 GaAs bulk material with a similar manganese concentration. Also the anisotropy field and coercive fields are significantly larger than for GaAs bulk material.

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 studied 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 sub-
strate • VERENA ZUMBEHR, ALBERT ANDREAS DÖRING, NIKI BENYOUCEF, and JANNEN PETER RETTMAYER — 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 nano-
structures. 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 Strickland-Keastanov (SSK) 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 microscopy) and optical (macro- and micro-
photoluminescence) properties of InGaAs QDs grown by DE on un-
doped (100) GaAs substrates at elevated growth temperatures in the range from 410 °C to 500 °C to preserve the crystal quality of QDs.

HL 85.110 Thu 18:00 P4
Optical properties of ZnO/ZnMgO nanowire heterostruc-
tures • NILS NEUBAUER1, BINGQIANG CAO2, MARIUS GRUNDMANN2, and FRANK CICERO1 — 1Molecular Nanophotonics Group, University of Leipzig, Linnéstraße 5, 04103 Leipzig — 2Semiconductor Physics Group, University of Leipzig, Linnéstraße 5, 04103 Leipzig.
ZnO nanowires are promising candidates for the fabrication of nanoscale 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 het-
terostructures even single-photon emission is a possible require-
ment for future communication technologies like quantum crypto-
graphy. We have investigated ZnO nanowires with a radial and axial ZnO/ZnMgO quantum well heterostructure. These core/shell nanos-
tuctures 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 properties were carried out in a photo luminescence setup. Excitation is done with a frequency quadru-
pled Nd:YVO4 laser in a TIRF (Total Internal Reflection Fluorescence)
configuration. The emitted light is collected confocally and is detected in a Hambury Brown-Twiss setup to study photon correlations.

HL 85.111 Thu 18:00 P4
Control of the carrier density of an inverted GaAs/A1xGa1-xAs 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 quantum dots 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 2DES. 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 un-
charged quantum dot • HEIKE SCHWÄRGER1, FLORIAN KLOTZ2, VALE GJONANOV2, JOHANNES KIERGEL2, CLAYTON C. LICKLE1, NIKI BENYOUCEF2, MARTIN BRANDT1, GEZA GIEBECZ1, and JONATHAN FINLEY2 — 1Max-Planck-Institut für Quantenoptik, Hans-Kopffren-Strasse 1, 85748 Garching — 2Walter 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 mea-
surements allow us to directly monitor the buildup of the nuclear 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 pump out 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 XES • RALF SCHUMANN, PHILIP R. GANZ2, FABRICE WILHOLT2, ANDREAS ROGALSKI2, and DANIEL M. SCHAUERT1 — 1Institute of Applied Physics/DFG-Center for Func-
tional Nanostructures, Karlsruhe Institute of Technology, Germany — 2European 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. We present a new understanding of the incorporation of Cu in the GaN host is desir-
able. 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 se-
ries 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] V. 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 GÖTTLICH, 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 with the response function of the instrument h(t) leads to a signif-
cient broadening of the resulting experimental intensity transients. 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 nu-
merical methods solve a set of linear equations: \[ I_{\text{true}}(t) = \int_{0}^{\infty} h(t) \cdot I_{\text{true}}(t) \, dt \] with the aim to reconstruct \( h(t) \). Both ways are very sensitive to experimentally inevitable noise, mak-
ing deconvolution a sophisticated task. We test different algorithms
and we refer to the pitfalls of the deconvolution for noisy data.

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-
trinsic, a growth process with a lower lattice mismatch, such as MOVPE, can be used. The strain relaxation of the GaN layers is determined by HRXRD. The resulting strains can be used to calculate the strain energy, which is an important factor in the growth of high-quality GaN layers.  

The paper also discusses the local density approximation and its application to GaN-based devices. The authors present experimental results that show the potential of GaN-based devices for future applications. The paper is a valuable contribution to the field of GaN research and will be of interest to researchers and engineers working in this area.
GaN/AlGaN quantum well structures — G. Cloudas, H.-J. Jönen, U. Rosso, and A. Hangleiter — Technische Universität Braunschweig, Institut für Angewandte Physik, Mendelssohnstr. 2, 38106 Braunschweig

The efficiency of GaN/AlGaN quantum well (QW) structures is quite low compared to GaN/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 GaN/GaN quantum structures is based on the observation that every dislocation in highly efficient c-plane GaN/GaN structures is decorated with a so-called V–p, a hexagonal-shaped inverted pyramid with (1011) 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 structures. The decrease of photon energies related to reduced barrier thickness the peak energies observed in photoluminescence decreased from 3.28 eV to 3.12 eV. 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.

U. Rosso, and A. 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 GaN/AlGaN 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 GaN quantum wells determined by X-ray diffraction measurements was 38% and 0.26 mm, respectively. The barrier width was varied for each sample between 4.15 nm, 3.04 nm, 1.30 nm, and 1.00 nm. With decreasing barrier thickness the peak energies observed in photoluminescence decreased from 3.28 eV to 3.12 eV. 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.

U. Rosso, and A. Hangleiter — Technische Universität Braunschweig, Germany

Polaritonic effects in wide-gap semiconductors as a function of temperature — M. Klemann, S. Shokhovets, G. Gobs, and O. Ambacher — Technische Universität Ilmenau, Ilmenau, Germany

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-z 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.

S. Shokhovets, G. Gobs, and O. Ambacher — Technische Universität Ilmenau, Ilmenau, Germany

Dielectric functions of wurzite GaN at elevated temperatures — C. Möller, S. Shokhovets, G. Gobs, K. Köhler, and O. Ambacher — Technische Universität Ilmenau, Ilmenau, 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 (1011) and (2021) 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.

C. Möller, S. Shokhovets, G. Gobs, K. Köhler, and O. Ambacher — Technische Universität Ilmenau, Ilmenau, Germany

Optoelectronical properties of InGaN quantum well light emitting diodes on semipolar GaN — J. Rass, M. Stastчёт, S. Ploch, T. Wernicke, P. Vogt, and M. Kiesel — Technische Universität 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 (1011) and (2021) 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.


Semiconductor Physics Division (HL)

Thursday
quenztchnik, 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$_{0.1}$Ga$_{0.9}$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 a bias 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 WOHL**$^1$, **JESSICA SCHLIEGEL**$^1$, **PATRICK VOOGT**$^1$,
  **SYLVIA HAGEDORN**$^2$, **SVEN EINPELT**$^2$, **MARKUS WEVERS**$^2$, and
  **MICHAEL KNESSEL**$^{1,2}$

$^1$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 based 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 AlGaN-based light-emitting diodes**

- **BASTIAN GALLER**, **ANSGER LAUBSCH**, **ANDREAS WOGICI**, **HANS-JÜRGEN LUGAUER**, **ALVARO GOMEZ-IGLESIAS**, **MATTHIAS SABATH**, and **BEERLICH HANS** — OSRAM Opto Semiconductors GmbH, Leibnistrasse 4, 93055 Regensburg, Germany

Several experiments investigating the efficiency droop in AlGaN-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, we applied uniaxial stress in order to reduce the carrier distribution. We study stress-induced carrier confinement in various AlGaN/InGaN quantum wells by examining the quantum efficiency as a function of temperature and current density.


HL 86 Quantum Dots: Growth and Characterization

Time: Friday 10:15–13:15

**Effects of in-situ annealing on site-selective InAs quantum dots grown on pre-structured GaAs substrates**

- **MATTHEW HELFRIICH**$^{1,2}$, **DANIEL RÄLCE**$^{1,2}$, **JOSHUA HENDRICKSON**$^3$, **MATHIAS GEHL**$^4$, **DONGCHEN HU**$^{1,2}$, **MICHAEL HETTERICH**$^{1,2}$, **STEPAN LENNÉ$^5$**, **MARTIN WEGENER**$^{1,2}$, **GALINA KHITROVA**$^6$, **HYATT M. GIBBS**$^6$, **HEINZ KALT**$^{1,2}$, and **DANIEL M. SCHADEIF**$^{1,2}$

$^1$JFZ-Center for Functional Nanostructures (CFN), Karlsruhe Institute of Technology (KIT),
$^2$Festkörperphysik, Hardenbergstr. 36, 10623 Berlin —
$^3$State Scientific Corp., 27-2 Wright Road, Hollis, NH 03040, U. S. A. —
$^4$College of Optical Sciences, University of Arizona, 1630 E. University Blvd., 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.

**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 excitation 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.

**Atomic structure of submonolayer grown InAs/GaAs quantum dots**


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 and 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) Si 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 In/III ratio are examined on differently prepared silicon surfaces including ex- and in-situ cleaning procedures. Additional improvements for the cleaning and growth is achieved by exposing the Si surface withGa 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 Nanostucturing 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 inscribe the precise transfer of holes defined on e-beam resist to the underlying silicon substrate. The diameter of the diameters 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 μm period.

**HL 86.6** Fri 11:30  FOE Anorg Growth of small-period Si/Ge quantum dot crystals by MBE — **Svetlana Borisova**, Julian C. Gerhardz, Yasin Eking, Gregor Müßler, and Dietlev Grützmacher — Institute of Bio- and Nano systems 1, Forschungszentrum Jülich, D-52425 Jülich, Germany — 2Laboratory 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 drawback of self-assembled Ge QDs is 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 minimal 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 tunneling microscopy (STM).

**HL 86.7** Fri 12:00  FOE Anorg Ultraviolet photoluminescence of zinc oxide quantum dots sputtered at room-temperature — **Gillian Kilian**, Reinhard Schneider, Dimitri Litvinov, Daugmayer Gerhass, Mikhail Fonin, Ulrich Rüdiger, Alfred Leitenstorfer, and Rudolf Bratschitsch — 1Center for Applied Photonics, Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany — 2Laboratorium 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 transmission 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 — **Tilmann Schwager, 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 time between 20s and 300s. 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.


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

**Semiconductor Physics Division (HL)**
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$_3$N$_4$ TEM membrane on which CNTs are grown by means of chemical vapour deposition. The CNTs 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.


Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Germany. 

Institute for Semiconductor and Solid State Physics, Johannes Kepler University Linz, Austria.

Semiconductor nanowires (NW) play a key role in future nanotechnologies. Despite 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 tend to increase the layer thickness along the [110] direction by changing the c-axis, while simultaneously reducing 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 86.10** Fri 12:45 FOE Anorg

Model and applications of local droplet etching — Christian Heyn. 

Institut für Angewandte Physik, Jungiusstr 11, 20555 Hamburg, Germany.

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.


**HL 87.3** Fri 10:45 POT 51 

Electrochemical deposition of ZnO for Flexible Electronic Devices — Miriam Schwarz and Vett Wagner. 

School of Engineering and Science, Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany.

Electrochemical deposition from aqueous zinc nitrate (Zn(NO$_3$)$_2$)$_2$ solution provides a simple way to deposit crystalline ZnO at low temperatures. Thus, it is a suitable process for flexible substrates like polyethylene terephthalat (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, Apurva Dev, Kathrin Sebald, and Tobias Voss. 

Institut für Festkörperphysik, Bremen, Germany.

The exposure of semiconductors to ultrashort laser pulses can lead to 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 $\times$ 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.
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 sulphurphore environment creating an extremely highly doped surface layer. We apply a similar approach for zinc oxide, where we show in previous work that antimony was incorporated to the first 260 nm, resulting in the tracing of a larger number of pulses leads to smaller ripple periods as well as steeper and deeper trestes. Our results are a promising step towards doping zinc oxide surface layers by ultrashort laser pulses.

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**Semiconductor Physics Division (HL)**

Friday

**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-leak atmosphere is analyzed. The origin of these defects will be discussed.

**HL 87.6 Fri 11:30 POT 51**

Metastable state of the VZn_H2 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 VZn_H2 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 (VZn_H2). VZn H2 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 3348.0 cm-1 which represent antisymmetric and symmetric combinations of the two separate O-H stretch modes, respectively. The energy difference between the ground and metastable state of the vacancy 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 STÎNÎR,* MATHIAS ALLARDT1, DANIEL SEVERIN2, MARKUS BENDER2, and JÖRG WEBER2** — 1Technische Universität Dresden, 01062 Dresden, Germany, 2GSF 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**

Zn1−x CdO thin films and heterostructures grown by pulsed laser deposition — **MARTIN LANGE, CHRISTOF P. DITRICH, HOLGER VON WENCKSTERN, MICHAEL LORENZ, and MARIUS GRUNDMANN** — Universität Leipzig, Institut für Experimentelle Physik II, Semiconductor Physics Group, Limestr. 5, D-04103 Leipzig, Germany

Efficient optoelectronic devices are based on heterostructures which requires a gap engineering of the CdO/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 observed.

We used mixed targets of ZnO and CdO and were therefore able to grow the Zn1−x CdO directly on the α-plane sapphire 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 Zn1−x CdO.

Finally, Zn1−x CdO was combined with ZnO thin films and ZnO nanowires in various heterostructures.


**HL 87.9 Fri 12:30 POT 51**

Strain-related defects in MgZn1−x O thin films — **FRIEDRICH SCHMIDT, HOLGER VON WENCKSTERN, and MARIUS GRUNDMANN** — Universität Leipzig, Abteilung Halbleiterphysik, Limnstraße 5, 04103 Leipzig

We investigated the influence of tensile and compressive strain, respectively, on the incorporation of deep levels defects in Mg0.1 Zn0.9 O thin films grown by pulsed-laser deposition on α-plane sapphire substrates. For ZnO it was recently shown that tensile strain induces a new defect level traceable via photoluminescence by the recombination line I12.[1] In order to investigate thin films under tensile and compressive strain, respectively, we chose Al-doped ZnO as buffer layer, because it offers 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 Mg0.1 Zn0.9 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 0 to 0.02. In concordance with ref. [1] we observe the I12 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.


**HL 87.10 Fri 12:45 POT 51**

Strain distribution in ZnO nanowires — **CHRISTOF P. DITRICH, MARTIN LANGE, FABIAN J. KLÜPPEL, RÜDiger SCHMIDT-GRUND, HOLGER VON WENCKSTERN, and MARIUS GRUNDMANN** — Universität Leipzig, Abteilung Halbleiterphysik, Institut für Experimentelle Physik 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 nanowires 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. We show that a thin film of ZnO microwires directly grown on a 6H-SiC substrate is a simple practical approach to study the strain distribution in ZnO microwires. The strain in the nanowires is continuously tunable by bending, which was verified by a 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 along 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
Eckehard Schöll
and nonequilibrium effects on relaxation oscillations in a quantum-dot
of the quantum-dot distribution is taken into account.
Carrier-carrier and carrier-phonon collisions are treated within the ef-
cal approach, where the laser field and active medium are described
under the injection of an external optical signal into the laser cavity.
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 influence laser dynamics[1]. With our simulations, we now investi-
gate 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 semiclassi-
cal 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 ef-
erative relaxation rate approximation. Inhomogeneous broadening
of the quantum-dot distribution is taken into account.
and nonequilibrium effects on relaxation oscillations in a quantum-dot

Optical Gain, Thermal Resistance and Antiguiding Factor of
Ga-based Laser Diodes from UV to Green — •Wolfgang
Scheibenzuber1, Ulrich Schwarz2, Teresa Lehmer3, Stephan
Lütgen2, and Uwe Strauß2 — 1Fraunhofer IAF, Tullastrasse 72,
D-79108 Freiburg, Germany — 2Osmar Opto Semiconductors GmbH,
Leibnizstrasse 4, D-93055 Regensburg, Germany
For highly efficient Ga-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, in-
ternal 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 electrolu-
minescence 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.

Implementing 330 nm UV-output by frequency doubling of a
miniaturized red AlGaInP-VECSEL emitting at 660 nm — •Hermann Kähle, Thomas Schwarzkopf, Marcus Escherfelder,
Wolfgang-Michael Schulz, Robert Rossbach, Michael Jetter,
and Peter Michler — Institut für Halbleiteroptik und Funktione
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-
onorganic vapour-phase epitaxy on GaAs substrates for an operation
wavelength of around 660 nm. Five QW packages are placed in
(Al0.55Ga0.45)0.51In0.49P cladding layers, which are lattice matched
to GaAs, in a resonant periodic gain design. Each package consists
of four QWs embedded in (Al0.33Ga0.67)0.51In0.49P barriers. The 3 λ
thick cavity is fabricated on an Al0.5Ga0.5As/MAs distributed
Bragg reflector. By inserting a BB0-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.

Thermal properties of high power vertical-external-cavity
surface-emitting lasers — •Alexej Chernikov1, Jens
Herrmann1, Maik Schellner1, Martin Koch1, Bernadette
Kunert1, Wolfgang Stolz2, Sangam Chatterjee2, Stephan
W. Koch1, Trien-Luan Wang1, Yoshi Kanaeda3, Joe M.
Yarbrough2, Jörg Hader4, and Jerome V. Moloney2
1Faculty of Physics and Material Sciences Center, Philippus-Universität
Marburg, Renthof 5, D-35032 Marburg, Germany — 2College of
Optical Sciences, The University of Arizona, 1630 East University Boule-
vard, Tucson, Arizona, 85721, USA

Parameter that connects the energetic shift of the wire luminescence
and the applied uniaxial stress.

Quantum Dot Lasers
Effects of Many-Body Coulomb Effects on Injection-Locked
36, 10623 Berlin, Germany — Physik, Sekr. EW 7-1, Technische Universität Berlin, Hardenbergstr.
Eckehard Schöll

Low temperature CVD-synthesis of nitrogen doped ZnO
thin films — •Sebastian Ehrmann, Stefan Lautenschläger,
Michael N. Hopmann, Andreas Lauper, Melanie Pinnisch,
Christian Reindl, Julian Benz, Peter J. Klair, and Bruno
K. Meyer1, Institut für 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 success-
ful 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) anal-
ysis. Furthermore, ZnO diode structures were fabricated and inves-
tigated 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 fea-
ture increases with increasing nitrogen content. The IV-measurements
reveal typical diode-like behaviour of the ZnO diode structures.

GaN-based Laser Diodes from UV to Green
Optical Gain, Thermal Resistance and Antiguiding Factor of
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 im-
plantation of zinc ions and thermal annealing at low oxygen partial
pressures increase its concentration. From photo- capacitance trans-
sients the photo-ionisation cross- section spectrum was calculated.

Semiconductor Physics Division (HL)
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 the device. Our results illustrate the substantial importance of the 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-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 ~25 dB.

Review of the performance of semiconductor lasers in the mid-infrared...
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 2-3 μm 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 2.0 μm but with different active region designs, optimized for barrier-pumping at 1.0 μm (GaAsSb-barriers) and 1.5 μm (GaSb-barriers). Both structures were characterized in pulsed mode in order to reduce thermal heating effects. At room temperature, the power efficiency of the 1.5 μm-pumped structure is 1.43-times higher than the 1.0 μm-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 1.5 μm-pumped structure. We attribute this effect to the reduced barrier height of the latter structure and thus increased heterobarrier leakage.

Investigation of heat dissipation in Mid-Infrared Quantum cascade lasers — Stefanie Mayer, Christian Schilling, Ralf Ostendorf, Quankui Yang, Rainer Löscher, 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 element analysis. The influence of different mounting techniques and of different heat spreaders on the temperature profile and the heat dissipation is investigated. Additionally, different active region designs, optimized for barrier-pumping at 1.0 μm and 1.5 μm have been send along 001-crystallographic direction. In this geometry we have reported on detailed investigation of complex susceptibilities.

We report on electric-field-induced second-harmonic generation (SHG) in the GaAs semiconductor in the vicinity of the band gap. The light is reflected 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 1.5 μm-pumped structure. We attribute this effect to the reduced barrier height of the latter structure and thus increased heterobarrier leakage.

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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 Schwager, Andrea Stemmann, Stefan Menda, 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-gap 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-gap thin film layer.


HL 89.5 Fri 11:15 POT 251

By altering the growth parameters for BaTiO$_3$/SrTiO$_3$ heterostructures we achieved matching of the refractive index for selected wavelength. 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 the initial AlAs layers. Reflectivity measurements confirm the existence of the air-gap thin film layer.

HL 89.6 Fri 11:30 POT 251
Effect of localized boron impurities on the line shape of the fundamental band gap transition in photoluminescence spectra of (B,Ga,In)As — Thomas Sanders, Jörn Teubert, Peter J. Klan, Andrew Lindsay, and Eoin O'Reilly — Institute of Experimental Physics I, Justus-Liebig University Giessen, Germany — Tyndall National Institute, Lee Maltings, Cork, Ireland

Photoluminescence (PL) as well as Raman scattering of individual NWs have been grown by the wet chemical solution liquid solid technique [2]. Time resolved measurements of circular polarization reveal rather trivial spin dynamics of donor localized electrons. Initially the degree of circular 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 is 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.

Surface acoustic wave induced electron tunneling from an InGaAs/GaAs wetting layer — Jens Pustinowski, Florian J. R. Schröter, Dirk Reuther, Andreas D. Wierck, Max Bichler, Kai Müller, John J. Finley, Achim Wixforth, and Hubert J. Klüpfel — Lehrstuhl für Experimentelle Physik I, Universität Augsburg, 86159 Augsburg, Germany — Lehrstuhl für Angewandte Festkörperphysik, 47480 Bochum, Germany — 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 focused into the wetting layer to lock the frequency of the SAW to 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 originates 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.


HL 89.7 Fri 12:00 POT 251
HL 89.8 Fri 12:15 POT 251
Optical orientation of Mn$^{2+}$ ions in bulk GaAs under application of weak longitudinal magnetic fields ($B$ ≤ 150 mT). The studied samples were grown by liquid phase epitaxy and Crochalski method and were doped with a low Mn acceptor concentration of 1 x 10$^{18}$ cm$^{-3}$. Time resolved measurements of circular polarization for donor-acceptor photoluminescence in Faraday geometry reveal non-trivial spin dynamics of donor localized electrons. Initially the degree of circular 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 is 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.
Excitonic Absorption Spectra with Energetic Disorder — DEAN HURON, JENS FÖRSTNER, MALTE V. REICHHOLD, and TOBIAS MEIER — Department of Physics and CeQFP, 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.


Exciton dynamics in potential traps and the possibility of Bose-Einstein condensation — •RICO SCHWARTZ1, NOBUKO NAKA2,3, JAN BRANDT4, CHRISTIAN SANFORD4, and HEINRICH STOLZ5 — 1Institut für Physik, Universität Rostock, D-18051 Rostock, Germany — 2Department of Physics, Kyoto University, Kyoto 606-8502, Japan — 3PRESTO, JST, 4-1-8 Honcho Kagawa-cho, Saitama 332-0012, Japan — 4Fakultät Physik, Technische Universität Dortmund, D-44221 Dortmund, Germany

Experiments on excitons in Cu2O 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]. Concomitantly, we reached exciton numbers in the order of 106 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.


HL 90.11 Fri 13:00 POT 254
Excitonics in Potential Traps and the Possibility of Bose-Einstein Condensation

HL 90.09 Fri 12:45 POT 251
Excitonic Absorption Spectra with Energetic Disorder

HL 90.12 Fri 13:15 POT 251
Zero-magnetic-field spin-splitting and the warping in the valence band of highly doped amorphic AlGaAs/GaAs Quantum Wells — •MICHAEL HIRMER, M. HIRMER, D. SCHUR, W. WEIGSCHREIDER, T. KORN, and C. SCHÜLLER — Institut für Experimentalphysik, 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∥. In our experiments, we focus on highly doped amorphic AlGaAs/GaAs QW. We utilize electronic interband 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 interband 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.


[2] Nextnano3 by Stefan Birner

HL 90: Intersectional Joint Session: Nano Plasmonic

Time: Friday 10:30–13:00

Invited Talk

HL 90.01 Fri 10:30 BAR 205
Plasmon Driven Higher Harmonics Generation — IN-YONG PARK, SEUNGCHUL KIM, JOON-HEE CHOI, and SEUNG-WOO KIM — Ultralight optics for ultraprecision research group, KAIST, Daejeon, Republic of Korea

Plasmon resonance enables field enhancement of a low-intensity fs pulse, permitting high harmonic generation with 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 microstructure. 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 wavelengths in the millimeter scale, can funnel through nano slits and nano slot antennas. The field enhancement is enormous, three orders of magnitude lower than those from literature [2]. Concomitantly, we reached exciton numbers in the order of 106 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.


Invited Talk

HL 90.02 Fri 11:00 BAR 205
Structure and Dynamics of Free Nanoparticles: From Charging to Time-Resolved Photoemission — •ECKHARD 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 nanoparticle measurements show properties dependent on 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 90.03 Fri 11:30 BAR 205
Terahertz Nano Plasmonics — •DAI-SIK KIM — Center for Sub-wavelength 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 electromagnetic waves in free space.

Invited Talk

HL 90.4 Fri 12:00 BAR 205  
Couloumb complexes: Electron emission from clusters in strong FEL pulses — Ulff 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 multipole charged by massive electron emission. We device a model, which we call Couloumb complexes [1], in order to investigate the emission process. It turns out that the electron spectra strongly depend upon the ionization rate. For high 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 understood in terms of our model containing only few parameters available from experiments.


Invited Talk

HL 90.5 Fri 12:30 BAR 205

HL 91: Joint Focussed Session: Theory and Computation of Electronic Structure: New Frontiers VIII

Time: Friday 11:15–12:45

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 raise 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 latter 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 — Ralph Hamachek, Christine Giorgetti, Xochity Lopez-Lozano, and Lucia Reining — 1LSI, Ecole Polytechnique, CNRS, CEA/DSM, Palaiseau, France — 2European Theoretical Spectroscopy Facility — 3University 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 uneffective 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 nanotubes (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 $$\varepsilon(q, q', \omega)$$ 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.


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 Rischlikon, 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.


HL 91.4 Fri 12:15 TRE Phy  
Impact ionization rates from ab initio calculations — Marton Voros, Dario Rocca, Giorgio Zimanyi, Giulia Galli, and Adam Galli — 1Budapest University of Technology and Economics, Department of Atomic Physics — 2UC Davis, Department of Chemistry — 3UC Davis, Department of Physics — 4Hungarian 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
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limit when building semiconductor-based solar cells. A thorough, 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.

Selective Excitation of Molecular Vibrations by Tunneling Electrons — Jessica Walkenhorst¹, Marius Wanko¹, Alberto Castro², and Angel Rubio¹ — 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 — 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.