Semiconductor Physics Division
Fachverband Halbleiterphysik (HL)

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Vice Chairs:
Kathrin Sebald,
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Gabriel Bester,
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Overview of Invited Talks and Sessions

(Lecture rooms H2, H10, H13, H14, H15, H16, and H17; Poster A)

Invited Talks

HL 5.1	Mon	9:30–10:00	H15	**Quantum optics with quantum dots in photonic wires** — •Jean-Michel Gerard
HL 6.6	Mon	11:15–11:45	H16	**Epitaxial paradigms of van der Waals bonded chalcogenide materials** — •Raffaella Calarco
HL 11.1	Mon	11:30–12:00	H10	**A clean single electron source using voltage pulses generating levitons.** — •Christian Glattli
HL 11.4	Mon	12:30–13:00	H10	**(De)coherence of single electron wavepackets in quantum Hall edge channels** — •Erwann Bocquillon, Arthur Marguerite, Vincent Freulon, Jean-Marc Berroir, Bernard Plaçais, Antonella Cavanna, Yong Jin, Gwendal Fève
HL 12.1	Mon	14:45–15:15	H2	**Surface chemistry of colloidal semiconductor nanocrystals** — •Zeger Hens
HL 13.1	Mon	14:45–15:15	H10	**Energy- and time-resolved detection of hot single-electron wave packets** — •Masaya Kataoka
HL 13.3	Mon	15:30–16:00	H10	**The reabsorption effect with single-electron sources** — •Géraldine Haack, Michael Moskalets
HL 13.5	Mon	16:45–17:15	H10	**Electronic states in a driven quantum contact** — •Mihajlo Vanevic, Julien Gabelli, Wolfgang Belzig, Bertrand Reulet
HL 13.10	Mon	18:15–18:45	H10	**Clocked single-electron transfer: quantized currents and electron pair partitioning** — •Frank Hohls
HL 15.7	Mon	16:15–16:45	H16	**Mechanical Control of Excitonic States in Quantum Dots** — Rinaldo Trotta, Javier Martín-Sánchez, •Armando Rastelli
HL 16.1	Mon	14:45–15:15	H17	**Advances in Raman Spectroscopy of Graphene and Layered Materials** — •Andrea C. Ferrari
HL 16.5	Mon	16:15–16:45	H17	**Thermodynamic picture of ultrafast conduction in graphene** — •Dmitry Turchinovich, Zoltan Mics, Klaas-Jan Tielrooij, Ivan Ivanov, Xinliang Feng, Klaus Müllen, Mischa Bonn
HL 22.8	Tue	11:45–12:15	H10	**Coherent Quantum Dynamics of Excitons in Atomically Thin Semiconductors** — •xiaoqin li
HL 26.1	Tue	9:30–10:00	H16	**Exploring spin quantum state decoherence in optically active quantum dots** — •Jonathan Finley
HL 30.1	Tue	11:00–11:30	H16	**On-chip quantum photonics with integrated quantum dot emitters** — •Mark Fox
HL 30.2	Tue	11:30–12:00	H16	**Quantum photonics with quantum dot single photons in silicon oxynitride waveguide circuits** — •Anthony Bennett, James Lee, David Ellis, Eoin Murray, Frederik Floether, Jonathon Griffiths, Thomas Meany, Ian Farrer, David Ritchie, Andrew Shields
HL 30.3	Tue	12:15–12:45	H16	**GaAs integrated quantum photonics** — •S. Höfling, C. P. Dietrich, A. Fiore, M. Thompson, M. Kamp
HL 30.4	Tue	12:45–13:15	H16	**Photonic integrated circuits with on-chip single-photon emitters based on III-V semiconductors** — •Mario Schwartz, Ulrich Rengstl, Thomas Herzog, Matthias Paul, Jan Kettler, Simone Luca Portalupi, Michael Jetter, Peter Michler

HL 37.4	Tue	15:30–16:00	H10	**Blasting semiconductor electrons with terahertz fields** — •Mackillo Kira
HL 40.1	Tue	14:45–15:15	H16	**On-chip generation, routing and detection of nonclassical light** — •Kai Müller, Kevin A. Fischer, Constantin Dory, Günther Reithmaier, Fabian Flassig, Konstantin G. Lagoudakis, Tomas Sarmiento, Michael Kaniber, Jonathan J. Finley, Jelena Vuckovic
HL 40.2	Tue	15:15–15:45	H16	**On-chip quantum optics using quantum dot microcavities and waveguide structures** — Pierce Munnelly, Matthias Karow, Arsenty Kaganskiy, Jan-Hindrik Schulze, Andre Strittmatter, Martin Kamp, Sven Rodt, Sven Höfling, Tobias Heindel, Christian Schneider, •Stephan Reizenstein
HL 41.1	Tue	14:45–15:15	H17	**Ultrafast carrier dynamics in monolayer graphene** — •Daniele Brida
HL 44.1	Wed	9:30–10:00	H10	**Rydberg excitons in cuprous oxide** — •Manfred Bayer
HL 44.11	Wed	12:45–13:15	H10	**From a loophole-free Bell test to a secure quantum Internet** — •Ronald Hanson
HL 48.5	Wed	11:00–11:30	H15	**Exciton-polariton thermodynamics in ZnSe-based microcavities** — •Sebastian Klembt, Emilien Durupt, Sanjoy Datta, Thorsten Klein, Yoan Léger, Augustin Baas, Charsten Kruse, Detlef Hommel, Anna Minguzzi, Maxime Richard
HL 49.1	Wed	9:30–10:00	H16	**Probing bandgap renormalization, excitonic effects, and interlayer coupling in 2D transition metal dichalcogenide semiconductors** — •Miguel M. Ugeda, Aaron Bradley, Sufei Shi, Felipe H. Jornada, Yi Zhang, Diana Qiu, Wei Ruan, Sebastian Wickenburg, Alexander Riss, Jiong Lu, Sung-Kwan Mo, Zahid Hussain, Zhi-Xun Shen, Feng Wang, Steven G. Louie, Michael F. Crommie
HL 49.5	Wed	11:15–11:45	H16	**Enhanced light-matter coupling and single-photon emission of atomically thin semiconductors** — •Rudolf Bratschitsch
HL 49.6	Wed	11:45–12:15	H16	**Optical Properties and Carrier Dynamics in Transition Metal Dichalcogenides** — •Alexander Steinhoff-List, Malte Rösner, Matthias Florian, Michael Lorke, Christopher Gies, Ji-Hee Kim, Deok-Soo Kim, Chanwoo Lee, Gang Hee Han, Mun Seok Jeong, Tim Wehling, Frank Jahnke
HL 58.1	Wed	14:45–15:15	H2	**Ultrafast excitonic and charge transfer dynamics in nanostructured organic polymer materials** — •Irene Burghardt, Robert Binder, Matthias Polkehn, Hiroyuki Tamura
HL 59.6	Wed	16:00–16:30	H10	**Discontinuous Galerkin Methods in Nano-Photonics** — •Kurt Busch
HL 68.1	Thu	9:30–10:00	H10	**Modifications of material and chemical properties of organic molecules driven by QED phenomena** — •Francisco Garcia-Vidal
HL 72.1	Thu	9:30–10:00	H16	**Group IV alloys: New tricks with Silicon** — •Detlev Grützmacher
HL 72.4	Thu	10:30–11:00	H16	**SiGe heterostructures for photonics interconnects** — •Giovanni Isella, Jacopo Frigerio, Andrea Ballabio, Daniel Chrastina, Vladyslav Vakarin, Papichaya Chaisakul, Laurent Vivien, Delphine Marris-Morini
HL 83.1	Thu	14:45–15:15	H16	**Electronic properties and applications of functionalized wide gap semiconductors** — •Martin Stutzmann
HL 84.1	Thu	14:45–15:15	H17	**Resonant plasmonic nanoantennas for mid-infrared spectroscopy and sensing** — •Frank Neubrech, Harald Giessen
HL 95.4	Fri	10:45–11:15	H10	**Nano-architectures and organic-inorganic hybrid material combinations for novel photovoltaic device concepts** — •Silke Christiansen
HL 99.1	Fri	9:30–10:00	H17	**Multifunctional 3D GaN: strategies for solid state lighting, electronics and sensing** — •Andreas Waag, J. Hartmann, Hao Zhou, S. Fündling, F. Steib, M. Mohajerani, Feng Yu, H.-H. Wehmann, A.E. Gad, D. Prades, D. Bichler, B. Huckenbeck, T. Schimpke, M. Mandl, I. Stoll, A. Avramescu, M. Strassburg, H.-J. Lugauer

Invited talks of the Tutorial "Plasmonics"

HL 1.1	Sun	16:00–16:45	H15	**Graphene and Metal Plasmonics for Mid-IR Biosensing** — •Hatice Altug
HL 1.2	Sun	16:45–17:15	H15	**Active 3D plasmonics** — •Na Liu
HL 1.3	Sun	17:30–18:00	H15	**Infrared nanoscopy and nano-FTIR spectroscopy by elastic light scattering from a scanning probe tip** — •Rainer Hillenbrand

HL 1.4	Sun	18:00–18:30	H15	**Complex functional plasmonics: Ultrafast hybrid nonlinear plasmonics** — •Harald Giessen

Invited talks of the joint symposium SYHP, "Fundamentals of Hybrid and Perovskite Photovoltaics"

See SYHP for the full program of the symposium.

SYHP 1.1	Mon	9:30–10:00	H1	**Perovskite Semiconductors: Opportunities and Challenges for Photovoltaic Materials Design** — •David B. Mitzi
SYHP 1.2	Mon	10:00–10:30	H1	**Perovskite Solar Cells: A new Paradigm in Photovoltaics** — •Mohammad Nazeeruddin
SYHP 1.3	Mon	10:30–11:00	H1	**Charge-Carrier Diffusion and Radiative Efficiencies in Hybrid Metal Halide Perovskites** — •Laura Herz
SYHP 1.4	Mon	11:15–11:45	H1	**Photovoltage losses in perovskite solar cells** — •Kristofer Tvingsted
SYHP 1.5	Mon	11:45–12:15	H1	**Computational screening of perovskite solar energy materials** — •Karsten W. Jacobsen

Invited talks of the joint symposium SYTI, "Topological Insulators"

See SYTI for the full program of the symposium.

SYTI 1.1	Wed	9:30–10:10	H1	**Topological insulators and topological superconductors** — •Shoucheng Zhang
SYTI 1.2	Wed	10:10–10:50	H1	**Three-dimensional topological insulators and superconductors** — •Yoichi Ando
SYTI 1.3	Wed	10:50–11:30	H1	**Interplay of magnetic and electronic states in pyrochlore iridates** — •Leon Balents
SYTI 1.4	Wed	11:40–12:20	H1	**Magnetic imaging of edge states** — •Kathryn Moler
SYTI 1.5	Wed	12:20–13:00	H1	**Sub-nm wide edge states at the dark side of a weak topological insulator** — •Markus Morgenstern

Invited talks of the joint symposium SYQS, "Quantum Effects in Magnetism"

See SYQS for the full program of the symposium.

SYQS 1.1	Wed	15:00–15:30	H1	**Magnonic macroscopic quantum states and supercurrents** — •Burkard Hillebrands, Dmytro A. Bozhko, Alexander A. Serga
SYQS 1.2	Wed	15:30–16:00	H1	**Elementary excitations of magnetic insulators and its heterostructures with metals** — •Gerrit Bauer
SYQS 1.3	Wed	16:00–16:30	H1	**Cavity Spintronics** — •Can-Ming Hu
SYQS 1.4	Wed	16:45–17:15	H1	**Hybrid Quantum Systems - Coupling Color Centers to Superconducting Cavities** — •Johannes Majer
SYQS 1.5	Wed	17:15–17:45	H1	**Quantum enhanced sensing with single spins in diamond** — •Fedor Jelezko

Invited talks of the joint symposium SYES, "Frontiers of Electronic-Structure Theory"

See SYES for the full program of the symposium.

SYES 1.1	Fri	9:30–10:00	H1	**Intrinsic Transport Coefficients and Momentum Space Berry Curvatures** — •Allan H MacDonald
SYES 1.2	Fri	10:00–10:30	H1	**Berry phase linked spin-orbit torques in Ferromagnetic and Antiferromagnetic systems** — •Jairo Sinova
SYES 1.3	Fri	10:30–11:00	H1	**Transport in Topological Insulators and Topological Superconductors: In Search of Majorana Fermions** — •Ewelina Hankiewicz
SYES 1.4	Fri	11:15–11:45	H1	**Engineering Topological Quantum States: From 1D to 2D.** — •Jelena Klinovaja
SYES 1.5	Fri	11:45–12:15	H1	**Skyrmions – Topological magnetization solitons for future spintronics** — •Stefan Blügel

Sessions

HL 1.1–1.4	Sun	16:00–18:30	H15	**Tutorial: Plasmonics**
HL 2.1–2.3	Sun	16:00–18:30	H18	**Tutorial: Hybrid and Perovskite Photovoltaics (Joint session of CPP, DF, DS and HL, organized by CPP)**
HL 3.1–3.5	Mon	9:30–12:15	H1	**Symposium SYHP: Fundamentals of Hybrid and Perovskite Photovoltaics (Joint session of CPP, DF, DS and HL, organized by CPP)**
HL 4.1–4.12	Mon	9:30–13:00	H13	**Spintronics: Nanostructures and Optics**
HL 5.1–5.8	Mon	9:30–12:15	H15	**Quantum Dots and Wires: Single Photon Sources**
HL 6.1–6.11	Mon	9:30–13:00	H16	**Two-dimensional Materials (Joint session of HL, DS and O, organized by HL)**
HL 7.1–7.10	Mon	9:30–12:30	H17	**Graphene: Theory (Joint session of DS, HL and TT, organized by HL)**
HL 8.1–8.11	Mon	9:45–13:00	H22	**Transport: Quantum Coherence and Quantum Information Systems - Experiment (Joint session of HL, MA and TT, organized by TT)**
HL 9.1–9.11	Mon	10:30–13:30	H24	**Graphene I: Structure and Dynamics**
HL 10.1–10.10	Mon	10:30–13:15	S054	**Plasmonics and Nanooptics: Light-Matter Interaction**
HL 11.1–11.4	Mon	11:30–13:00	H10	**Focus Session: Single Particle Sources for Electronic Devices I (Joint session of HL and TT, organized by HL)**
HL 12.1–12.12	Mon	14:45–18:30	H2	**Photovoltaics (Joint session of HL and DF, organized by HL)**
HL 13.1–13.10	Mon	14:45–18:45	H10	**Focus Session: Single Particle Sources for Electronic Devices II (Joint session of HL and TT, organized by HL)**
HL 14.1–14.10	Mon	14:45–17:45	H13	**Spintronics: Transport and Theory**
HL 15.1–15.13	Mon	14:45–18:45	H16	**Quantum Dots and Wires: Fabrication and Devices**
HL 16.1–16.8	Mon	14:45–17:45	H17	**Graphene: Transport (Joint session of DS, HL and TT, organized by HL)**
HL 17.1–17.10	Mon	15:00–17:45	H18	**Transport: Topological Insulators - 2D (Joint session of DS, HL, MA, O and TT, organized by TT)**
HL 18.1–18.11	Mon	15:00–18:00	S054	**Plasmonics and Nanooptics I: Microscopy**
HL 19.1–19.9	Mon	15:00–17:30	H38	**Hybrid and Perovskite Photovoltaics I (Joint session of CPP, DS and HL, organized by CPP)**
HL 20.1–20.7	Mon	15:45–17:45	H51	**Frontiers of Electronic Structure Theory: Focus on Topology and Transport**
HL 21.1–21.4	Mon	17:45–18:45	H17	**Graphene: Fabrication (Joint session of DS, HL and TT, organized by HL)**
HL 22.1–22.12	Tue	9:30–13:15	H10	**Ultrafast Phenomena I (Joint session of HL and O, organized by HL)**
HL 23.1–23.12	Tue	9:30–13:00	H13	**Oxide Semiconductors I**
HL 24.1–24.8	Tue	9:30–12:00	H14	**Carbon-based Nanostructures**
HL 25.1–25.10	Tue	9:30–12:30	H15	**Quantum Information Systems (Joint session of HL and TT, organized by HL)**
HL 26.1–26.3	Tue	9:30–11:00	H16	**Quantum Dots and Wires: Quantum Optics I**
HL 27.1–27.12	Tue	9:30–13:00	H17	**Zinc Oxide and Zinc Selenide**
HL 28.1–28.12	Tue	9:30–12:45	H22	**Transport: Quantum Coherence and Quantum Information Systems - Theory 1 (Joint session of HL, MA and TT, organized by TT)**
HL 29.1–29.8	Tue	10:45–13:00	H37	**Hybrid and Perovskite Photovoltaics II (Joint session of CPP, DS and HL, organized by CPP)**
HL 30.1–30.4	Tue	11:00–13:15	H16	**Focus Session: On-Chip Quantum Photonics I**
HL 31.1–31.3	Tue	12:15–13:00	H14	**Silicon-based Semiconductors I**
HL 32.1–32.4	Tue	14:00–15:00	H22	**Transport: Quantum Coherence and Quantum Information Systems - Theory 2 (Joint session of HL, MA and TT, organized by TT)**
HL 33.1–33.7	Tue	14:00–16:00	H24	**Frontiers of Electronic Structure Theory: Focus on Topology and Transport I**
HL 34.1–34.5	Tue	14:00–15:15	H31	**Magnetic Semiconductors I (Joint session of HL and MA, organized by MA)**
HL 35.1–35.51	Tue	15:00–19:00	Poster A	**Poster I**
HL 36.1–36.38	Tue	15:00–19:00	Poster A	**Poster Ib**
HL 37.1–37.4	Tue	14:45–16:00	H10	**Ultrafast Phenomena II**

HL 38.1–38.4	Tue	14:45–15:45	H13	**Oxide Semiconductors II**
HL 39.1–39.4	Tue	14:45–15:45	H14	**Silicon-based Semiconductors II**
HL 40.1–40.3	Tue	14:45–16:00	H16	**On-Chip Quantum Photonics II**
HL 41.1–41.3	Tue	14:45–15:45	H17	**Graphene: Optics (Joint session of HL and TT, organized by HL)**
HL 42.1–42.6	Tue	14:00–15:30	H37	**Organic Electronics and Photovoltaics I (Joint session of CPP, DS, HL and O, organized by CPP)**
HL 43.1–43.5	Wed	9:30–13:00	H1	**Symposium SYTI: Topological Insulators: Status Quo and Future Directions (Joint session of DS, HL, MA, O and TT, organized by TT)**
HL 44.1–44.11	Wed	9:30–13:15	H10	**Optical Properties I**
HL 45.1–45.8	Wed	9:30–11:45	H11	**Hybrid and Perovskite Photovoltaics III (Joint session of CPP, DS and HL, organized by CPP)**
HL 46.1–46.6	Wed	9:30–11:30	H13	**Organic Semiconductors**
HL 47.1–47.7	Wed	9:30–11:45	H14	**Quantum Hall Effect**
HL 48.1–48.7	Wed	9:30–12:00	H15	**Quantum Dots and Wires: Microcavities**
HL 49.1–49.9	Wed	9:30–13:00	H16	**Focus Session: Many-body effects in two-dimensional materials (Joint session of HL and O, organized by HL)**
HL 50.1–50.13	Wed	9:30–13:15	H17	**Gallium Nitride: Fabrication and Characterization**
HL 51.1–51.13	Wed	9:30–13:15	H22	**Transport: Graphene (Joint session of DS, DY, HL, MA, O and TT, organized by TT)**
HL 52.1–52.10	Wed	9:30–12:15	H32	**Spintronics (incl. quantum dynamics) (Joint session of HL, MA and TT, organized by MA)**
HL 53.1–53.42	Wed	9:30–13:30	Poster A	**Poster II**
HL 54.1–54.10	Wed	10:30–13:00	H24	**Frontiers of Electronic Structure Theory: Focus on Topology and Transport II**
HL 55.1–55.11	Wed	10:30–13:15	S051	**Photonics and Nanooptics I: Nonlinear Response**
HL 56.1–56.10	Wed	10:30–13:00	S053	**2D Materials: Growth**
HL 57.1–57.3	Wed	12:15–13:00	H15	**Quantum Dots and Wires: Quantum Optics II**
HL 58.1–58.12	Wed	14:45–18:30	H2	**Organic Photovoltaics and Electronics**
HL 59.1–59.12	Wed	14:45–18:30	H10	**Optical Properties II**
HL 60.1–60.8	Wed	14:45–17:15	H13	**III-V Semiconductors (no Nitrides)**
HL 61.1–61.9	Wed	14:45–17:30	H16	**Quantum Dots and Wires: Transport Properties**
HL 62.1–62.13	Wed	14:45–18:30	H17	**Gallium Nitride: Optical and Electronic Properties**
HL 63.1–63.5	Wed	15:00–17:45	H1	**Symposium SYQS: Quantum Signatures in Magnetism (Joint session of HL, MA, O and TT, organized by MA)**
HL 64.1–64.8	Wed	15:00–18:30	H11	**Focus Session: Semiconductor Heteroepitaxy on Nanopatterned Substrates**
HL 65.1–65.12	Wed	15:00–18:30	H24	**Frontiers of Electronic Structure Theory: Focus on Topology and Transport III**
HL 66.1–66.10	Wed	15:00–17:45	H32	**Topological Insulators (Joint session of DS, HL, O, and TT, organized by MA)**
HL 67.1–67.7	Wed	18:15–20:30	Poster A	**Frontiers of Electronic Structure Theory: Focus on Topology and Transport**
HL 68.1–68.9	Thu	9:30–12:30	H10	**Metal-Semiconductor Hybrids**
HL 69.1–69.9	Thu	9:30–13:15	H11	**Focussed Session: Oxide Semiconductors for Device and Energy Applications 1**
HL 70.1–70.12	Thu	9:30–13:00	H13	**Semiconductor Lasers I**
HL 71.1–71.12	Thu	9:30–13:00	H15	**Quantum Dots and Wires: Optical Properties**
HL 72.1–72.8	Thu	9:30–12:45	H16	**Focus Session: Functionalization of Semiconductors I**
HL 73.1–73.13	Thu	9:30–13:15	H17	**Heterostructures and Interfaces (Joint session of HL and O, organized by HL)**
HL 74.1–74.13	Thu	9:30–13:00	H23	**Transport: Molecular Electronics and Photonics 1 (Joint session of CPP, DS, HL, MA, O and TT, organized by TT)**
HL 75.1–75.11	Thu	9:30–12:45	H40	**Organic Electronics and Photovoltaics II (Joint session of CPP, DS, HL and O, organized by CPP)**
HL 76.1–76.9	Thu	10:30–13:15	H24	**Frontiers of Electronic Structure Theory: Focus on Topology and Transport IV**
HL 77.1–77.9	Thu	10:30–12:45	S053	**Graphene III: Electronic Properties**
HL 78.1–78.11	Thu	10:30–13:30	S054	**2D Materials beyond Graphene: Dynamics and Excitation**

HL 79.1–79.8	Thu	11:15–13:15	H8	**Focus Session: Physics and Application of Emergent 2D-semiconductors and their Heterostructures 1**
HL 80.1–80.13	Thu	14:45–18:30	H2	**Hybrid and Perovskite Photovoltaics IV (Joint session of CPP, DF, DS and HL, organized by HL)**
HL 81.1–81.8	Thu	14:45–17:15	H10	**Topological Insulators I (Joint session of DS, HL, O and TT, organized by HL)**
HL 82.1–82.3	Thu	14:45–15:30	H13	**Semiconductor Lasers II**
HL 83.1–83.6	Thu	14:45–17:15	H16	**Focus Session: Functionalization of Semiconductors II**
HL 84.1–84.8	Thu	14:45–17:30	H17	**Novel Functional Materials I**
HL 85.1–85.4	Thu	15:00–17:00	H8	**Focus Session: Physics and Application of Emergent 2D-semiconductors and their Heterostructures 2**
HL 86.1–86.7	Thu	15:00–16:45	H11	**Oxide Semiconductors for Device and Energy Applications 2**
HL 87.1–87.4	Thu	15:00–16:00	H23	**Transport: Molecular Electronics and Photonics 2 (Joint session of CPP, DS, HL, MA, O and TT, organized by TT)**
HL 88.1–88.13	Thu	15:00–18:15	H24	**Frontiers of Electronic Structure Theory: Focus on Topology and Transport V**
HL 89.1–89.6	Thu	16:00–17:45	H13	**Quantum Dots and Wires: Lasing**
HL 90.1–90.42	Thu	16:00–19:00	Poster A	**Poster III**
HL 91.1–91.19	Thu	16:00–19:00	Poster A	**Poster IIIb (Joint session of DS and HL, organized by HL)**
HL 92.1–92.37	Thu	16:00–19:00	Poster A	**Postersession DS/HL**
HL 93.1–93.7	Thu	16:15–18:30	H23	**Transport: Spintronics and Magnetotransport (Joint session of DS, HL, MA and TT, organized by TT)**
HL 94.1–94.5	Fri	9:30–12:15	H1	**Symposium SYES: Frontiers of Electronic Structure Theory: Focus on Topology and Transport (Joint session of DS, HL, MA, MM and O, organized by O)**
HL 95.1–95.7	Fri	9:30–12:00	H10	**Novel Functional Materials II**
HL 96.1–96.6	Fri	9:30–11:30	H13	**Magnetic Semiconductors**
HL 97.1–97.8	Fri	9:30–12:00	H15	**Topological Insulators II (Joint session of DS, HL O and TT, organized by HL)**
HL 98.1–98.5	Fri	9:30–11:45	H16	**Focus Session: Functionalization of Semiconductors III**
HL 99.1–99.9	Fri	9:30–12:30	H17	**Gallium Nitride: Devices**
HL 100.1–100.9	Fri	9:30–12:00	H40	**Organic Electronics and Photovoltaics III (Joint session of CPP, DS, HL and O, organized by CPP)**
HL 101.1–101.10	Fri	10:30–13:00	S051	**Graphene IV: Electronic Properties and Structure**

Annual General Meeting of the Semiconductor Physics Division

Thursday 18:00–19:00 H13

- Report of the Chairman
- Miscellaneous

HL 1: Tutorial: Plasmonics

Organizer: Harald Giessen (Universität Stuttgart)

The tutorial Plasmonics and Nanooptics covers highly topical subjects in the fields of nanooptics and plasmonics. The topics include novel methods of bottom-up fabrications of functional plasmonic nanostructures with DNA-origami (Na Liu, University of Heidelberg und MPI for Intelligent Systems, Stuttgart), complex functional plasmonics with hybrid systems (Harald Giessen, University of Stuttgart), application as novel sensors (Hatice Altug, EPFL Lausanne, Switzerland), as well as infrared plasmonics with novel 2D materials such as graphene and hexagonal boron nitride (Rainer Hillenbrand, Nanogune San Sebastian, Spain).

The tutorial is aiming at students and postdocs who would like to get an overview of the fields of plasmonics and nanooptics, as well as at researchers who are interested in the most exciting new developments directly from leading scientists in the field.

Time: Sunday 16:00–18:30 Location: H15

Tutorial HL 1.1 Sun 16:00 H15

Graphene and Metal Plasmonics for Mid-IR Biosensing — •Hatice Altug — Bionanophotonics Systems Laboratory, EPFL Lausanne, Switzerland

Mid-IR absorption spectroscopy is a powerful label-free biosensing technique enabling chemical identification of molecules through their vibrational fingerprints. However, the method is not effective in detecting nanometric biomolecules due to the large size-mismatch with several microns long Mid-IR light. By engineering on-chip plasmonic nano-antennas, we overcome this fundamental limitation and enhance intrinsic signals of molecules by many orders of magnitude. Using extreme field concentration we also monitor in real-time and in-situ biomolecular interactions from low quantities of molecules. Most recently we showed that graphene could revolutionize biosensing due to its exceptional opto-electronic properties. Graphene plasmons can be tuned by electrostatic gating, in contrast to conventional plasmonic materials such as noble metals. By exploiting this unique feature we demonstrated a dynamically tunable plasmonic Mid-IR biosensor that can extract complete optical properties of proteins over a broad spectrum.In addition, the extreme light confinement in graphene*up to two orders of magnitude higher than in metals*produces an unprecedentedly strong overlap with nanometric biomolecules, enabling superior sensitivity. The combination of tunable spectral selectivity and enhanced sensitivity of graphene opens exciting prospects for sensing, not only proteins but also a wide range of chemicals and thin films.

Tutorial HL 1.2 Sun 16:45 H15

Active 3D plasmonics — •Na Liu — Kirchhoff Institute for Physics, University of Heidelberg — MPI for Intelligent Systems, Stuttgart, Germany

Active control of three-dimensional configuration is one of the key steps towards smart plasmonic nanostructures with desired functionalities. We lay out a multi-disciplinary strategy to create active 3D plasmonic nanostructures, which execute DNA-regulated conformational changes on the nanoscale.

Construction of 3D reconfigurable plasmonic nanostructures witnesses major technological limitations, arising from the required subwavelength dimensions and controlled 3D motion. There have been considerable efforts on integration of plasmonic nanostructures with active platforms using top-down techniques. Here we lay out and implement a multi-disciplinary strategy to create active 3D plasmonic nanostructures by merging plasmonics and DNA nanotechnology on the nanoscale. First, we show the creation of a reconfigurable plasmonic switch, which can execute DNA-regulated conformational changes. In one role, DNA works as molecular platform for organizing plasmonic nanoparticles into a 3D architecture. In the other role, DNA is used as fuel to drive the constructed 3D plasmonic switch along fully programmable routes. Simultaneously, the 3D plasmonic switch serves as optical reporter, which transduces its own conformational information into optical circular dichroism changes upon external stimuli in real time. We also demonstrate the first plasmonic walker.

Coffee Break

Tutorial HL 1.3 Sun 17:30 H15

Infrared nanoscopy and nano-FTIR spectroscopy by elastic light scattering from a scanning probe tip — •Rainer Hillenbrand — CIC nanoGUNE, San Sebastian, Spain

With the development of scattering-type scanning near-field optical microscopy (s-SNOM) [1] and nanoscale FTIR spectroscopy [2,3], the analytical power of IR and THz imaging has been brought to the nanometer scale. The spatial resolution of about 10 - 20 nm opens a new era for modern nano-analytical applications such as chemical identification, free-carrier profiling and near-field mapping of plasmons.

s-SNOM and nano-FTIR spectroscopy are based on elastic light scattering from AFM tips. Acting as an optical antenna, the tip convert the illuminating light into strongly concentrated near fields at the tip apex, providing a means for localized excitation of molecule vibrations, plasmons or phonons in the sample surface. Recording the tip-scattered light yields nanoscale-resolved IR images and spectra, beating the diffraction limit by orders of magnitude.

After a brief overview of fundamentals and applications, recent achievements such as IR-spectroscopic nanoimaging of polymers and proteins [4] will be presented, as well as the launching and mapping of ultra-confined plasmons in graphene [5,6].

[1] F. Keilmann, R. Hillenbrand, Phil. Trans. R. Soc. Lond. A 362, 787 (2004) [2] F. Huth, et al., Nature Mater. 10, 352 (2011) [3] F. Huth, et al., Nano Lett. 12, 3973 (2012) [4] I. Amenabar, et al., Nat. Commun. 4:2890 (2013) [5] J. Chen et al., Nature 487, 77 (2012) [6] P. Alonso Gonzalez et al., Science 344, 1369 (2014)

Tutorial HL 1.4 Sun 18:00 H15

Complex functional plasmonics: Ultrafast hybrid nonlinear plasmonics — •Harald Giessen — 4th Physics Institute and Research Center SCoPE, University of Stuttgart

We are going to present several different concepts on ultrafast nonlinear hybrid plasmonics. Both second- and third-harmonic processes are studied. The first concept incorporates strong local nonlinearities such as nanocrystals of nonlinear materials like LiNbO3 and ITO into gaps of plasmonic nanoantennas [1]. The second concept investigates the nonlinearities of the metals itself, particularly the influence of the localized density of states in the d-band and its influence on the nonlinear optical processes [2]. The third concept uses Miller's rule to enhance the optical nonlinearity by tailoring the linear response such that the first order susceptibility is resonant with the second harmonic light [3]. This leads to a strong and reproducible enhancement of the nonlinear response. Our general method is particularly well suited to incorporate also localized quantum emitters into the gap and investigate nonlinear optical processes on the single particle level.

[1] B. Metzger et al., Nano Lett. 14, 2867 (2014). [2] B. Metzger et al., Opt. Lett. 39, 5293 (2014). [3] B. Metzger et al., Nano Lett. 15, 3917 (2015).

HL 2: Tutorial: Hybrid and Perovskite Photovoltaics (Joint session of CPP, DF, DS and HL, organized by CPP)

Organizers: Lukas Schmidt-Mende (Universität Konstanz), Vladimir Dyakonov (Universität Würzburg) and Christoph Lienau (Universität Oldenburg)

Tremendous progress has been achieved in the performance of hybrid solar cells, with efficiencies now exceeding 20 % for devices based on organometallic halide perovskites. Aim of this tutorial is to introduce this topic of perovskite solar cells to prepare for the following symposium (SYHP) and allow vivid scientific discussions. A description of current state-of-the-art device fabrication methods and solar cell architectures will be given and their role on the device performance explained. The device physics will be discussed and charge carrier generation and recombination mechanisms in perovskite films explained and compared to other material systems. Additionally the important role of electronic structure of the different layers in hybrid perovskite will be covered.

Time: Sunday 16:00–18:30 Location: H18

Tutorial HL 2.1 Sun 16:00 H18

Perovskite photovoltaics: Synthesis, structure and device architecture — •Pablo Docampo — LMU Munich, Germany

Recently, organic-inorganic hybrid perovskites have been proven to be excellent photovoltaic materials, exhibiting outstanding light absorption, high carrier mobility and facile solution processability. Besides the manufacturing low costs of perovskite thin-films, the power conversion efficiencies demonstrated for this class of materials is already at the same level as poly-crystalline silicon and other thin film photovoltaic technologies. The pursuit of efficiency in the field of metal halide perovskite solar cells has been achieved mainly through the improvement to perovskite deposition processing and optimization of the device architecture.

In this tutorial I will focus on three topics. Firstly, the evolution of the device architecture, starting from sensitized mesoscopic solar cells to planar heterojunction devices employing organic contacts. Secondly, the commonly employed perovskite deposition techniques with special emphasis on the morphological quality of the prepared perovskite films. Thirdly, the perovskite structure and its stability both towards moisture and other factors such as UV-light, temperature and atmosphere. I will link these different aspects with device performance characteristics and introduce recent developments in the field towards surmounting the challenges the technology is currently facing from a materials point of view.

Tutorial HL 2.2 Sun 16:50 H18

Charge Carrier Generation and Recombination in Organic and Perovskite Solar Cells — •Andreas Baumann — Bayerisches Zentrum für Angewandte Energieforschung (ZAE Bayern), Magdalene-Schoch-Str. 3, D-97074 Würzburg

The new star on the photovoltaic (PV) horizon, are the so called organometal halide perovskite solar cells. This new kind of thin-film PV technology has experienced a tremendous, yet not seen increase in power conversion efficiency (PCE) compared to other types of PV technologies. Up to now the solar cell efficiency on lab scale could be improved from 3.8% in 2008 to above 20% in 2015 being already competitive with commercially available PV technologies. Especially this boost in PCE values has attracted attention of many researchers from all different PV research fields. Thereby, perovskite PV is one of the most promising thin film PV technologies regarding low-cost manufacturing combined with high PCE. However, the working principle of these solar cells is yet not completely understood and is strongly discussed in literature. Phenomena, such as the often observed anomalous hysteresis in the current-voltage characteristics or the giant dielectric constant and its impact on charge carrier generation and recombination are highly debated topics with so far different given possible explanations.

In this tutorial, the processes of charge carrier generation and recombination in perovskite solar cells will be highlighted and compared to those in well studied organic solar cells. Thereby, the aim is to give an overview of the published data on these processes in order to present the current status of research.

Tutorial HL 2.3 Sun 17:40 H18

The electronic structure in hybrid perovskite layers and devices — •Selina Olthof — University of Cologne, Institute for Physical Chemistry, Luxemburger Straße 116, 50939 Köln, Germany

The performance of optoelectronic devices strongly depends on the appropriate energetic alignment of the participating transport levels which directly influence the charge transport through the different layers. In order to optimize these interfaces in a non-trial-and-error fashion, one needs to know the conduction band minimum and valence band maximum of the perovskites to be able to select ideal transport layers as well as contact materials. While commonly vacuum level alignment is assumed at the interface to the substrate, this is actually rarely found in devices. Interfacial states, interface dipoles, and band bending can (and do) significantly alter the energy level landscape.

In this tutorial I will discuss the electronic structure of perovskites and introduce common measurement techniques that can shed a light on their energetic properties as well as the interface alignment relevant for devices. Combining reports from literature with our own recent results on the versatile electronic nature of this material I will elucidate the interplay between electronic structure and overall device performance.

HL 3: Symposium SYHP: Fundamentals of Hybrid and Perovskite Photovoltaics (Joint session of CPP, DF, DS and HL, organized by CPP)

Time: Monday 9:30–12:15 Location: H1

Invited Talk HL 3.1 Mon 9:30 H1

Perovskite Semiconductors: Opportunities and Challenges for Photovoltaic Materials Design — •David B. Mitzi — Duke University, Edmund T. Pratt Jr. School of Engineering, Durham, NC 27708-0300 USA

Organic-inorganic and related halide-based perovskites (e.g., those based on Pb halide frameworks) have attracted substantial recent interest for solar cell and other optoelectronic technologies, because of the large optical absorption coefficients, high carrier mobilities, long minority carrier lifetimes, and relatively benign defects and grain boundaries. Indeed, these materials have enabled an unprecedented rapid improvement in photovoltaic (PV) performance to levels above 20% power conversion efficiency. Despite the great promise, challenges for the current generation of PV materials include replacing lead with more environmentally benign metals, improving PV device stability (moisture, UV and air) and controlling hysteresis. This talk will explore beyond the current focus on three-dimensional (3-D) lead(II)-based perovskites, to highlight the outstanding structural, chemical and electronic flexibility of the perovskite family. Particular focus will be afforded to systems in which divalent lead is replaced with other metal cations exhibiting a lone pair of electrons, such as Sn, Bi and Sb, since these systems share some of the beneficial electronic structure characteristics of the Pb-based systems. Further discovery within the perovskite structural

and chemical space may offer prospects to solve the current technological challenges for perovskite PV and yield important opportunities for energy materials design.

Invited Talk HL 3.2 Mon 10:00 H1

Perovskite Solar Cells: A new Paradigm in Photovoltaics — •Mohammad Nazeeruddin — EPFL, GMF, Sion Switzerland

Perovskite solar cells exhibited significant leapfrog in efficiency due to a broad absorption, high optical absorption coefficient, very low exciton binding energy, long carrier diffusion lengths, efficient charge collection, and very high open circuit potential similar to III-IV semiconductors. Unlike silicon solar cells, perovskite solar cells can be developed a variety of low-temperature solution process from inexpensive raw materials. By engineering compositional ratio of perovskite absorber, film formation using anti-solvent, and interface engineering of charge transport materials a remarkable power conversion efficiency of over 21% has been demonstrated, highlighting the unique photovoltaic properties of perovskite materials. In this talk, we present the current progress in perovskite solar cells, various deposition methods for perovskite absorbing layer, synthesis and characterization of novel hole transporting materials, and highlight crucial challenges and prospects

Invited Talk HL 3.3 Mon 10:30 H1

Charge-Carrier Diffusion and Radiative Efficiencies in Hybrid Metal Halide Perovskites — •Laura Herz — University of Oxford, Oxford, UK

Hybrid metal halide perovskites (stoichiometry AMX_3) have recently emerged as low-cost active materials in PV cells with power conversion efficiencies in excess of 20%. In addition, hybrid perovskites show prospects for applications in low-cost light-emitting diodes and lasers.

Here we discuss how parameters essential for photovoltaic operation, such as charge carrier recombination and diffusion lengths are altered with substitutions of the organic A cation (e.g. methylammonium versus formamidinium), the metal M cation (e.g. Pb^{2+} or Sn^{2+}) and the halide X anion (I versus Br). We analyze distinct charge-carrier recombination mechanisms, such as trap-mediated, bi-molecular (electron-hole) and Auger recombination, which show different dependences on composition and temperature.

We use these insights to predict charge-carrier diffusion lengths and radiative efficiencies in the limit of ultra-low trap-related recombination, which could potentially be reached through further advances in material processing. We find that for hybrid lead iodide perovskites with typical charge-carrier mobilities of $\sim 30 cm^2/(Vs)$, charge-carrier diffusion lengths under solar irradiation are unlikely to exceed $\sim 10 \mu m$ even if all trap-related recombination is eliminated. We further show that if high radiative efficiencies are to be obtained for intermediate charge-carrier densities ($n \sim 10^{14} cm^{-3}$), trap-related recombination lifetimes have to exceed microseconds.

15 min. break.

Invited Talk HL 3.4 Mon 11:15 H1

Photovoltage losses in perovskite solar cells — •Kristofer Tvingsted — Experimental Physics VI, Julius Maximilians Universität, Würzburg, Germany

Perovskite PVs have reached significant power conversion efficiency in a very short time period. Apart from providing a rather high photocurrent, they also retain a comparatively high open circuit voltage (VOC). The VOC of most solar cells is however far from its potential upper limit due to charge carrier recombination of various types, whose origin must be accurately determined. Herein, I summarize what we have learned about these photovoltage losses by studying the radiative part of recombination in Perovskites. By accurate determination of the present solar cells radiative efficiency, that is their ability to emit light, we conclude how far the solar cells are from their own thermodynamic upper limit and further, how they relate to a reference OPV cell. We evaluate the carrier density dependence of the radiative efficiency and associate it to the ideality factor, which in itself represents a uniform figure of merit for the dominant type of recombination. We show that, as the perovskite steady state photoluminescence is strong at open circuit conditions, but substantially quenched only at short circuit, they perform in this respect just as an ideal solar cell should do, and also very different from most OPVs or DSSC cells studied so far. Substantially improving the radiative efficiency to increase the open circuit voltage is a promising route to put these new photovoltaic converters in efficiency parity with the best inorganic counterparts.

Invited Talk HL 3.5 Mon 11:45 H1

Computational screening of perovskite solar energy materials — •Karsten W. Jacobsen — CAMD, Dept. of Physics, Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark

In the talk I shall describe computational efforts to idenfity new materials for efficient light absorption with particular focus on materials in the perovskite structure and water splitting. The materials have to obey a number of criteria in order to work for light absorption and water splitting depending on the particular design of the device. We consider in particular stability, appropriate bandgap and bandstructure for visible light absorption, and an adequate line-up of band edges to the water redox potential. We also identify descriptors to determine defect-sensitivity of the materials.

We have considered several classes of materials with most emphasis on the cubic perovskite structure and derivatives like double perovskites and layered perovskites (Ruddlesden-Popper and Dion-Jacobson phases) with anions O, N, F, or S. Also a range of Sn and Pb based organic and inorganic perovskites have been considered with different combinations of the anions I, Br, and Cl. The possibilities of band gap tuning using atomic-level heterostructures or strain will also be touched upon.

I shall finally mention presently available open databases of relevance for energy materials including the Computational Materials Repository (https://cmr.fysik.dtu.dk) where the discussed data are made publicly available.

HL 4: Spintronics: Nanostructures and Optics

Time: Monday 9:30–13:00 Location: H13

HL 4.1 Mon 9:30 H13

Nuclear spin polarization in the electron spin-flip Raman scattering of singly charged (In,Ga)As/GaAs quantum dots — •Philipp Waldkirch[1], J. Debus[1], D. Kudlacik[1], V. F. Sapega[2], D. Dunker[1], P. Bohn[1], F. Passmann[1], D. Braukmann[1], J. Rautert[1], D. R. Yakovlev[1,2], D. Reuter[3], A. D. Wieck[4], and M. Bayer[1,2] — [1]Experimentelle Physik 2, Technische Universität Dortmund, 44227 Dortmund, Germany — [2]Ioffe Institute, Russian Academy of Sciences, 194021 St. Petersburg, Russia — [3]Department Physik, Universität Paderborn, 33098 Paderborn, Germany — [4]Angewandte Festkörperphysik, Ruhr-Universität Bochum, 44780 Bochum, Germany

We show that resonant, two-color spin-flip Raman scattering (SFRS) cannot only be used to manipulate carrier spins in a singly charged ensemble of (In,Ga)As QDs [1], but can also sensitively indicate the coupling of carrier spins to the surrounding nuclear spin bath, i.e., to study the central spin problem [2]. This method allows for monitoring the dynamic nuclear spin polarization directly through the Overhauser shift of the electron-SFRS line, while its width is determined by nuclear spin fluctuations. The rapid temporal decay of the Overhauser shift with slightly increasing temperature is caused by phonon-induced electron spin-flips that depolarize the nuclear spin system. The mechanism of the two-color SFRS is discussed together with the electron-nuclear hyperfine interaction and Pauli exclusion principle.

[1] J. Debus et al., Phys. Rev. B **90**, 235404 (2014)
[2] J. Debus et al., Phys. Rev. B **92**, 195421 (2015)

HL 4.2 Mon 9:45 H13

Spin Dynamics in Single Wurtzite GaAs Nanowires — •Florian Dirnberger, Stephan Furthmeier, Andreas Bayer, Joachim Hubmann, Benedikt Bauer, Moritz Forsch, Josef Zweck, Elisabeth Reiger, Christian Schüller, Tobias Korn, and Dominique Bougeard — Institut für Experimentelle und Angewandte Physik, Universität Regensburg, D-93040 Regensburg, Deutschland

Spin orbit coupling (SOC) in semiconductor nanowires (NWs) is cur-

rently attracting great interest regarding the application of spintronic and spin-orbitronic concepts. The action of this relativistic effect can be experimentally captured through its influence on the spin dynamics in the material. In contrast to electrical spin injection by means of ferromagnetic contacts, optical orientation with circularly polarized light provides a contact-free, non-invasive method to investigate the spin dynamics in semiconductors.

In this contribution, we demonstrate for the first time efficient optical spin orientation in single free-standing wurtzite (WZ) GaAs/AlGaAs core-shell nanowires. Our WZ nanowires are stacking-fault-free over lengths of several μm. We investigated the intrinsic spin dynamics in time-resolved micro-photoluminescence measurements on single NWs and observed long spin lifetimes up to $\tau_s = 1.5$ ns. The spin dynamics further reveal an anisotropic SOC for the studied NWs, which is counterintuitive compared to bulk WZ semiconductors. We present a model of the observed electron spin dynamics which highlights the major role of the interface SOC in these nanowires.

HL 4.3 Mon 10:00 H13

Fe doped InAs: what is the exchange interaction? — •Ye Yuan[1], René Hübner[1], Kay Potzger[1], Fang Liu[1], Maciej Sawicki[2], Tomasz Dietl[2], Manfred Helm[1], and Shengqiang Zhou[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Institute of Physics, Polish Academy of Sciences, Warsaw, Poland

Fe doped InAs layers have been prepared by ion implantation and pulsed laser annealing. Fe ions exist in the +3 valence state when located in Indium sites, which indicates that Fe atoms do not introduce free carriers in the InAs layer and only act as the local spins. However, (In, Fe)As or (In, Fe)As n-type doped with Se exhibits properties typical to a blocked superparamagnet, as proven by both static and dynamic magnetic measurements. This is most probably due to the formation of Fe-rich nanoregions in the InAs matrix, similarly to the case of Cr-doped ZnTe [1]. However, the p-type doping with Zn increases both the saturation magnetization and the Curie temperature. A systematic comparison between (In, Fe)As, (In, Fe)As: Zn and (In, Fe)As: Se leads to the re-affirmation of the pd-exchange as the key gradient in dilute ferromagnetic semiconductors [2].

[1]. K. Kanazawa et al., Nanoscale, 6, 14667-14673 (2014) [2]. T. Dietl et al., Science, 287, 1019-1022 (2000)

HL 4.4 Mon 10:15 H13

Weak (Anti)Localization in Tubular Semiconductor Nanowires with Spin-Orbit Coupling — •Paul Wenk[1], Michael Kammermeier[1], John Schliemann[1], Sebastian Heedt[2], and Thomas Schäpers[2] — [1]Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany — [2]Peter Grünberg Institute and JARA-Fundamentals of Future Information Technology, Forschungszentrum Jülich, 52425 Jülich, Germany

Motivated by recent experiments we compute analytically the quantum mechanical correction to the Drude conductivity in tubular semiconductor systems of zincblende type. Focusing on the lowest conduction band, we include linear Rashba and Dresselhaus spin-orbit coupling (SOC) and compare the results for nanorods of standard growth directions $\langle 100\rangle$, $\langle 111\rangle$ and $\langle 110\rangle$. The motion on the quasi two-dimensional surface is considered diffusive in both directions: transverse as well as along the cylinder axis. It is shown that both Dresselhaus and Rashba SOC affect the spin relaxation rates. We detect a crossover from weak localization to weak anti-localization depending on SOC strength as well as dephasing and scattering rate.

* * *

[1] S. Kettemann, PRL **98** 176808 (2007)
[2] P. Wenk *et al.*, PRB **83** 115301 (2011)
[3] S. Heedt *et al.*, Nanoscale **7** 18188 (2015)

HL 4.5 Mon 10:30 H13

Spin-orbit coupling effects in nanowires using the k.p method — •Tiago de Campos[1,3], Paulo Eduardo Faria Junior[1], Guilherme Sipahi[1,2], and Jaroslav Fabian[3] — [1]Universidade de São Paulo — [2]State University of New York at Buffalo — [3]Universität Regensburg

The search for Majorana fermions is a hot subject nowadays. One of the possibilities for realization of such experiments is a hybrid that couples a nanowire with a s-wave superconductor in the presence of an external magnetic field [1]. To understand the nanowire's role in this setup, we need a realistic band structures including spin-orbit effects. To consider the spin-orbit effects, it is common to use models that take into account only the first conduction band. Although these reduced models have been successfully in determine some physical properties, a more realistic description of the spin-orbit coupling between the bands is required to further investigate possible ways to realize the Majorana fermions. In this study we use a state of the art k.p Hamiltonian, which has the Dresselhaus and Rashba spin-orbit coupling built on the Hamiltonian from the beginning, together with the envelope function approach [2] to determine the band structure of zincblende InSb and wurtzite InAs nanowires. We analyze how the quantum confinement change the coupling between the bands and extracted the effective masses and the spin-splitting parameters that can be used in effective models.

[1] J. Alicea, Rep. Prog. Phys. 75, 076501 (2012). [2] P. E. Faria Junior and G. M. Sipahi, J. Appl. Phys. 112, 103716 (2012).

HL 4.6 Mon 10:45 H13

***g*-factor properties of electrons and holes confined in quantum dots emitting at telecom wavelengths** — •Janina Schindler[1], Vasilii V. Belykh[1], Dmitri R. Yakovlev[1,2], Evgeny A. Zhukov[1], Matusala Yacob[3], Johann P. Reithmaier[3], Mohamed Benyoucef[3], and Manfred Bayer[1,2] — [1]Experimentelle Physik 2, TU Dortmund, 44227 Dortmund, Germany — [2]Ioffe Institute, Russian Academy of Sciences, 194021 St. Petersburg, Russia — [3]Institute of Nanostructure Technologies and Analytics, University of Kassel, 34132 Kassel, Germany

Spins in semiconductor quantum dots (QDs) are considered as highly attractive systems for future applications in the solid-state quantum information processing. In that context, the characterization of g-factors is very important to assess the spin dynamics for the semiconductor physics in general and for tailoring nanostructures in particular, since the dynamics are sensitive to shape anisotropies as well as spin-state mixing. We study electron and hole g-factors and dephasing times in a novel InAs/InAlGaAs/InP quantum dot ensemble by measuring time-resolved pump-probe ellipticity. The emission of the QDs lies in the telecommunication wavelength range around 1.55 μm, which is highly interesting for information-processing applications. We observe a surprisingly strong deviation of the electron g-factor from the Roth-Lax-Zwerdling equation, a strong dispersion of the hole g-factor and a significant out-of-plane anisotropy of the g-factors, in contrast to nearly isotropic in-plane properties.

30 min. Coffee Break

HL 4.7 Mon 11:30 H13

Low Field Nuclear Magnetic Resonance in Gallium Arsenide detected via Spin Noise Spectroscopy — •Fabian Berski[1], Jens Hübner[1], Michael Oestreich[1], Arne Ludwig[2], A. D. Wieck[2], and Mikhail Glazov[3] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstr. 2, D-30167 Hannover, Germany — [2]Angewandte Festkörperphysik, Ruhr-Universität Bochum, 44780 Bochum, Germany — [3]Ioffe Institute, Polytechnicheskaya 26, 194021 St.-Petersburg, Russia

The hyperfine interaction between donor electron spins and lattice magnetic moments in III-V semiconductor materials is a challenge for quantum information processing. However, the ubiquitous interaction also provides all-optical access to the spin dynamics of the nuclear system, which may serve as long-lived solid-state qubits.

We present highly sensitive spin noise measurements on an ensemble of non-interacting donor bound electrons (D^0X) in a nearly perfect, high purity Gallium Arsenide host matrix [1]. The experiment distinctly reveals the finite Overhauser shift of an electron spin precession at zero external magnetic field and a second contribution around zero frequency stemming from the electron spin components parallel to nuclear spin fluctuations. Moreover, at very low frequencies, features related with time-dependent nuclear spin fluctuations are clearly resolved making it possible to study the intricate nuclear spin dynamics at zero and low magnetic fields.

[1] Berski, et al., Phys. Rev. Lett. **115**, 176601 (2015).

HL 4.8 Mon 11:45 H13

Elliott-Yafet spin relaxation revisited — •Svenja Vollmar[1,2] and Hans Christian Schneider[1] — [1]Department of Physics and Research Center of OPTIMAS, University of Kaiserslautern — [2]Graduate School of Excellence Materials Science in Mainz

By computing the dynamics of the reduced electronic density matrix,

we present a new analysis of the Elliott-Yafet spin relaxation mechanism, i.e. the spin relaxation due to incoherent electron-phonon scattering [1,2,3]. In our approach spin dynamics is described correctly without approximating mixed spin states by pure spin states, as done in Yafet's original treatment [3]. Our approach is therefore also valid for pronounced spin mixing. The central new quantity introduced in our calculation is a torque matrix element that determines the spin dynamics in a transparent fashion.

For the special case of Kramers degenerate bands we use this result to derive a novel expression for the close-to-equilibrium spin relaxation-time. To this end, we determine the reduced density matrix for a spin polarized system with arbitrary spin mixing in quasi-equilibrium [4].

[1] A. W. Overhauser, Phys. Rev. 89, 689 (1953).
[2] R. J. Elliott, Phys. Rev. 96, 266 (1954).
[3] Y. Yafet, Solid State Physics 14, 1 (1963).
[4] A. Baral, S. Vollmar, S. Kaltenborn, H.C. Schneider, arXiv: 1505.01432.

HL 4.9 Mon 12:00 H13

Impurity dominated spin dynamics in GaAs in the vicinity of the metal-to-insulator transition — •Jan Gerrit Lonnemann[1], Eddy Patrick Rugeramigabo[2], Jens Hübner[1], and Michael Oestreich[1] — [1]Institute for Solid State Physics, Leibniz Universität Hannover, Appelstr. 2, D-30167 Hannover, Germany — [2]Laboratory of Nano and Quantum Engineering, Leibniz Universität Hannover, Schneiderberg 39, D-30167 Hannover, Germany

Several theoretical works treat the spin dynamics in zinc-blende semiconductors. We present extremely low excitation Hanle depolarization measurements on well characterized n-doped MBE grown GaAs in the vicinity of the metal-to-insulator transition (MIT). This doping concentration regime is of special interest because around the MIT at $2*10^{16}\,\mathrm{cm}^{-3}$ extremely long spin lifetimes are experimentally observed [1]. Spin relaxation in this regime is dominated by the impurity states because the merging of impurity and conduction band does not take place below $8*10^{16}\,\mathrm{cm}^{-3}$. We conclude from our measurements that the well known D'yakonov Perel mechanism is dominating in slightly metallic samples. Furthermore there is no evidence of spin relaxation by hopping transport (HT) above the MIT that has been predicted as the main mechanism of relaxation for the impurity band regime [2]. In contrast our measurements show a metal-like behavior of the electrons in the impurity band.

[1] M. Römer et al.; *Phys. Rev. B*, **81**, 075216 (2010).
[2] G.A. Intronati et al.; *Phys. Rev. Lett.*, **108**, 016601 (2012).

HL 4.10 Mon 12:15 H13

Novel properties of the Mn^{2+} spin-flip Raman scattering in ZnMnSe quantum wells — •Henning Moldenhauer[1], Carolin Lüders[1], Philipp Waldkirch[1], Dennis Kudlacik[1], Victor Sapega[2], Jörg Debus[1], Andreas Waag[3], and Manfred Bayer[1,2] — [1]Experimentelle Physik 2, Technische Universität Dortmund, 44227 Dortmund, Germany — [2]Ioffe Institute, Russian Academy of Sciences, 194021 St. Petersburg, Russia — [3]Institut für Halbleitertechnik, Technische Universität Braunschweig, 38106 Braunschweig, Germany

Diluted magnetic semiconductors (DMS) are promising materials for novel types of devices based on the tailoring of their spin properties leading to the field of semiconductor spintronics. Even though there has been a continuous study on Mn-based DMS during the last decades, several questions on the carrier-Mn ion interactions are still unanswered. We extend considerably the picture of the spin-flip Raman scattering (SFRS) of the Mn^{2+} ions by studying it in Faraday and tilted geometries in ZnMnSe quantum wells with Mn concentrations below 4%. We demonstrate that the paramagnetic Mn^{2+} resonances are caused by exchange interactions with conduction band electrons as well as hyperfine interactions with the Mn^{2+} nuclear spins. To verify this mechanism we apply radio-frequency (RF) fields, combined with resonant SFRS, to observe an impact of the nuclear spin depolarization on the Mn^{2+} SFRS signals. Surprisingly, the anti-Stokes Mn^{2+} scattering process is observed and also affected by the RF-fields.

HL 4.11 Mon 12:30 H13

Hole spin coherence in coupled GaAs/AlAs quantum wells — •Christian Gradl, Michael Kempf, Johannes Holler, Dieter Schuh, Dominique Bougeard, Christian Schüller, and Tobias Korn — Universität Regensburg, 93040 Regensburg, Germany

Due to its p-like character, the valence band in GaAs-based heterostructures offers rich and complex spin-dependent phenomena. Especially for some low-symmetry growth directions, a strong anisotropy of the hole g factor with respect to the in-plane magnetic field direction is theoretically predicted. Therefore, we perform time-resolved Kerr rotation measurements on an undoped [113]-grown double quantum well (QW) structure to resolve the spin dynamics of hole ensembles at low temperatures. Our gated system consists of two QWs with different well widths, which we use for the spatial separation of the optically excited electron-hole pairs. Thus, we are able to create hole ensembles with spin lifetimes of several hundreds of picoseconds in the broader QW without any doping. This allows the observation of a strong hole g factor anisotropy by varying the magnetic field direction in the QW plane. The experimental g factor values are in very good agreement with theoretical predictions. Furthermore, we observe an unexpected additional non-precessing component in the Kerr signal for certain in-plane magnetic field directions. This might have its origin in a precession axis that is tilted relative to the magnetic field due to the crystal structure of this low-symmetry growth direction.

HL 4.12 Mon 12:45 H13

Time-resolved electrical detection of the Spin Galvanic effect after ps optical excitation — •Manfred Ersfeld[1], Ivan Stepanov[1], Mihail Lepsa[2], and Bernd Beschoten[1] — [1]2nd Institute of Physics, RWTH Aachen University, Germany — [2]Peter Grünberg Institut (PGI-9), Forschungszentrum Jülich GmbH, Germany

Direct conversion of electron spin precession in semiconductor heterostructures into a detectable electrical voltage plays an important role in many spintronic concepts. Here we report on the first time-resolved electrical measurement of the spin galvanic effect (SGE) probed by spin dependent photo-voltages in n-InGaAs. Phase triggering of electron spin coherence is achieved by circularly polarized picosecond laser pulses. Electron spin precession in a transverse external magnetic field can be directly monitored as voltage oscillations using a phase-triggered sampling oscilloscope as a probe. The strong crystal axis anisotropy of the spin-orbit interaction allows analyzing the predicted dependence of the spin-dependent photo-voltage on the strength of the spin-orbit interaction. In contrast to previous theoretical predictions, the amplitude of the SGE does not depend on the spin-orbit coupling strength.

HL 5: Quantum Dots and Wires: Single Photon Sources

Time: Monday 9:30–12:15 Location: H15

Invited Talk HL 5.1 Mon 9:30 H15

Quantum optics with quantum dots in photonic wires — •Jean-Michel Gerard — Institute for Nanosciences and Cryogenics, Grenoble, France

Over the last 20 years, quantum dots have been fruitfully combined with optical microcavities to perform quantum optics experiments and to develop quantum light sources for QIPC. In this talk, I will show that the very basic photonic wire geometry opens an attractive alternative avenue in this context [1]. I will noticeably introduce the Photonic Trumpet (PT) [2], formed by a high-index single-mode waveguide and a conical tapering. Nearly perfect single-mode emission, low-divergence Gaussian radiation pattern, linear polarization control, efficient wavelength tuning based on strain effects, and high efficiency single photon emission (> 0.75 photon per pulse) are reported for a single quantum dot embedded in a PT. The PT also appears as a very promising platform to explore the unique optical properties of one-dimensional atoms[3] and hybrid optomechanical systems where the interaction between the two-level quantum system and mechanical modes is mediated by strain [4]. Work done with J. Claudon, J Bleuse, M Munsch, P Stepanov and with the groups of JP Poizat, O Arcizet, A Auffèves, M Richard (CNRS I. Néel Grenoble) and N Gregersen (DTU), who are gratefully acknowledged. [1] For a review see J Claudon et al Chem Phys Chem 14, 1393 (2013); [3] M. Munsch et al, PRL 110, 177402 and 239902(E) (2013) ; P Stepanov et al APL 106, 041112 (2015) :

[4] D. Valente et al, New J. Phys 14, 083029 (2012); Phys Rev A 86, 022333 (2012) [5] I. Yeo et al, Nat. Nano. 9, 106 (2014)

HL 5.2 Mon 10:00 H15

Phase super-resolution with N00N-states generated by on demand single-photon sources — •M. Müller, H. Vural, S. L. Portalupi, and P. Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen, Allmandring 3, 70569 Stuttgart, Germany

Quantum metrology is a promising scientific field taking advantage of the probably most fundamental aspect of quantum mechanics, namely entanglement. Enhanced optical phase sensing for instance, which utilizes multi-photon entangled states has attracted a lot of attention in the community. Up to now, so called path-entangled N00N states have been generated by light sources possessing probabilistic photon statistics, e. g., parametric-down conversion. Here we present the experimental generation of two-photon N00N states with a single quantum emitter making use of the radiative biexciton-exciton cascade in a single semiconductor quantum dot. A resonant and coherent two-photon excitation process ensures the deterministic preparation of the quantum dot states. The subsequently emitted single-photons possess a reasonable indistinguishability for the production of the excitonic and biexcitonic two-photon N00N states. Phase super-resolution, i. e., a reduced de-Broglie wavelength of the photonic wave packet, expressed by pronounced oscillations with twice the single photon frequency, is observed. Theoretical calculations are in excellent agreement with the experimental results, allowing for a complete description of the system. Prospects and limitations related to optical phase measurements with a precision beating the standard quantum limit involving quantum dot single-photon sources will be discussed.

HL 5.3 Mon 10:15 H15

Semiconductor source of single photons frequency matched to Rb — •Jan-Philipp Jahn[1], Lucas Béguin[1], Mathieu Munsch[1], Andreas Kuhlmann[1], Martina Renggli[1], Yongheng Huo[2], Fei Ding[3], Rinaldo Trotta[2], Oliver G. Schmidt[3], Armando Rastelli[2], Philipp Treutlein[1], and Richard J. Warburton[1] — [1]Department of Physics, University of Basel, Switzerland — [2]Johannes Kepler University Linz, Austria — [3]IFW Dresden, Germany

Semiconductor quantum dots are excellent single-photon sources, providing triggered single-photon emission at a high rate and high spectral purity. Independently, atomic ensembles have emerged as one of the best quantum memories for single photons, providing high efficiency storage and long memory lifetimes. In this project, we combine these two physical systems to exploit the best features from both worlds. We have characterized a new type of self-assembled GaAs/AlGaAs quantum dots that emits lifetime-limited ($\Delta\nu \sim 1.42$GHz) single-photons at a wavelength compatible with Rb atoms [1]. Fine tuning of the photon frequency to address the Rb D2-line is achieved via strain. To overcome the inherent bandwidth mismatch between the two disparate systems we excite the QD in the Rayleigh scattering regime. This allows a temporal shaping of the QD photons in pulsed resonant excitation, a prerequisite to achieve high storage efficiencies. Furthermore we performed pulsed Hong-Ou-Mandel measurements to directly quantify the indistinguishability, which constitutes a key aspect for quantum information networks. [1] Jahn et.al. arXiv:1508.06461

HL 5.4 Mon 10:30 H15

An electrically driven cavity-enhanced source of indistinguishable photons with 61% overall efficiency — •Tobias Heindel[1], Alexander Schlehahn[1], Alexander Thoma[1], Pierce Munnelly[1], Martin Kamp[2], Sven Höfling[2,3], Christian Schneider[2], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, Berlin, Germany — [2]Technische Physik, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [3]SUPA, School of Physics and Astronomy, University of St Andrews, St Andrews, United Kingdom

Single semiconductor quantum dots (QDs) integrated into photonic microstructures are promising candidates for the realization of high-fidelity and high-speed quantum-light sources [1]. Besides a high single-photon flux and vanishing multi-photon emission probabilities, the photon-indistinguishability is a crucial attribute for quantum information processing schemes.

In this work, we report on state-of-the-art electrically triggered sources of single and indistinguishable photons. Exploiting the Purcell-effect and the highly-directional emission of electrically contacted QD micropillar cavities operated at excitation repetition rates up to 1.2 GHz, we extract cavity-enhanced single-photon emission with record-high efficiencies of $(61 \pm 11)\,\%$. Moreover, two-photon interference experiments reveal a photon-indistinguishability of $(41.1 \pm 9.5)\,\%$ under pulsed current injection at 487 MHz.

[1] G.-C. Shan et al., Front. Phys. 9, 170 (2014)

30 min. Coffee Break

HL 5.5 Mon 11:15 H15

Single-photon emission at a rate of 143 MHz from deterministic quantum-dot microlenses triggered by a mode-locked VECSEL — •Alexander Schlehahn[1], Mahmoud Gaafar[2], Max Vaupel[2], Manuel Gschrey[1], Peter Schnauber[1], Jan-Hindrik Schulze[1], Sven Rodt[1], André Strittmatter[1], Wolfgang Stolz[2], Arash Rahimi-Iman[2], Tobias Heindel[1], Martin Koch[2], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, 10623 Berlin, Germany — [2]Department of Physics and Material Sciences Center, Philipps-Universität Marburg, 35032 Marburg, Germany

We report on the realization of an ultra-bright quantum-dot (QD) based single-photon source. The source consists of a deterministic QD microlens and is excited by a mode-locked vertical-external-cavity surface-emitting laser (ML-VECSEL). The frequency-doubled ML-VECSEL operates at a wavelength of 508 nm and features pulse widths of 4.2 ps at a repetition rate of 494 MHz, being about 6 times faster than conventional Ti:sapphire lasers. This unique and compact combination allows us to achieve single-photon fluxes of (143 ± 16) MHz collected by the first lens of the setup, corresponding to a photon-extraction efficiency of $(29 \pm 3)\%$ with $g^{(2)}(0)$ below 0.03 [1]. Beyond this proof of principle under non-resonant excitation, our concept is perfectly suited for the application of resonant excitation schemes using wavelength-tunable ML-VECSELs and spectrally matched QDs to generate indistinguishable single photons at high rates.

[1] A. Schlehahn et al., Appl. Phys. Lett. 107, 041105 (2015)

HL 5.6 Mon 11:30 H15

Enhanced in-situ cathodoluminescence lithography for the deterministic fabrication of quantum light sources — •Arsenty Kaganskiy, Manuel Gschrey, Alexander Schlehahn, Jan-Hindrik Schulze, Ronny Schmidt, Tobias Heindel, Sven Rodt, André Strittmatter, and Stephan Reitzenstein — Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstraße 36, D-10623

Future nanophotonic devices will rely on the development of sources for indistinguishable single photons and entangled photon pairs based on self-assembled quantum dots (QDs). Preselected QDs with the mentioned properties need to be deterministically embedded into photonic structures to enhance their photon extraction efficiency. In order to meet this requirement we developed a deterministic technology platform named enhanced in-situ cathodoluminescence lithography (eCLL) [1]. By using marker structures the eCLL technique allows for a detailed spectral pre-characterization of QD properties such as emission energy, fine-structure splitting (FSS) and decay time of excitonic complexes before integrating the QDs with high alignment accuracy into, e.g., microlenses. In this way, QDs with small FSS can be selected and integrated into microlenses in order to realize efficient sources of polarization entangled photon pairs. Moreover, the eCLL technique allows for a direct comparison of the QD properties before and after the processing. For instance we observed a two-fold shortening of the decay time that could be related to a moderate Purcell effect.

[1] A. Kaganskiy et al., Rev. Sci. Instrum. 86 (2015), 073903.

HL 5.7 Mon 11:45 H15

Efficient single-photon sources based on deterministic quantum-dot microlenses with backside gold mirrors — •Sarah Fischbach[1], Esra Yarar Tauscher[1], Peter Schauber[1], Ronny Schmidt[1], Jan-Hindrik Schulze[1], Alexander Thoma[1], Alexander Schlehahn[1], Benjamin Wohlfeil[2], Sven Burger[2], André Strittmatter[3], Tobias Heindel[1], Sven Rodt[1], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, Germany — [2]Zuse-Institut Berlin (ZIB), Germany — [3]Institut für Experimentelle Physik, Otto-von-Guericke-Universität Magdeburg, Germany

By utilizing single semiconductor quantum dots (QDs) advances in creating single-photon sources (SPSs) have been made, enabling close to ideal single-photon emission in terms of $g^{(2)}(0)$ as well as the photon-

indistinguishability. Applications in the field of quantum communications, however, require highest photon extraction efficiencies at precisely defined emission wavelengths at the same time.
Here, we report on a novel approach to realize high fidelity SPSs by combining a single QD, deterministically integrated within a monolithic microlens, with a backside gold mirror. FEM-simulations are carried out to determine the optimum device geometry. The mirror is realized via a flip-chip process with thermo-compression gold bonding, while microlenses are patterned by in situ three-dimensional electron-beam lithography at cryogenic temperatures. In that way, bright QDs with preselected spectral features can be chosen to optimize their photon extraction efficiency.

HL 5.8 Mon 12:00 H15

Exploring dephasing in deterministic quantum-dot microlenses by Hong-Ou-Mandel interferometry — •Alexander Thoma[1], Peter Schnauber[1], Manuel Gschrey[1], Marc Seifried[1], Janik Wolters[1], Jan-Hindrik Schulze[1], André Strittmatter[1], Sven Rodt[1], Alexander Carmele[2], Andreas Knorr[2], Tobias Heindel[1], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, TU Berlin, Berlin, Germany — [2]Institut für Theoretische Physik, TU Berlin, Berlin, Germany

Bright quantum light sources based on single semiconductor quantum dots (QDs) integrated into photonic microstructures are key building blocks for the realization of advanced quantum computation schemes. Further advancement beyond proof-of-principle studies towards applications in quantum information technology will rely on deterministic device processing and profound knowledge of the underlying mechanism affecting their quantum optical properties. In this work we probe time-dependent dephasing processes in deterministic QD-microlenses [1]. In particular, we explore the photon-indistinguishability as a function of the time δt elapsed between consecutive photon emission events to gain experimental access to the underlying decoherence processes at a ns time-scale. Gradually increasing δt from 2 ns to 12 ns results in a plateau-like behaviour at low δt with visibilities close to unity, while the visibility decreases for larger δt ($>$ 8 ns). Our experimental observations are theoretically described by a non-Markovian noise process in agreement with fluctuating charge carriers in the QD's vicinity.

[1] A. Thoma et. al, arXiv:1507.05900 (2015)

HL 6: Two-dimensional Materials (Joint session of HL, DS and O, organized by HL)

Time: Monday 9:30–13:00 Location: H16

HL 6.1 Mon 9:30 H16

Boundary conditions for transition-metal dichalcogenide monolayers in the continuum model — •Csaba Géza Péterfalvi, Andor Kormányos, and Guido Burkard — Department of Physics, University of Konstanz, D-78464 Konstanz, Germany

We derive the boundary conditions for MoS_2 and similar transition-metal dichalcogenide honeycomb (2H polytype) monolayers with the same type of $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian within the continuum model around the K points. [1] In an effective 2-band description, the electron-hole symmetry breaking quadratic terms are also taken into account. We model the effect of the edges with a linear edge constraint method that has been applied previously to graphene. Focusing mainly on zigzag edges, we find that different reconstruction geometries with different edge-atoms can generally be described with one scalar parameter varying between 0 and 2π. We analyze the edge states and their dispersion relation in MoS_2 in particular, and we find good agreement with the results of previous density functional theory calculations for various edge types.

[1] Cs. G. Péterfalvi, A. Kormányos, G. Burkard, arXiv:1509.00184 (2015).

HL 6.2 Mon 9:45 H16

High Q-factor in WSe2 Nano-electromechanical resonator — •Antoine Reserbat-Plantey[1], Nicolas Morell[1], Ioannis Tsioutsios[1], Kevin Schädler[1], François Dubin[2], Frank Koppens[1], and Adrian Bachtold[1] — [1]ICFO, The Insitutue for Photonic Sciences, Barcelona, ES — [2]INSP, Université Paris 6, Paris, FR

Atomically thin nano-electromechanical systems (2D-NEMS) combine extremely low mass resonators having resonant frequencies in the MHz-GHz range, wide tunability, low damping and exotic non-linearities. Atomically thin 2D semi-conductors such as transition metal dichalcogenides (TMD) have extremely rich optical properties (direct band gap, spin valley, embedded quantum emitters), which are intrinsically linked to their low dimensionality. Optical and electronic properties of WSe2, an emblematic TMD, have been intensively studied while there is no extensive nanomechanical investigation of this system. Here we show a new generation of semiconductor 2D-NEMS made of monolayer of WSe2. We record mechanical and photoluminescence spectra of WSe2 nanoresonators down to cryogenic temperatures. We measure mechanical quality factor Q>47000 at T=3.5 K, which is the highest value reported so far for 2D-NEMS in this temperature range. Combining ultra-low dissipation resonators with the very rich optical properties of TMD, paves the way for novel type of optomechanical experiments with 2D materials.

HL 6.3 Mon 10:00 H16

Landau levels and Shubnikov-de Haas oscillations in monolayer transition metal dichalcogenide semiconductors — •Andor Kormányos[1], Péter Rakyta[2], and Guido Burkard[1] — [1]Physics Department, University of Konstanz — [2]Department of Theoretical Physics, Budapest University of Technology and Economics

We study the Landau level (LL) spectrum using a multi-band $\mathbf{k}\cdot\mathbf{p}$ theory in monolayer transition metal dichalcogenide semiconductors [1]. We find that in a wide magnetic field range the LL can be characterized by a harmonic oscillator spectrum and a linear-in-magnetic field term which describes the valley degeneracy breaking. The effect of the non-parabolicity of the band-dispersion on the LL spectrum is also discussed. Motivated by recent magnetotransport experiments, we use the self-consistent Born approximation and the Kubo formalism to calculate the Shubnikov-de Haas oscillations of the longitudinal conductivity. We investigate how the doping level, the spin-splitting of the bands and the broken valley degeneracy of the LLs affect the magnetoconductance oscillations. We consider monolayer MoS_2 and WSe_2 as concrete examples and compare the results of numerical calculations and an analytical formula which is valid in the semiclassical regime. Finally, we briefly analyze the recent experimental results [Cui et al., Nat. Nanotechnol. **10**, 534 (2015)] using the theoretical approach we have developed.

[1] New J. Phys. **17**, 103006 (2015).

HL 6.4 Mon 10:15 H16

Second-harmonic generation in MoS2 monolayers coupled to resonant nanoantennas — •Franz Johannes Friedrich Löchner[1], Stefan Fasold[1], Antony George[2], Paul Douglas Harrison[1], Christoph Menzel[1], Andrey Turchanin[2], Isabelle Staude[1], Falk Eilenberger[3], Frank Setzpfandt[1], and Thomas Pertsch[1] — [1]Institute of Applied Physics, Abbe Center of Photonics , Friedrich-Schiller-Universität Jena, 07743 Jena, Germany — [2]Institute of Physical Chemistry, Friedrich-Schiller-Universität Jena, 07743 Jena, Germany — [3]Fraunhofer Institute for Applied Optics and Precision Engineering, 07745 Jena, Germany

Two-dimensional monolayers of transition metal dichalcogenides (TMDs), a new class of direct band-gap semiconductors, recently have attracted a lot of attention due to their pronounced excitonic emission lines and strong second-order nonlinearity.

Coupling TMDs to resonant nanoantennas allows to further enhance these effects by concentrating the exciting optical field into a small volume. Such enhancement has been shown for excitonic emission using plasmonic nanoantennas. However, nonlinear optical effects in TMD-nanoantenna systems have not been studied yet.

In our contribution, we report on experimental investigations of second-harmonic generation in molybdenum disulfide (MoS2) monolayers coupled to nanoantennas, resonant at the exciting fundamental-harmonic wavelength. Polarization resolved measurements show the profound impact which the presence of the nanoantenna has on the second-harmonic radiation generated by the MoS2-monolayer.

HL 6.5 Mon 10:30 H16

Electrochemical growth and characterization of molybdenum sulfide layers for thin film transistors — •Talha Nisar,

Torsten Balster, and Veit Wagner — Jacobs University Bremen gGmbH, Campus Ring 1, 28759 Bremen, Germany

Molybdenum disulfide has attracted considerable interest for its great potential in the field of nanoelectronics due to its semiconducting and 2D nature. It has been successfully deposited by the Scotch tape method resulting in high-mobility transistors with an area of a few square microns. The state-of-the-art method for the growth of crystalline molybdenum disulfide single and multilayers is chemical vapor deposition.
In our study we use electrochemical deposition as an alternative approach to grow large area molybdenum sulfide layers. For this purpose, ammonium tetrathiomolybdate (ATTM) has been used as precursor material for the electrodeposition in cathodic regime with respect to Ag/AgCl reference electrode. The obtained layers are amorphous as could be confirmed by Raman measurements. In addition, in the UV-VIS spectra of the MoS_x (x=2..3) layer a transition at 2.4 eV is visible, which could be related to oxygen contamination. Further annealing steps in an Ar/H_2 atmosphere with an additional sulfur source at temperatures above 600°C are necessary to remove the oxygen and to convert the layer into crystalline MoS_2. The converted layer has to be transferred onto SiO_2/Si substrates for thin film transistor applications.

30 min. Coffee Break

Invited Talk HL 6.6 Mon 11:15 H16

Epitaxial paradigms of van der Waals bonded chalcogenide materials — •Raffaella Calarco — Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5-7, 10117 Berlin, Germany

In recent years it has become clear that materials with covalent bonding in only two dimensions (2D) have attractive properties for devices. The bonding in the third dimension, which is between individual layers, occurs by van der Waals (vdW) forces, which are weaker if compared to the covalent bonding. Materials used in conventional devices are instead characterized by covalent bonding in three dimensions (3D). In the present contribution, I shed some light on understanding the mechanisms that determine the interface structure between 2D and 3D or 2D materials. To study possible options for altering the bonding configurations of the 2D-3D interface GeTe-Sb2Te3 layers are deposited by molecular beam epitaxy on top of five different surface reconstructions-passivation of the Si(111). The 2D-2D interface is best studied using graphene as a substrate. Finally, I address the most crucial issue: The realization of vdW epitaxy in Sb2Te3-GeTe superlattices. Such superlattices, if compared to their alloy counterpart, show impressive performances highly attractive for future non-volatile memory applications.

HL 6.7 Mon 11:45 H16

Transparent Conducting Materials: Insights from High-Throughput — •Pino D'Amico[1,2], Alice Ruini[1,2], Alessandra Catellani[2], Arrigo Calzolari[2], Marco Fornari[3,5], and Marco B. Nardelli[4,5] — [1]FIM-UNIMORE, Modena, Italy — [2]CNR-NANO S3, Modena, Italy — [3]Central Michigan Univ., Mt. Pleasant, USA — [4]Univ. of North Texas, Denton, USA — [5]Duke Univ., Durham, USA

Good electrical conductivity and optical transparency in the visible domain are the physical properties required in order to have Transparent Conducting Material (TCM). Various semiconductors becomes TCM when doped and up to now their discovery has followed an a-posteriori path: take a material and investigate its physical properties in order to see if it is a good TCM. Thanks to the large amount of data available in the AFLOWLIB repository[1], we use instead an inverse-design approach in order to search for new possible TCMs: starting from the paradigmatic case of ZnO[2] we have identified the physical descriptors representing a TCM and extracted from the database a list of materials having the required characteristics using highthroughput techniques. We investigated doped structures of resulting materials inserting substitutional elements in a systematic way with a given concentration. We will present an accurate study of both conductivity and optical properties of the doped structures obtained by means of a newly developed numerical tool based on Boltzmann theory and dielectric function calculations[3] and reliyng on an efficient ab-initio tight-binding representation of the lattice structures[4]. [1]www.aflowlib.org; [2]ACS Photonics 1, 703 (2014); [3]preprint(2015); [4]arXiv:1509.02558 (2015).

HL 6.8 Mon 12:00 H16

Investigating the Potential of TMD Monolayers as Photodetectors — •Maja Feierabend[1], Gunnar Berghäuser[2], and Ermin Malic[2] — [1]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, TU Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Chalmers University of Technology, Department of Physics, SE-412 96 Gothenburg, Sweden

Transition metal dichalcogenides (TMDs) are promising materials for technological application in the area of optoelectronics. Due to the direct band gap and the extraordinarily strong Coulomb interaction, TMDs exhibit efficient light-matter coupling and tightly bound excitons [1]. As atomically thin materials, they are very sensitive to changes in the surrounding environment. This motivates a functionalisation approach, where external molecules are non-covalently attached to the material surface to control its optical properties.

Here, we theoretically investigate functionalized TMDs based on the density matrix formalism combined with tight-binding wave functions. Considering exemplary spiropyran molecules exhibiting a strong dipole moment, we predict pronounced spectral red-shifts and the appearance of an additional side-peak in the absorption spectrum of functionalized TMDs. Interestingly, we also observe a further peak splitting due to the intervalley coupling between the high-symmetry K/K' points. The predicted pronounced changes in optical spectra of TMDs show their potential for technological application in photodetectors.

[1] G. Berghäuser and E. Malic, PRB 89, 125309 (2014)

HL 6.9 Mon 12:15 H16

Investigation of excitonic resonances in monolayer MoSe2 for strong coupling experiments at room temperature — •Nils Lundt[1], Aleksander Maryński[2], Grzegorz Sek[2], Oliver Iff[1], Sefaattin Tongay[3], Sven Höfling[1,4], and Christian Schneider[1] — [1]Chair for Apllied Physics, University of Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Institute of Physics, Wrocław University of Technology, Wybrzeze Wyspiańskiego 27, 50-370 Wrocław, Poland — [3]School for Engineering of Matter, Transport, and Energy, Arizona State University, Tempe, Arizona 85287, United States — [4]SUPA, School of Physics and Astronomy, University of St. Andrews, St. Andrews KY 16 9SS, United Kingdom

We studied the temperature evolvement of the reflectivity of a MoSe2 monolayer. From this investigation we deduced the dependence of linewidth and oscillator strength on temperature. The results were used for transfer matrix simulations of strong coupling reflectivity spectra, expected if the MoSe2 monolayer is integrated into a micro-cavity. These calculations should evaluate, if strong coupling can be observed in MoSe2 monolayers at room temperature. Calculations were conducted for different cavity designs such as an open cavity approach, a monolithic cavity and for the coupling to a Tamm Plasmon. Moreover, we present results of excitation power dependent photoluminescence studies on MoSe2 monolayers.

HL 6.10 Mon 12:30 H16

Localized states from WSe_2 as promising candidates for new single-photon sources — •Sven Borghardt[1], Jhih-Sian Tu[1], Florian Winkler[2], Detlev Grützmacher[1], and Beata Kardynal[1] — [1]PGI-9, Forschungszentrum Jülich, Jülich, Germany — [2]ER-C, Forschungszentrum Jülich, Jülich, Germany

An emission of single photons from WSe_2 monolayers (ML) has been recently demonstrated but the origin of the emission is still not clear. The aim of our research is to understand its origin and then control the localized emission in this material to harvest the unique properties of the material for new applications in quantum photonics.

Samples prepared by exfoliation from synthetic crystals and also grown with CVD are measured using polarization resolved μ-photoluminescence (PL) as well as time-resolved PL.

Our results show linearly polarized emission doublet lines with an energy splitting of up to a few meV. The samples show a high density of such lines close to the sample edges. We attribute the linear polarization of the localized states to a mixing of K- and K'-states. There is an evidence of an alignment of the polarization of emission with the crystal lattice. PL from the localized states decays faster with the temperature than the one from the free exciton states. Chemical modification of the samples is further used in an attempt to manipulate the emission from the localized states.

HL 6.11 Mon 12:45 H16

Theoretical studies of transition metal dichalcogenides for the use in electron holography — •Sven Borghardt[1], Zeila Zanolli[4], Matthieu Verstraete[3], Florian Winkler[2], Juri Barthel[2], Rafal Dunin-Borkowski[2], and Beata Kardynal[1]

— [1]PGI-9, Forschungszentrum Jülich, Jülich, Germany — [2]ER-C, Forschungszentrum Jülich, Jülich, Germany — [3]PCPM, Université Catholique de Louvain, Louvain-la-Neuve, Belgium — [4]PGI-2 and IAS, Forschungszentrum Jülich, Jülich, Germany

Few-layer transition metal dichalcogenides (TMDs) represent a new family of materials with promising properties for new optoelectronic nano-devices. Their well-known and tailorable thickness render them an ideal system for quantitative electron holography.

Here, we present the simulation of the effect of charge reorganisation due to bonding on the phase acquired by electrons passing through few layer TMD structures in electron holography experiments. This is done by simulating the phases for potentials from density functional theory calculations in comparison with ones obtained from the independent-atom approximation. The results show in an impressive way that neglecting the atomic bonding and the associated small change in the overall charge distribution leads to an overestimation of the average electron phase by approximately 5% for the analyzed materials. Comparison with experimental data confirms this conclusion.

Building on the results for pristine materials, we present calculations for single defects and heterostructures composed of different materials from the transtition-metal dichalcogenide family.

HL 7: Graphene: Theory (Joint session of DS, HL and TT, organized by HL)

Time: Monday 9:30–12:30 Location: H17

HL 7.1 Mon 9:30 H17

Instantaneous Quantum Time Reversal Mirror in Graphene — •Phillipp Reck[1], Cosimo Gorini[1], Arseni Goussev[2], Mathias Fink[3], and Klaus Richter[1] — [1]Institut für Theoretische Physik, Universität Regensburg — [2]Department of Mathematics and Information Sciences, Northumbria University, Newcastle Upon Tyne, UK — [3]Ecole Supérieure de Physique et Chimie Industrielle, CNRS, PSL Research University, Paris, France

The physicists' fascination for time inversion goes back a long time, as testified by the famous 19th-century argument between Loschmidt and Boltzmann concerning the arrow of time. Both metaphysical and practical considerations intrigued generations of scientists, who have ever since strived to devise and implement time-inversion protocols – in particular, different forms of "time mirrors" for classical waves such as sound- and electromagnetic-waves (see e.g. [1-2]), and recently an instantaneous time mirror for water waves [3].

Here we propose the realization of instantaneous Time Mirrors for quantum systems. These are controlled time discontinuities acting on wavefronts as mirrors in time and leading to distinct wavefunction echoes. More precisely, our Quantum Time Mirror exploits up to now unrelated concepts of wavefront time inversion and population reversal in two-level systems, the latter quintessential to spin echoes. It can be implemented in a relativistic Dirac-like system, e.g. graphene.

[1]M. Fink , IEEE Trans. Ultr. Ferroel. Freq. Control, 39, 555, (1992)

[2]G. Lerosey, et al., Phys. Rev. Lett. 92, 193904 (2004)

[3]V. Bacot, et al., preprint (2015)

HL 7.2 Mon 9:45 H17

Plasmon signature in Dirac-Weyl liquids — •Johannes Hofmann — TCM Group, Cavendish Laboratory, University of Cambridge, UK

I shall discuss theoretically as a function of temperature the plasmon mode arising in three-dimensional Dirac liquids, i.e., systems with linear chiral relativistic single-particle dispersion, within the random phase approximation. It is found that whereas no plasmon mode exists in the intrinsic (undoped) system at zero temperature, there is a well-defined finite-temperature plasmon with superlinear temperature dependence, rendering the plasmon dispersion widely tunable with temperature. The plasmon dispersion contains a logarithmic correction due to the ultraviolet-logarithmic renormalization of the electron charge, manifesting a fundamental many-body interaction effect as in quantum electrodynamics. The plasmon dispersion of the extrinsic (doped) system displays a minimum at finite temperature before it crosses over to the superlinear intrinsic behavior at higher temperature, implying that the high-temperature plasmon is a universal feature of Dirac liquids irrespective of doping. This striking characteristic temperature dependence of intrinsic Dirac plasmons along with the logarithmic renormalization is a unique manifestation of the three-dimensional relativistic Dirac nature of quasiparticle excitations and serves as an experimentally observable signature of three-dimensional Dirac materials.

HL 7.3 Mon 10:00 H17

Finite temperature and electric field effects in the RKKY interaction in graphene and bilayer graphene — •Nicolas Klier[1], Sangeeta Sharma[2], Oleg Pankratov[1], and Sam Shallcross[1] — [1]Theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7-B2, 91058 Erlangen — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle

The Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction in Bernal stacked bilayer graphene [1,2] is shown to have a particularly rich dependence on temperature and a layer symmetry breaking electric field. Depending on whether we consider the chemical potential or particle number as the fixed variable we find that an electric field may tune the RKKY between ferromagnetic (FM) and anti-ferromagnetic (AFM) coupling, or an oscillatory and AFM coupling.

[1] N. Klier, S. Shallcross, and O. Pankratov, *P*hys. Rev. B **90**, 245118, 2014.

[2] N. Klier, S. Shallcross, S. Sharma, and O. Pankratov, *P*hys. Rev. B **92**, 205414, 2015.

HL 7.4 Mon 10:15 H17

The Electronic Structure of Graphene from Dyson-Schwinger Equations with Partially Screened Coulomb Interactions — •Manon Bischoff[1], Katja Kleeberg[2], Dominik Smith[2], Lorenz von Smekal[2], and Björn Wellegehausen[2] — [1]Johannes Gutenberg Universität, Mainz, Deutschland — [2]Justus Liebig Universität, Gießen, Deutschland

We have studied the possibility of a semimetal-insulator transition via spin-density or charge-density wave formation with partially screened Coulomb interactions in graphene from the coupled Dyson-Schwinger equations (DSEs) for the electronic excitations and their Lindhard screening on the honeycomb lattice. In the limit of purely static Lindhard screening these DSEs close on themselves and no further truncation is necessary. With appropriate boundary conditions they can then be solved numerically by fixed-point iteration. This is particularly efficient on graphical processing units (GPUs). After validating the static approximation from Monte-Carlo simulations on smaller lattices with appropriate boundary conditions, it allows to study much larger sheets than in the ab-initio simulations, e.g., to search for Miransky scaling, and to include cases where the latter break down because of a fermion-sign problem as for charge-density wave formation, for example.

HL 7.5 Mon 10:30 H17

Ab-initio lattice Monte-Carlo simulations of the Neck-disrupting Lifshitz transition in mono-layer graphene — •Michael Koerner, Dominik Smith, and Lorenz von Smekal — Institut fuer Theoretische Physik, Justus-Liebig-Universitaet Giessen

We study the effects of inter-electron interactions on the neck-disrupting Lifshitz transition, which is characterized by a change of topology of the Fermi surface. The Lifshitz transition is known to occur within a pure tight-binding description of mono-layer graphene when an external chemical potential drives the Fermi surface away from half-filling and across the saddles at the M-points. At these Van Hove singularities the density of states diverges logarithmically without interactions. We employ ab-intio Monte-Carlo simulations, which account for the full many-body physics of interacting electrons. We choose a partially screened Coulomb potential which combines the screening from localized electron states at short distances with the unscreened long-range Coulomb tails characteristic of graphene at half filling. Our goal is to determine whether interactions change the character of the topological transition, such that a real phase transition in the thermodynamic sense may occur, possibly in combination with chiral superconductivity.

HL 7.6 Mon 10:45 H17

Tight-binding description of spin-orbit coupling in graphene due to adatoms — •Susanne Irmer, Denis Kochan, Klaus Zollner, Martin Gmitra, Tobias Frank, and Jaroslav Fabian — University of Regensburg, Regensburg, Germany

We present realistic effective tight-binding models for proximity spin-orbit coupling in graphene due to adatoms at top, bridge, and hollow positions. The models are built from symmetry arguments and fitted to ab initio calculations for a variety of adsorbants, such as H [1], F [2], Cu, and CH3 [3]. For each of these adatoms we provide magnitudes for orbital couplings to the adsorbants, as well as the intrinsics, Rashba, and pseudospin-inversion asymmetry (PIA) couplings. Our models can be used to study spin relaxation, spin Hall effect, and spin transport using quantum transport models.

This work was supported by the DFG SFB 689 and GRK 1570, and by the European Union Seventh Framework Programme under Grant Agreement No. 604391 Graphene Flagship.

[1] M. Gmitra, D. Kochan, J. Fabian, Phys. Rev. Lett. 110, 246602 (2013)

[2] S. Irmer, T. Frank, S. Putz, M. Gmitra, D. Kochan, J. Fabian, Phys. Rev. B 91, 115141 (2015)

[3] K. Zollner, T. Frank, S. Irmer, M. Gmitra, D. Kochan, J. Fabian, arXiv:1507.02820

30 min. Coffee Break

HL 7.7 Mon 11:30 H17

Ab initio studies of excitations in monolayer black phosphorus — •Tobias Frank[1], Marcin Kurpas[1], Martin Gmitra[1], Rene Derian[2], Ivan Stich[2], and Jaroslav Fabian[1] — [1]Universität Regensburg, Regensburg, Germany — [2]Slovak Academy of Sciences, Bratislava, Slovakia

Monolayer black phosphorus, or phosphorene, represents an ideal system to study many-body electron-electron and electron-hole interactions due to its strong anisotropy driven 1d electronic nature. In particular, the size of the fundamental band gap value and excitonic binding energies remain unresolved given the different gap values of 1.6 to 2.4 eV [1] obtained by many-body GW calculations. We present our contribution to this issue studying excitations in phosphorene employing quantum monte carlo (QMC) calculations. We show the evolution of finite size effects of the fundamental and optical gap, with respect to relatively large supercell sizes in the theoretical framework of diffusion monte carlo (DMC) explicitly including electronic correlations. Our studies point to a significant influence of electron correlation on the fundamental gap as well as to a strong anisotropic nature of the excitonic state. Furthermore we address the question of a multiconfigurational ground state in monolayer black phosphorus. This work is supported by the DFG GRK 1570, SFB 689, and European Union Seventh Framework Programme under Grant Agreement No. 604391 Graphene Flagship.

[1] A. N. Rudenko, Shengjun Yuan, and M. I. Katsnelson, Phys. Rev. B 92 085419 (2015)

HL 7.8 Mon 11:45 H17

Phase structure of graphene from Hybrid Monte-Carlo simulations — •Pavel Buividovich[1], Lorenz von Smekal[2], Dominik Smith[2], and Maksim Ulybyshev[1] — [1]Regensburg University, Institute for Theoretical Physics, D-93053 Regensburg, Universitatstr. 31 — [2]Giessen University, Institute for Theoretical Physics, D-35392 Gießen, Heinrich-Buff-Ring 16

We study the phase structure of monolayer graphene in the parametric space of on-site and nearest-neighbour interactions using the Hybrid Monte-Carlo algorithm similar to those used in lattice QCD simulations. Our simulation code allows us to perform ab-initio simulations on lattices as big as 36x36 unit cells. We numerically determine the boundaries of the charge density wave, spin density wave and the Kekule distortion phases. We also confront the results with analytic studies based on Schwinger-Dyson equations, which allow to reach even larger lattice sizes, up to 5000x5000 unit cells.

HL 7.9 Mon 12:00 H17

Quantum Monte-Carlo study of graphene in external magnetic field — •Maksim Ulybyshev — Institute of Theoretical Physics, University of Regensburg, D-93053 Germany, Regensburg, Universitatsstrasse 31

Recent experimental results indicate that graphene turns into insulator in sufficiently strong magnetic field. However, the exact nature of this state is still elusive and there are some discrepancies between theoretical predictions and experimental results. To resolve this discrepancies extensive simulations of graphene in external magnetic field were performed using Hybrid Monte Carlo algorithm. Insulating state was observed in agreement with experiment. Mass gap and various order parameters were measured.

HL 7.10 Mon 12:15 H17

Interaction-induced conductance from zero modes in a clean magnetic graphene waveguide — •Laura Cohnitz[1], Wolfgang Häusler[2,3], Alex Zazunov[1], and Reinhold Egger[1] — [1]Institut für Theoretische Physik, Heinrich-Heine-Universität, D-40225 Düsseldorf, Germany — [2]Institut für Physik, Universität Augsburg, D-86135 Augsburg, Germany — [3]Institut für Theoretische Physik, Universität Hamburg, D-20355 Hamburg, Germany

We consider a waveguide formed in a clean graphene monolayer by a spatially inhomogeneous magnetic field. The single-particle dispersion relation for this waveguide exhibits a zero-energy Landau-like at band, while finite-energy bands have dispersion and correspond, in particular, to snake orbits. For zero-mode states, all matrix elements of the current operator vanish, and a finite conductance can only be caused by virtual transitions to finite-energy bands. We show that Coulomb interactions generate such processes. In stark contrast to finite-energy bands, the conductance is not quantized and shows a characteristic dependence on the zero-mode filling. Transport experiments thereby offer a novel and highly sensitive probe of electron-electron interactions in clean graphene samples. We argue that this interaction-driven zero-mode conductor may also appear in other physical settings and is not captured by the conventional Tomonaga-Luttinger liquid description.

HL 8: Transport: Quantum Coherence and Quantum Information Systems - Experiment (Joint session of HL, MA and TT, organized by TT)

Time: Monday 9:45–13:00 Location: H22

HL 8.1 Mon 9:45 H22

Tunable coupling between fixed-frequency superconducting transmon qubits — •Stefan Filipp[1], David C. McKay[2], Easwar Magesan[2], Antonio Mezzacapo[2], Jerry M. Chow[2], and Jay M. Gambetta[2] — [1]IBM Research - Zurich, 8803 Rueschlikon, Switzerland — [2]IBM TJ Watson Research Center, Yorktown Heights, NY, USA

The controlled realization of qubit-qubit interactions is essential for both the physical implementation of quantum error-correction codes and for reliable quantum simulations. Ideally, the fidelity and speed of corresponding two-qubit gate operations is comparable to those of single qubit operations. In particular, in a scalable superconducting qubit architecture coherence must not be compromised by the presence of additional coupling elements mediating the interaction between qubits. Here we present a coupling method between fixed-frequency transmon qubits based on the frequency modulation of an auxiliary circuit coupling to the individual transmons. Since the coupler remains in its ground state at all times, its coherence does not significantly influence the fidelity of consequent entangling operations. Moreover, with the possibility to create interactions along different directions, our method is suited to engineer Hamiltonians with adjustable coupling terms. This property can be utilized for quantum simulations of spins or fermions in transmon arrays, in which pairwise couplings between adjacent qubits can be activated on demand.

HL 8.2 Mon 10:00 H22

Concentric transmon qubit featuring fast tunability and an anisotropic magnetic dipole moment — •Jochen Braumüller[1], Martin Sandberg[2], Michael R. Vissers[2], Andre Schneider[1], Steffen Schlör[1], Lukas Grünhaupt[1], Hannes Rotzinger[1],

Michael Marthaler[1], Alexander Lukashenko[1], Amadeus Dieter[1], Alexey V. Ustinov[1,3], Martin Weides[1,4], and David P. Pappas[2] — [1]Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany — [2]National Institute of Standards and Technology, Boulder, Colorado 80305, USA — [3]National University of Science and Technology MISIS, Moscow 119049, Russia — [4]Johannes Gutenberg University, Mainz, 55128 Mainz, Germany

We present a planar qubit design based on a superconducting circuit that we call concentric transmon. While employing a straightforward fabrication process using Al evaporation and lift-off lithography, we observe qubit lifetimes and coherence times in the order of 10 μs. We systematically characterize loss channels such as incoherent dielectric loss, Purcell decay and radiative losses. The implementation of a gradiometric SQUID loop allows for a fast tuning of the qubit transition frequency and therefore for full tomographic control of the quantum circuit. Due to the large loop size, the presented qubit architecture features a strongly increased magnetic dipole moment as compared to conventional transmon designs. This renders the concentric transmon a promising candidate to establish a site-selective passive direct $\hat{Z}$ coupling between neighboring qubits, being a pending quest in the field of quantum simulation.

HL 8.3 Mon 10:15 H22

Quasiparticle-Induced Decoherence of Microscopic Two-Level-Systems in Superconducting Qubits — •Alexander Bilmes[1], Jürgen Lisenfeld[1], Sebastian Zanker[1], Michael Marthaler[2], Gerd Schön[2], Georg Weiss[1], and Alexey V. Ustinov[1] — [1]PHI, KIT, 76131 Karlsruhe, Germany — [2]TFP, KIT, 76131 Karlsruhe, Germany

Parasitic Two-Level-Systems (TLS) are one of the main sources of decoherence in superconducting nano-scale devices such as SQUIDs, resonators and quantum bits (qubits), although the TLS' microscopic nature remains unclear. We use a superconducting phase qubit to detect TLS contained within the tunnel barrier of the qubit's Al/AlOx/Al Josephson junction. If the TLS transition frequency lies within the $6 - 10$ GHz range, we can coherently drive it by resonant microwave pulses and access its quantum state by utilizing the strong coupling to the qubit. Our previous measurements of TLS coherence in dependence of the temperature indicate that quasiparticles (QPs), which diffuse from the superconducting Al electrodes into the oxide layer, may give rise to TLS energy loss and dephasing [1]. Here, we probe the TLS-QP interaction using a reliable method of *in-situ* QP injection via an on-chip dc-SQUID that is pulse-biased beyond its switching current. The QP density is calibrated by measuring associated characteristic changes to the qubit's energy relaxation rate. We will present experimental data which show the QP-induced TLS decoherence in good agreement to theoretical predictions.

[1] J. Lisenfeld et al., PRL **105**, 230504 (2010)

HL 8.4 Mon 10:30 H22

Transmon qubits enter circuit nano-electromechanics — •Daniel Schwienbacher[1,2], Matthias Pernpeintner[1,2,3], Friedrich Wulschner[1,2], Philip Schmidt[1,2,3], Frank Deppe[1,2,3], Achim Marx[1], Rudolf Gross[1,2,3], and Hans Huebl[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [2]Physik-Department, TU München, 85748 Garching, Germany — [3]Nanosystems Initiative Munich (NIM), 80799 München, Germany

The field of cavity nano-electromechanics combines nano-scale mechanical elements with microwave circuits for the investigation of the light-matter interaction on a quantum level. In this context ground state cooling, electromechanically induced transparency effects, as wells as state transfer between the mechanical and photonic modes have been demonstrated. Recently, Abdi et al.[1] have proposed the integration of a nanomechanical beam into the capacitor of a transmon qubit, which is in turn coupled to a microwave resonator and predicted enhanced electro-mechanical coupling rates as well as the preparation of mechanical Fock states and the generation of three-partite entanglement. Here, we present an experimental study concerning the integration of a nanomechanical beam, a transmon qubit, and a microwave resonator on a single chip. We will discuss fabricational aspects and first spectroscopy data of the device.

We thankfully acknowledge financial support by the DFG via the collaborative research center SFB 631.

[1] Mehdi Abdi et al., PRL **114**, 173602 (2015)

HL 8.5 Mon 10:45 H22

Thermal microwave states acting on a superconducting qubit — •Jan Goetz[1,2], Miriam Müting[1,2], Max Haeberlein[1,2], Friedrich Wulschner[1,2], Edwar Xie[1,2,3], Peter Eder[1,2,3], Michael Fischer[1,2], Frank Deppe[1,2], Kirill Fedorov[1,2], Hans Hübl[1,2], Frank Deppe[1,2,3], Achim Marx[1], and Rudolf Gross[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [2]Physik-Department, TU München, 85748 Garching, Germany — [3]Nanosystems Initiative Munich (NIM), Schellingstraße 4, 80799 München, Germany

We analyze the influence of broadband thermal states in the microwave regime on the coherence properties of a superconducting (transmon) qubit coupled to a transmission line resonator. We generate the thermal states inside the resonator by heating a 30 dB attenuator to emit blackbody radiation into a transmission line. In the absence of thermal fluctuations, the qubit coherence time is limited by relaxation. We find that the relaxation rate is almost unaffected by the presence of a thermal field inside the resonator. However, such states induce significant dephasing which increases quadratically with the number of thermal photons, whereas for a coherent population of the resonator, the increase shows a linear behavior. These results confirm the different photon statistics, being Poissonian for a coherent population and super-Poissonian for a thermal population of the resonator.

This work is supported by the German Research Foundation through SFB 631 and FE 1564/1-1, EU projects CCQED, PROMISCE, the doctorate program ExQM of the Elite Network of Bavaria.

HL 8.6 Mon 11:00 H22

Displacement of squeezed propagating microwave states — •Kirill G. Fedorov[1], P. Yard[1,2], S. Pogorzalek[1,2], P. Eder[1,2,3], M. Fischer[1,2,3], J. Goetz[1,2], F. Wulschner[1,2], E. Xie[1,2,3], F. Deppe[1,2,3], A. Marx[1], and R. Gross[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [2]Physik-Department, Technische Universität München, 85748 Garching, Germany — [3]Nanosystems Initiative Munich (NIM), Schellingstraße 4, 80799 München, Germany

The displacement of propagating quantum states of light is a fundamental operation for quantum communication. It can be applied to fundamental studies of macroscopic quantum coherence and has an important role in quantum teleportation protocols with continuous variables. We study an experimental implementation of this operation for propagating squeezed microwave states. We generate these states using a Josephson parametric amplifier and implement the displacement operation using a specific cryogenic directional coupler. We demonstrate that even for strong displacement amplitudes we do not observe any degradation of the reconstructed quantum states. Furthermore, we confirm that path entanglement generated using displaced squeezed states, also stays constant over a wide range of the displacement power.

We acknowledge support by the German Research Foundation through SFB 631 and FE 1564/1-1, the EU project PROMISCE, and Elite Network of Bavaria through the program ExQM.

15 min. break

Invited Talk HL 8.7 Mon 11:30 H22

Coherent Suppression of Quasiparticle Dissipation in a Superconducting Artificial Atom — •Ioan Pop — Physikalisches Institut, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany — Department of Applied Physics, Yale University, New Haven, CT 06520, USA

We demonstrate immunity to quasiparticle dissipation in a Josephson junction. At the foundation of this protection rests a prediction by Brian Josephson from fifty years ago: the particle-hole interference of superconducting quasiparticles when tunneling across a Josephson junction [1]. The junction under study is the central element of a fluxonium artificial atom, which we place in an extremely low loss environment and measure using radio-frequency dispersive techniques [2]. Furthermore, by using a quantum limited amplifier (a Josephson Parametric Converter) we can observe quantum jumps between the 0 and 1 states of the qubit in thermal equilibrium with the environment. The distribution of the times in-between the quantum jumps reveals quantitative information about the population and dynamics of quasiparticles[3]. The data is entirely consistent with the hypothesis that our system is sensitive to single quasiparticle excitations, which opens new perspectives for quasiparticle monitoring in low temperature devices.

[1] B. D. Josephson, Physics Letters **1**, 251 (1962)

[2] I. M. Pop et al., Nature **508** (2014)
[3] U. Vool et al., PRL **113** (2014)

HL 8.8 Mon 12:00 H22

Tunable superconducting resonators with integrated trap structures for coupling with ultracold atomic gases — •Benedikt Ferdinand[1], Daniel Bothner[1,2], Dominik Wiedmaier[1], Dieter Koelle[1], and Reinhold Kleiner[1] — [1]Physikalisches Institut and Center for Quantum Science (CQ) in LISA$^+$, Universität Tübingen, Auf der Morgenstelle 14, D-72076 Tübingen, Germany — [2]Kavli Institute of Nanoscience, Delft University of Technology, PO Box 5046, 2600 GA, Delft, The Netherlands

We intend to investigate a hybrid quantum system where ultracold atomic gases play the role of a long-living quantum memory, coupled to a superconducting qubit via a coplanar waveguide transmission line resonator. As a first step we developed a resonator chip containing a Z-shaped trapping wire for the atom trap. In order to suppress parasitic resonances due to stray capacitances, and to achieve good ground connection we use hybrid superconductor - normal conductor chips. As an additional degree of freedom we add a ferroelectric capacitor making the resonators voltage-tunable. We furthermore show theoretical results on the expected coupling strength between resonator and atomic cloud.

HL 8.9 Mon 12:15 H22

Quantum correlations in microwave frequency combs — •Thomas Weissl[1], Erik Tholén[2], Daniel Forchheimer[1,2], and David B. Haviland[1] — [1]KTH- Royal Institute of Technology, 106 91 Stockholm, Sweden — [2]Intermodulation Products AB, 823 93 Segersta, Sweden

Non-linear superconducting resonators are used as parametric amplifiers in circuit quantum electrodynamics experiments [1]. When pumped below threshold the pump correlates vacuum fluctuations in the signal and idler bands giving rise to two-mode squeezed vacuum. When a non-linear oscillator is pumped with a frequency comb complex multipartite entangled states can be created as demonstrated in similar experiments in the optical domain [2]. We present a method to generate and measure microwave frequency combs by up- and down-conversion from intermediate frequencies. The comb is generated and analyzed using a multi-frequency lock-in amplifier. From transmission measurements we extract correlation- and quasi-probability functions.
[1] E. Tholén et al., APL **90**, 253509 (2007)
[2] M. Chen et al., PRL **112**, 120505 (2014)

HL 8.10 Mon 12:30 H22

Microwave experiments with quantum phase-slip in superconducting AlO_x nanowires — •Sebastian T. Skacel[1], Marco Pfirrmann[1], Jan N. Voss[1], Micha Wildermuth[1], Julian Münzberg[1], Lucas Radtke[1], Sebastian Probst[1], Martin Weides[1,2], J. E. Mooij[1,3], Hannes Rotzinger[1], and Alexey V. Ustinov[1] — [1]Physikalisches Institut, Karlsruher Institut für Technologie, D-76131 Karlsruhe, Germany — [2]Institute of Physics, Johannes Gutenberg University Mainz, D-55128 Mainz, Germany — [3]Kavli Institute of Nanoscience, Delft University of Technology, 2628 CJ Delft, The Netherlands

Superconducting nanowires in the quantum phase slip (QPS) regime allow to study the flux and phase dynamics in duality to Josephson junction systems. We experimentally study QPS effects of nanowires which are embedded in a resonant microwave circuit. The samples are probed at ultra-low microwave power and applied magnetic field at mK temperatures. The AlO_x nanowires, with a sheet resistance in the kΩ range, are fabricated by sputter deposition of aluminium in a controlled oxygen atmosphere. The wires are defined with conventional electron beam lithography into hydrogen silsesquioxane (HSQ) down to a width of 15-30 nm.
We present the single layer process fabrication and measurements of nanowires galvanically coupled to a superconducting lumped element microwave resonator.

HL 8.11 Mon 12:45 H22

Localized quantum phase slips in TiN nanowires — •Ina Schneider[1], Tatyana Baturina[1,2], and Christoph Strunk[1] — [1]Inst. f. Exp. und Angewandte Physik, Uni Regensburg — [2]Inst. f. Semiconductor Physics, RAS, Novosibirsk, Russia

We investigate TiN nanowires with 780 nm length and widths ranging from 50-780 nm close to the superconductor/insulator transition. In zero magnetic field the superconducting transition of wider wires resembles that of macroscopic films, while narrower wires develop a finite and T-independent resistance down to the lowest temperatures. In perpendicular magnetic field B a pronounced nonmontonic magnetoresistance occurs. The $R(T)$-curves at fixed B show a reentrant insulating behavior very similar to that of Coulomb-blockaded linear arrays of Josephson junctions [1].

The $I(V)$-characteristics display a characteristic cross-over from the dc-Josephson effect towards Coulomb blockade at very low voltages and temperatures within a globally superconductive-like $I(V)$. In the linear regime, the magnetoresistance displays strong fluctuations. We interpret our results in terms of disordered Josephson networks with a B-dependent Josephson coupling energy that favors coherent quantum phase slips at certain B.
[1] A. Ergül, et al., NJP **15**, 095014 (2014).

HL 9: Graphene I: Structure and Dynamics

Time: Monday 10:30–13:30 Location: H24

HL 9.1 Mon 10:30 H24

The electronic structure of graphene superlattices revisited — •Pilkwang Kim[1] and Cheol-Hwan Park[2] — [1]Department of Physics and Astronomy, Seoul National University, Seoul, Korea — [2]Department of Physics and Astronomy, Seoul National University, Seoul, Korea

We present the calculated electronic structure of graphene superlattices, which are graphenes under lateral, periodic potential. Previous studies on a graphene superlattice [1-3] have reported anisotropic group velocity renormalization, emergence of new zero-energy points, conductance resonance, etc. However, several features manifested in the electronic structure obtained from our numerical calculations, e.g., the movement of the Dirac points in momentum space, cannot be explained by the theories introduced in those studies. In this presentation, we discuss the reason why there are features in the electronic structure of graphene superlattices that were not captured by previous theories. We also discuss electronic structure obtained by using first- and higher-order perturbation calculations.

1.Park, C.-H., Yang, L., Son, Y.-W., Cohen, M. L. & Louie, S. G. New generation of massless Dirac fermions in graphene under external periodic potentials. Phys. Rev. Lett. 101, 126804 (2008). 2.Barbier, M., Vasilopoulos, P. & Peeters, F. M. Dirac electrons in a Kronig-Penney potential: Dispersion relation and transmission periodic in the strength of the barriers. Phys. Rev. B 80, 205415 (2009). 3.Brey, L. & Fertig, H. A. Emerging Zero Modes for Graphene in a Periodic Potential. Phys. Rev. Lett. 103, 046809 (2009).

HL 9.2 Mon 10:45 H24

Confinement effects in quasiparticle interference on epitaxial graphene nanoflakes — •Julia Tesch[1], Philipp Leicht[1], Felix Blumenschein[1], Tomas Löfwander[2], Luca Gragnaniello[1], and Mikhail Fonin[1] — [1]Universität Konstanz, Konstanz, Germany — [2]Chalmers University of Technology, Göteborg, Sweden

In the search for suitable materials to be used in nanoscale electronic devices, graphene quantum dots, ribbons and flakes have attracted increased attention amongst researchers, as they allow for a combination of graphene's linear electronic dispersion relation with interesting physical phenomena arising from the size quantization of the structures.

We present a comprehensive study of epitaxial graphene nanoflakes on noble metal surfaces by means of low-temperature scanning tunneling microscopy and spectroscopy. The analysis of quasiparticle interference patterns produced by elastic scattering at defects allows for a clear identification of graphene-related contributions visible as ringlike *inter-* and *intravalley* features within the Fourier transform images [1]. Lateral electronic confinement within these elongated flakes gives rise to additional scattering intensity related to transitions between the

flake's transverse modes [2]. Additionally, we discuss the influence of edge configuration, lattice symmetry breaking and quasiparticle lifetime on the scattering, by comparison of the experimental results with tight-binding calculations of realistic graphene nanoflakes.

[1] P. Leicht *et al.*, ACS Nano **8**, 3735 (2014); [2] A. Bergvall *et al.*, Phys. Rev. B **87**, 205431 (2013).

HL 9.3 Mon 11:00 H24

Electron interference in ballistic graphene nanoconstrictions — •Johannes Aprojanz[1], Jens Baringhaus[1], Mikkel Settnes[2], Stephen Power[2], Anti-Pekka Jauho[2], and Christoph Tegenkamp[1] — [1]Leibniz Universität Hannover, Institut für Festkörperphysik, 30167 Hannover, Germany — [2]Technical University of Denmark, DTU Nanotech, Center for Nanostructured Graphene (CNG), 2800 Kgs. Lyngby, Denmark

Graphene nanoconstrictions (GNCs) are a central building block of future carbon electronic devices. However, the synthesis of constrictions with well-defined edges is challenging. Here, we use the tip of a scanning tunneling microscope (STM) for the local etching of graphene, which allows to define GNCs with variable dimensions of down to 1 nm. The GNCs are etched into fully ballistic graphene nanoribbons hosted on the sidewalls of SiC mesa structures [1]. Due to the highly precise etching technique as well as the exceptional electronic quality of the graphene (e.g. mean free path $> 10\ \mu$m), this system is ideal to study coherent transport phenomena. Therefore, the transport characteristics of constrictions with various dimensions are recorded by means of a variable temperature 4-tip-STM. Electron interference at the abrupt graphene interfaces gives rise to characteristic conductance peaks and transport gaps. Their appearance is described by a tight-binding and recursive Green's function approach which especially highlights the robustness of the resonances features against temperature as well as disorder.

[1] Baringhaus et al., Nature **506**, 349 (2014)

HL 9.4 Mon 11:15 H24

Graphene on Ru(0001) as a playground for the studies of the graphene-metal interaction — Elena Voloshina[1], Nikolai Berdunov[2], and •Yuriy Dedkov[2,3] — [1]HU Berlin, Germany — [2]SPECS GmbH, Germany — [3]IHP Frankfurt (Oder), Germany

We employ a combination of surface science methods (ARPES, STM/STS, AFM) and DFT calculations for the studies of the lattice mismatched graphene-Ru interface. Our results demonstrate a site-selective interaction (*strong* vs *weak*) between graphene and metal in the moiré lattice. In these studies we show that graphene-*hills* in this structure can be used as an array of electro-mechanical elastic nano-resonantors with very high resonance frequency (in the THz range). On the next step we modify the graphene-Ru interaction via intercalation. Here the scanning probe microscopy and spectroscopy were used to study the crystallographic structure and electronic properties of the uniform free-standing graphene layers obtained by intercalation of oxygen monolayer in the *strongly* bonded graphene/Ru(0001) interface. Spectroscopic data show that such graphene layer is heavily *p*-doped with the Dirac point located at 552 meV above the Fermi level, that corroborates our ARPES data. Experimental data are understood within DFT and the observed effects are in good agreement with the theoretical data.

Invited Talk HL 9.5 Mon 11:30 H24

Direct view on non-equilibrium carriers in graphene with time-resolved ARPES — •Isabella Gierz — Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany

The linear band structure of graphene bares great potential for optoelectronic applications ranging from Terahertz lasing to efficient light harvesting. We explore the response of the Dirac carriers in lightly hole-doped epitaxial graphene samples to three different excitation schemes: interband transitions for $\hbar\omega_{\mathrm{pump}} > 2\mu_{\mathrm{e}}$, free carrier absorption for $\hbar\omega_{\mathrm{pump}} < 2\mu_{\mathrm{e}}$, and resonant phonon excitation for $\hbar\omega_{\mathrm{pump}} = 200$ meV. Time- and angle-resolved photoemission spectroscopy (tr-ARPES) allows us to map the transient population of the Dirac cone in momentum space over a large energy window of several electron Volts down to arbitrarily small excitation energies.

We find a short-lived population-inverted state for interband excitation [1], a simple metallic relaxation behaviour for free carrier absorption [1], and indications for a transient enhancement of the electron-phonon coupling constant when resonantly driving the in-plane phonon in bilayer graphene [2]. Furthermore, by improving the temporal resolution to ∼10 fs, we were able to identify impact ionization as the primary thermalization channel within the first ∼25 fs [3].

[1] Gierz et al., Nature Materials 12, 1119 (2013)
[2] Gierz et al., PRL 114, 125503 (2015)
[3] Gierz et al., PRL 115, 086803 (2015)

HL 9.6 Mon 12:00 H24

Electronic properties of ytterbium interaction with graphene on Ir(111) — Hendrik Vita[1], •Stefan Böttcher[2], and Karsten Horn[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]SPECS Surface Nano Analysis GmbH, Berlin, Germany

The intercalation of metals in between graphene monolayers and a substrate is interesting from several points of view, for example in order to understand the effect of symmetry lowering in the interaction of the metal states with the specific graphene π bands in the region of the "Dirac cone". Here we present a study of the intercalation of a rare earth metal, Yb, in between graphene and Ir(111). Ytterbium exhibits an s-type valence band, making it possible to compare the electronic structure to the widely studied cases of alkali metals used as intercalates in graphene intercalation compounds. Using core level spectroscopy we follow the deposition of Yb and the evolution of the intercalated phase. LEED studies show that the structural arrangement of the intercalated Yb thin film leads to a $(\sqrt{3}\times\sqrt{3})$R30° phase. Angle-resolved photoemission reveals that the interaction between the metal states and the graphene π band near the K point induces an extremely strong n-type doping. Hybridization-induced band gaps open in the π band at binding energies of 0.3 eV and 1.6 eV due to the interaction with the strongly localized metal 4 *f* states. We compare our data with other weakly and strongly interacting intercalated metal layers.

HL 9.7 Mon 12:15 H24

Plasma-assisted CVD graphene synthesis and characterization on nickel substrates — •Patricia Pop-Ghe, Lisa Krückemeier, Nicolas Wöhrl, and Volker Buck — Faculty of Physics and CENIDE, University of Duisburg-Essen, Lotharstr, 1, 47057 Duisburg, Germany

This work presents the synthesis of graphene by plasma-assisted chemical vapour deposition on polycrystalline nickel foils. It is initiated by the comparison of the mechanisms in CVD and plasma-assisted CVD on a nickel substrate and focusses on the development of a growth model for both sides of the substrate within the experimental results. In detail, the differences in graphene growth at the front and at the back side of the substrate are investigated and correlated to specific influence factors. It is shown that growth mode as well as expansion and quality of graphene sheets can be adjusted by process temperature and time respectively since carbon solubility and diffusion in nickel both hold strong temperature and time dependencies. The strong time dependance of graphene growth is further indicative of a reconstructional nature of graphene formation, which is further discussed in the developed growth model. In addition the influence of the substrate is investigated by comparing results from graphene growth on polycrystalline nickel foils and nickel single crystal(111) substrates, as well as graphene on nickel (synthesized graphene) and silicon dioxide substrates (transferred graphene). Raman mappings are demonstrated to confirm the quality of the synthesized graphene.

HL 9.8 Mon 12:30 H24

Determination of the optical constants of graphene at the carbon K-edge by transmission spectroscopy — •Christine Jansing[1], Hans-Christoph Mertins[1], Andreas Gaupp[1], Andrey Sokolov[2], Markus Gilbert[1], Andreas Schümmer[1], Hud Wahab[3], Heiko Timmers[3], Suk-Ho Choi[4], and Dominik Legut[5] — [1]Münster University of Applied Sciences, Stegerwaldstr. 39, D-48565 Steinfurt — [2]HZB, Albert Einstein Str. 15, D-12489 Berlin — [3]University of New South Wales, Canberra, ACT 2600, Australia — [4]Kyung Hee University, Yongin 446-701, Korea — [5]IT4Innovations Center, VSB-Technical University of Ostrava, CZ-708 33 Ostrava, Czech Republic

The transmission of linearly polarized synchrotron radiation through quasi-free-standing graphene, supported by a Si3N4-membrane, has been measured across the carbon K-edge. From the measured absorption spectrum, that represents the imaginary part, the real part of the refractive index has been extracted via a Kramers-Kronig transformation. Based on these detailed optical parameters, reflection spectra have been simulated for linearly polarized soft x-ray light incident on graphene-metal systems. Importantly, the simulations include the interference of light reflected from graphene and from light reflected from

the metallic substrate, respectively. In addition the optical constants are compared to the ones obtained by various density function theory calculations using single-electron framework as well as the more complex many-body approaches to the electronic structure of free-standing graphene.

HL 9.9 Mon 12:45 H24

Origins of contact resistance in graphene-metal edge-contacts — •Bernhard Kretz[1], Christian Søndergaard Pedersen[2], Daniele Stradi[2], Aran Garcia-Lekue[1,3], and Mads Brandbyge[2] — [1]Donostia International Physics Center, E-20018 San Sebastian, Spain — [2]Center for Nanostructured Graphene, DTU Nanotech, Tech. Uni. of Denmark, DK-2800 Kongens Lyngby, Denmark — [3]IKERBASQUE, Basque Foundation for Science, E-48013 Bilbao, Spain

The transport properties of graphene-metal contacts play an important role in the design of graphene-based devices. Recent studies demonstrate the advantages of the edge-contact geometry over conventional surface contacts.[1,2] However, significantly different conclusions are reached regarding the influence of the metal on the conductance properties of edge-contacts: while simulations indicate that the contact resistance is of the same order of magnitude for different metals,[2] experiments reveal a strong metal-dependence.[1] The possible origins of these discrepancies are explored by studying the transport properties of graphene edge-contacts with different metals, different edge conformations, terminations and adsorption distances. We employ a density functional theory (DFT) based non-equilibrium Green-function (NEGF) approach, using the TranSIESTA code. Our results will offer insights towards a better understanding of the conductance properties of graphene-metal contacts deviating from ideal interfaces.

[1] Wang et al. Science 342, 2013; Chu et al. ACS Nano 8, 2014
[2] Matsuda et al., J. Phys. Chem. C 114, 2010

HL 9.10 Mon 13:00 H24

Magnetically confined quantum dots in graphene revealed by scanning tunneling spectroscopy — •Nils Freitag[1], Peter Nemes-Incze[1], Larisa Chizova[2], Colin R. Woods[3], Roman V. Gorbachev[3], Yang Cao[3], Andre K. Geim[3], Kostya S. Novoselov[3], Florian Libisch[2], and Markus Morgenstern[1] — [1]II. Institute of Physics B, RWTH Aachen, Otto-Blumenthal Street, 52074 Aachen, Germany — [2]Institute for Theoretical Physics, Vienna University of Technology, Wiedner Hauptstraße 8-10, 1040 Vienna, Austria — [3]School of Physics & Astronomy, University of Manchester, Manchester, United Kingdom

Confining graphene's chiral massless charge carriers by carving out nano-structures to circumvent Klein-tunneling suffers from disordered edges, impeding the control of the quasi-relativistic particles. Here, we use the electrostatic potential of an STM tip in combination with an homogeneous magnetic field to confine electrons in graphene without edges[1]. The confinement becomes visible as a fourfold charging sequence at B>2T, as expected from valley and spin degeneracy. Up to 40 charging peaks are observed in the hole and electron sector with charging energies of 5-10meV. Characteristic spatial charging patterns created by potential modulations of the commensurate G on BN are found[2].

[1] G. Giavaras and F. Nori, PRB 85, 165446 (2012)
[2] C. R. Woods et al., Nat. Phys. 10(6), 451-456 (2014)

HL 9.11 Mon 13:15 H24

Controling intramolecular Hydrogen-transfer by Gate-tunable STM — •Shai Mangel[1], Christian Dette[1], Katharina Polyudov[1], Paul Punke[1], Roberto Urcuyo[1], Marko Burghard[1], Soon Jung Jung[1], and Klaus Kern[1,2] — [1]Max-Planck-Institute for Solid State Research, D-70569 Stuttgart — [2]École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

The atomic level control of the electron transport has important advantages for many applications, such as molecular electronics, solar cells and sensors. Electron transport properties can be controlled by the intramolecular reaction which reshape the electronic configuration without any significant change in the conformation. The STM-induced tautomerization, i.e the interconversion between two isomers due to the migration of Hydrogen, was observed in the form of telegraphic noise. Several methods to control the intramolecular Hydrogen-transfer by changing the chemical environment of the molecule have been developed, such as locating adatoms or introducing defects. However, these affect the molecules only in the nm range. In this work, using the gate-tunable STM, we demonstrate a global control of the chemical environment of the substrate which results in the changing of the switching rate of the Hydrogen-transfer. The system we have used is a molecular network of phthalocyanine on graphene. Understanding and controlling the influence of the field-effect on the molecules, will be crucial for the construction of future molecular devices for energy and information usages.

HL 10: Plasmonics and Nanooptics: Light-Matter Interaction

Time: Monday 10:30–13:15 Location: S054

Invited Talk HL 10.1 Mon 10:30 S054

Hybrid plasmonic-photonic resonances for emitter control — •Femius Koenderink — Center for Nanophotonics, FOM Institute AMOLF, Amsterdam, The Netherlands

Plasmonic nanostructures match light to molecular length scales by hybridizing photons with charge density oscillations in noble metals. Plasmonics is pursued for many prospective uses ranging from sensing, spectroscopy, and microscopy, to the development of ultrabright single photon sources and broadband cavity QED for quantum information processing. I will report on our effort to use plasmonics to completely control when, into which direction, and with what polarization and wavefront single nanosources emit. I will particularly focus on Fourier-space polarimetry on single nano-antenna structures, as well as distributed periodic and quasiperiodic plasmonic structures for directional fluorescent, and lasing sources. Also, I will discuss the surprising physics of hybridizing plasmonics and dielectric nanophotonics. Recently we showed that, counter to conventional cavity perturbation theory, plasmonic structures can improve the quality factor of an already high-Q (exceeding 1 million) microtoroid. Finally, I will argue that hybrid plasmon-cavity structures can combine cavity Q-factors with plasmonic mode volumes.

HL 10.2 Mon 11:00 S054

Coherent and periodic energy transfer between widely separated and cavity-coupled nanoantennas — Martin Aeschlimann[1], Tobias Brixner[2], Benjamin Frisch[1], Bert Hecht[3], Bernhard Huber[2], •Matthias Hensen[4], Christian Kramer[2], Enno Krauss[3], Thomas Löber[5], Walter Pfeiffer[4], Martin Piecuch[1], and Philip Thielen[1] — [1]Department of Physics and Research Center OPTIMAS, TU Kaiserslautern, 67663 Kaiserslautern, Germany — [2]Department of Physical and Theoretical Chemistry, Würzburg University, 97074 Würzburg, Germany — [3]Experimental Physics 5, Würzburg University, 97074 Würzburg, Germany — [4]Faculty of Physics, Bielefeld University, 33615 Bielefeld, Germany — [5]Nano Structuring Center, TU Kaiserslautern, 67663 Kaiserslautern, Germany

We present a device that couples two widely separated ($d \approx 2\lambda_0$) nanoantennas via an extended plasmon mode in a metallic cavity of elliptical shape. As predicted by finite-difference time-domain simulations a coherent back and forth transfer of energy between the antennas is observed in experiments. Samples were made out of atomically-flat single crystalline gold plates and the temporal dynamics of plasmonic excitations was investigated by time-resolved photoelectron emission microscopy. The device depicts an all-plasmonic analogue of the quantum mechanical Tavis-Cummings model and it is particularly suited to study the interaction of deterministically positioned quantum systems coupled to the incorporated nanoantennas.

HL 10.3 Mon 11:15 S054

Far-field interferometry of weak plasmonics scatterers — •Christian Dicken[1], Daniela Wolf[1], Thorsten Schumacher[1], Klas Lindfors[2], Harald Giessen[3], and Markus Lippitz[1] — [1]Institute of Experimental Physics III, University of Bayreuth, Germany — [2]Department of Chemistry, Nanooptics Group, University of Cologne, Germany — [3]Institute of Experimental Physics IV, University of Stuttgart, Germany

Low-loss noble metals like gold and silver are at the heart of plasmonics. Yet, many applications focus on metals with higher losses and less pronounced optical response. We discuss how a simple mirror and a dielectric spacer layer turn a transmission experiment into an interferometer. This scheme is used by us in a simple model to optimize the sensitivity to small changes of the optical response of weak scatterers. In particular, we present interferometrically detected magnetic hysteresis loops of sub-100nm nickel disks and compare the data with our model.

HL 10.4 Mon 11:30 S054

Photoluminescence Enhancement by laterally ordered Ag/Alq_3:ZnPc/Ag Nanocavities — •Verena Kolb[1] and Jens Pflaum[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Center of Applied Energy Research (ZAE Bayern), 97074 Würzburg

Plasmonic nanostructures provide a perfect possibility to tailor the photoluminescence (PL) of organic semiconductors. In this contribution we present PL investigations on silver nanoprism arrays prepared by shadow nanosphere lithography and resonantly coupled to the luminescence of ZnPc (zinc phthalocyanine) molecules. Confocal PL measurements revealed a strong increase of the fluorescence of ZnPc thin films deposited on top of the nanoprisms. Co-evaporation into an Alq_3 (tris(8-hydroxyquinoline)aluminum) matrix at low concentrations of 4% leads to further increase, which can be explained by the reduction of non-radiative processes caused by exciton-exciton-annihilation and quenching at metal/organic interface. Lateral structuring of the organic layer and capping by silver result in periodically ordered Ag/Alq_3:ZnPc/Ag hybrid structures with PL enhancement factors up to 700 after geometrical correction. Complementary FDTD simulations confirm the pronounced spectral overlap between the localized surface plasmon resonance and the highest PL mode and thus, are able to prove the enhancement to be of plasmonic origin.

HL 10.5 Mon 11:45 S054

Optical rotation reversal and circular dichroism in resonantly and off-resonantly coupled plasmonic nanosystems — •Mario Hentschel[1,2], Vivan E. Ferry[3], A. Paul Alivisatos[1], and Harald Giessen[2] — [1]Materials Science Division, Lawrence Berkeley National Laboratory, Berkeley, CA, United States — [2]4th Physics Institute and Research Center SCoPE, University of Stuttgart, Germany — [3]Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, United States

In a system consisting of two resonant L-shaped particles we show that the sign of the circular dichroism spectrum in a plasmonic system can be controllably changed through small geometric perturbations that change the energetic ordering of the hybridized modes [1]. This mechanism is distinct from geometrical changes that explicitly change the handedness of the system. Secondly, we investigate the role of resonant coupling in chiral plasmonic systems, and whether the formation of collective plasmonic modes in a handed assembly of metallic nanostructures is a necessary condition for a chiroptical response. We show in experiment and simulation that off-resonant coupling between spectrally detuned nanostructures arranged with structural chirality leads to a clear yet weak chiroptical response [2]. We interpret our results in the framework of scattering between the individual constituents that in turn leads to a chiroptical farfield response. [1] M. Hentschel et al., ACS Photonics 2, 1253 (2015) [2] V. E. Ferry, M. Hentschel, and A. Paul Alivisatos, Nano Lett. 15, DOI 10.1021/acs.nanolett.5b03970

HL 10.6 Mon 12:00 S054

Enantiomorphic chiral near-fields in locally chiral plasmonic lattices — •Martin Schäferling, Xinghui Yin, Maxim Nesterov, Harald Giessen, and Thomas Weiss — 4th Physics Institute and Research Centers SCoPE and SimTech, University of Stuttgart, Germany

Chiral near-fields, which interact strongly with chiral molecules, can be obtained by illuminating geometrically chiral plasmonic nanostructures with circularly polarized light [1,2]. Fields with opposite handedness can be used to probe the chiroptical properties of chiral molecules with enhanced sensitivity. However, the field pairs generated by periodic arrangements of chiral nanostructures are, in general, not enantiomorphic. Additionally, such structures exhibit a chiroptical far-field response even in absence of chiral probe molecules. Both effects hamper the implementation of plasmonically enhanced chiroptical spectroscopy schemes.

In this contribution, we discuss periodic arrangements of simple achiral building blocks where the resulting superstructure is geometrically achiral, but still provides left- and right-handed geometrically chiral substructures. Due to their symmetry, such configurations provide enantiomorphic chiral near-fields, but no chiroptical far-field response. We show how to identify all such arrangements of plasmonic nanodiscs in a 4×4 unit cell that additionally provide C_4 symmetry and compare the simulated chiroptical near-field response of selected examples.

[1] Y. Tang and A. E. Cohen, Science **332**, 333 (2011).
[2] M. Schäferling et al., Phys. Rev. X **2**, 031010 (2012).

HL 10.7 Mon 12:15 S054

Circular Dichroism Spectroscopy on Individual Plasmonic Nanoparticles — •Julian Karst[1], Nikolai Strohfeldt[1], Mario Hentschel[1], Harald Giessen[1], and Na Liu[2] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart, Germany — [2]Max-Planck-Institute for Intelligent Systems, Stuttgart, Germany

Chirality is one of the most important basic principles of nature. We analyze the chiroptical response of single chiral plasmonic nanostructures. We utilize dark field circular dichroism spectroscopy to study the response of individual 3D chiral plasmonic Au-nanostructures. A customized spectroscopy setup for the visible spectral range is used. Transmission and scattering spectra are measured with a bright field and dark field spectroscopy setup, respectively. With large area ensembles of achiral and chiral plasmonic nanostructures we determine the influence of several optical components in the light path as well as the influence of fabrication defects. We show that individual chiral plasmonic oligomers in C_1 and C_4 configuration exhibit a mirror symmetry in the circular dichroism spectra for the right- and left-handed enantiomers. However, we see clear differences in the response of C_1-symmetric Au-nanostructures compared to the polarization conversion suppressing C_4-symmetric structures. The successful measurements of the chiroptical response of single chiral three dimensional plasmonic oligomers pave the way for studying more complex individual DNA based chiral plasmonic nanostructures.

HL 10.8 Mon 12:30 S054

Device design from stacked metasurfaces by use of a modified S-Matrix formalism — •Jan Sperrhake, Christoph Menzel, and Thomas Pertsch — Institut für angewandte Physik, Abbe Center of Photonics, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena

Artificial subwavelength structures called metamaterials (MM) are one of the most promising approaches in modern photonics for full control of light with respect to its polarization and spectral properties. By using MM made of complex shaped 3D elements almost arbitrary optical functionalities can be integrated into thin films. However, as the fabrication of 3D MM is usually difficult, complexity of the optical response might be achieved instead by choosing 2D metasurfaces (MS) and stacking them. In this contribution, we propose a method for efficiently treating and optimizing stacked complex homogeneous MS to create integrated, highly functional optical devices. A theoretical framework for fast numerical calculation is given by means of a modified scattering matrix formalism providing full information about phase, amplitude and polarization of the desired reflected and transmitted fields. As we will show with some examples this will pave the way towards simpler structures and easier fabrication, while maintaining and even increasing the range of accessible optical functionalities. A preprint of the paper is available at http://arxiv.org/abs/1511.09239.

HL 10.9 Mon 12:45 S054

Efficiency analysis of a finite-difference modal method for the derivation of electromagnetic fields — •Izzatjon Allayarov, Martin Schäferling, Maxim Nesterov, and Thomas Weiss — 4th Physics Institute and Research Center SCoPE, University of Stuttgart, Germany

Accurate numerical derivation of electromagnetic fields is important for many questions such as modeling the enhanced spontaneous emission due to the Purcell effect. Finite element methods (FEM) offer high accuracy, but are slow and tedious to implement. For periodic systems, the Fourier modal method (FMM) is a fast and reliable alternative. However, the underlying Fourier basis cannot resolve high contrasts of the dielectric constant accurately, which is especially problematic when fields close to such interfaces should be calculated.

We present an implementation of a finite difference basis for modal methods (FDMM) [1], which can exactly model arbitrary steps in the dielectric constant. We compare the accuracy and the calculation time to standard FMM as well as to FEM. Our results indicate that the ac-

curacy of the fields is higher for the FDMM compared to the FMM for comparable calculation times.

Additionally, we will discuss the possibility to combine this finite-difference basis with the coordinate transformation methods that have already been applied to the FMM [2]. This will allow for precise calculations of non-rectangular geometries using the FDMM.

[1] I. Semenikhin, and M. Zanuccoli, JOSA A **30**, 2531 (2013).
[2] T. Weiss et al., Opt. Express **17**, 8051 (2009).

HL 10.10 Mon 13:00 S054

Analytical model for hybrid magnetoplasmonics — •Dominik Floess[1], Thomas Weiss[1], Sergei Tikhodeev[2], and Harald Giessen[1] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart, Germany — [2]A. M. Prokhorov General Physical Institute, Russian Academy of Sciences, Moscow

In recent years, the hybrid plasmonic construction kit was expanded by magneto-optical materials, which offer magnetic tuning and non-reciprocal effects. By utilizing localized surface plasmons, the magneto-optical response of dielectric thin films can be resonantly amplified and spectrally tailored. While the experimental realization of such systems received considerable attention, so far there is no profound theoretical description that goes beyond numerical simulations. Here we present an intrisically non-reciprocal coupled oscillators model that reveals the underlying physics inside such systems and yields analytical expressions for the resonantly enhanced magneto-optical response. The predictions of the model are in good agreement with full numerical simulations of typical sample geometries as well as experiments. This includes modal dispersion, optical rotation and ellipticity.

HL 11: Focus Session: Single Particle Sources for Electronic Devices I (Joint session of HL and TT, organized by HL)

Organizers: Rolf Haug (Universität Hannover) and Janine Splettstößer (Chalmers University)

Time: Monday 11:30–13:00 Location: H10

Invited Talk HL 11.1 Mon 11:30 H10

A clean single electron source using voltage pulses generating levitons. — •Christian Glattli — Nanoelectronics Group, Service de Physique de l'État Condensé CEA-Saclay, 91191 Gif-sur-Yvette, France

A simple approach to realize an on-demand electron soource is to apply a voltage pulse on a contact of the conductor such that the resulting current pulse injects a single charge in the conductor. At first sight, the idea seems too naive to produce something useful. However it appears that this procedure perfectly works [1]. More surprisingly it contains a rich physics: the generation of a new kind of excitation carrying a single particle: a leviton. The method was theoretically considered 20 years ago by L. Levitov and collaborators [2] who found that a voltage pulse with Lorentzian shape produces a minimal excitation, i.e. such that the number of excitations generated is not larger than the number of injected charges.

In this talk, I will present the recent experimental generation of levitons. I will also show electron quantum optics applications, reporting a two-leviton quantum interference experiment, the electrical analog of the Hong Ou Mandel experiment with photons which reveal perfect electron coherence. Finally using electron quantum tomography [3] an almost complete picture of the Leviton wave-function can be experimentally given.

[1] J. Dubois et al, Nature 502, 659-663 (2013).
[2] Levitov et al., J. Math. Phys. 37, 4845*4856 (1996).
[3] T. Jullien et al., Nature 514, 603*607 (2014)

HL 11.2 Mon 12:00 H10

Feedback Control of Waiting Times — •Tobias Brandes — TU Berlin, Institut für Theoretische Physik

Feedback control is known as a versatile tool for controlling quantum transport. So far most approaches deal with a control of stationary quantities (such as charge and heat currents). In this talk I will address the direct control of a temporal correlation function, the waiting time distribution, under feedback conditions. Within a simple transport model, I try to analyse possible connections to the thermodynamics of information and (with C. Emary) to optimal control theory.

HL 11.3 Mon 12:15 H10

Squeezing of shot noise using feedback controlled single-electron tunneling — •Timo Wagner[1], Johannes C. Bayer[1], Eddy P. Rugeramigabo[1], Philipp Strasberg[2], Tobias Brandes[2], and Rolf J. Haug[1] — [1]Institut für Festkörperphysik, Leibniz Universität, D-30167 Hannover, Germany — [2]Institut für Theoretische Physik, TU Berlin, D-10623 Berlin, Germany

Quantum feedback control has been studied intensively in quantum optics for a variety of different mechanism and systems [1]. Here we demonstrate the squeezing of shot noise in a quantum dot (QD) using an exclusively electronic feedback loop. Therefore the single-electron counting statistics [2, 3] is monitored in real-time with a coupled quantum point contact (QPC) and the deviation from a target rate is fed back periodically to speed up or slow down the process. With increasing feedback response we observe a stronger squeezing and faster freezing of the charge current fluctuations. The measurements confirm previous theoretical predictions [4] and show that the feedback loop is very robust even under stronger experimental restrictions. Our technique is analog to the generation of squeezed light with in-loop photodetection in quantum optics [1, 5].

[1] H. M. Wiseman, *Quantum Measurment and Control*, Cambridge University Press, Cambridge (2009)
[2] S. Gustavson, et al., Surf. Sci. Rep. 64, 191 (2009)
[3] N. Ubbelohde, et al., Nature. Com. 3, 612 (2012)
[4] T. Brandes, Phys. Rev. Lett. 105, 06060 (2010)
[5] S. Machida, Y. Yamamoto, Opt. Commun. 57, 290 (1986)

Invited Talk HL 11.4 Mon 12:30 H10

(De)coherence of single electron wavepackets in quantum Hall edge channels — •Erwann Bocquillon[1,2], Arthur Marguerite[2], Vincent Freulon[2], Jean-Marc Berroir[2], Bernard Plaçais[2], Antonella Cavanna[3], Yong Jin[3], and Gwendal Fève[2] — [1]Physikalisches Institut (EP3), Universität Würzburg, Würzburg, Germany — [2]Laboratoire Pierre Aigrain, Ecole Normale Supérieure, Paris, France — [3]Laboratoire de Photonique et Nanostructures, Marcoussis, France

The ballistic propagation of electronic waves along the quantum Hall edge channels of a two dimensional electron gas bears strong analogies with photon optics. Ballistic and one-dimensional propagation are provided by the chiral quantum Hall edge states and electronic beam splitters can be implemented using quantum point contacts. These analogies have inspired a whole set of experiments and provide an efficient tool to understand electronic propagation in quantum conductors.

In this talk, I will present how one can implement electron quantum optics experiments down to a single charge resolution using an on-demand single electron emitter. In particular, we generate two indistinguishable quasiparticles that we characterize via their interference on a beamsplitter in an electronic analogue of the Hong-Ou-Mandel experiment. The visibility of two-particle interferences reveals decoherence effects due to interactions with the environment, and especially with other co-propagating edge channels. These implementations of electron quantum optics experiments pave the way to more complex ones, such as the tomography of a single electron.

HL 12: Photovoltaics (Joint session of HL and DF, organized by HL)

Time: Monday 14:45–18:30 Location: H2

Invited Talk HL 12.1 Mon 14:45 H2

Surface chemistry of colloidal semiconductor nanocrystals — •Zeger Hens — Physics and Chemistry of Nanostructures, Ghent University, Krijgslaan 281-S3, B9000 Gent, Belgium

Colloidal semiconductor nanocrystals or quantum dots are hybrid nano-objects composed of an inorganic, crystalline core capped by organic surface ligands. This talk addresses recent advances in the understanding of this ligand shell. First, solution NMR will be introduced as a unique, in-situ analysis technique for identifying and quantifying these ligands and for analysing ligand exchange reactions. This has recently led to the classification of nanocrystal/ligand nanocrystals based on the ligand binding motif, where use is made of the covalent bond classification scheme that was originally introduced for the classification of metal complexes. It is shown how this classification enables ligand exchange reaction to be rationalized and predicted and how this now provides researchers with an extensive toolbox to tweak nanocrystal properties at will by changing their surface chemistry. In the last part of the talk, the extension of the approach to metal oxide nanocrystals is addressed. It is shown that these feature a markedly different surface chemistry, which enables for example their use as colloidal nanocatalysts.

HL 12.2 Mon 15:15 H2

Combined Black Silicon Textures for Advanced Antireflective Surfaces — •Maria Gaudig[1,2], Jens Hirsch[1,3], Alexander N. Sprafke[2], Dominik Lausch[3], Norbert Bernhard[1,3], and Ralf B. Wehrspohn[2,4] — [1]Anhalt University of Applied Sciences, Technologies of Photovoltaics Group, Bernburger Str. 55, D-06366 Köthen — [2]Martin Luther University Halle-Wittenberg, Institute of Physics, Group microMD, Heinrich-Damerow-Str. 4, D-06120 Halle (Saale) — [3]Fraunhofer Center for Silicon Photovoltaics CSP, Otto-Eißfeldt-Straße 12, D-06120 Halle (Saale) — [4]Institute for Mechanics of Materials IWM, Walter-Hülse-Str. 1, D-06120 Halle (Saale)

Black silicon (b-Si) promises with its extremely low reflectivity to become a real alternative to wet chemical textured silicon in the PV industry. In this work, the nano texturing is realized with a maskless SF6/O2 plasma etch process. Compared to the wet chemical texturing, this method provides benefits like reduced silicon waste, independence of prior surface treatment and crystal orientation and the variation of the texture forms by different plasma processes by different plasma processes. We showed two different plasma textures with absorption about 95 %: (I) a needle like texture (needle height/width ~ 500/100-200 nm) with a strong antireflection and (II) parabolic pits (height/width ~ 2/1 micron) with improved light trapping. In this contribution, we want to go one step further and combine these two techniques to exploit the optical benefits of both textures. For this purpose, the two etch processes are applied successively on the wafer. The experimental data will be discussed and advantages will be highlighted.

HL 12.3 Mon 15:30 H2

Improved light harvesting and carrier collection using transparent nano-textured back contacts in sub-micron chalcopyrite absorber solar cells — •Wiebke Ohm[1,2], Wiebke Riedel[1,2], Ümit Aksünger[2], Martha Ch. Lux-Steiner[1,2], and Sophie Gledhill[1,2] — [1]Fachbereich Physik, Freie Universität Berlin, Berlin, Germany — [2]Institut für Heterogene Materialsysteme, Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

We investigate bifacial $Cu(In,Ga)Se_2$ (CIGS) solar cells on glass/F:SnO_2 substrates with ZnO nanorods (NR) at the back contact and a reduced absorber thickness ($<1\,\mu m$). Optical simulations of reflection and depth resolved absorption were used to show the potential of ZnO NR in bifacial sub-micron CIGS solar cells to increase the short-circuit current J_{SC}. Next to anti-reflection properties a shift of the absorption closer to the pn-junction was identified for back side illumination enhancing charge carrier collection resulting in an overall J_{SC} increase by up to 30 %. The anti-reflection effect of ZnO NR at the solar cell back contact was observed using optical measurements and the anti-reflection enhancement was estimated resulting in a maximum photo current increase of 2 %. An overall 5 % increase in J_{SC} with NR was achieved, identified in I-V measurements for back side illumination. The external quantum efficiency, however, show that parasitic absorption in the NR-based back contact limits the photo current enhancement, whereas in a wide wavelength range 20 % J_{SC} increase is demonstrated.

HL 12.4 Mon 15:45 H2

Hybrid charge transfer excitons at ZnMgO/P3HT interfaces — •Moritz Eyer, Sergey Sadofev, Joachim Puls, and Sylke Blumstengel — Institut für Physik, Humboldt-Universität zu Berlin

The performance of hybrid photovoltaic devices is strongly related to the efficiency of the charge separation process. In photovoltaic operation excitons generated in the organic and inorganic part diffuse to the interface of the heterojunction. It is suggested that prior to full charge separation a hybrid charge transfer exciton (HCTE) is formed i.e. a coulombically bound charge pair residing on both sides of the interface. Only after dissociation of such a pair a photocurrent is generated.

The formation of HCTE is experimentally verified in planar ZnMgO/poly(3-hexylthiophene) (P3HT) heterojunction devices via electroluminescence (EL) measurements [1]. Radiative recombination across the interface produces EL in the near infrared spectral region. The energy offset ΔE_{IO} between the conduction band minimum of ZnMgO and the P3HT highest unoccupied molecular orbital is tuned systematically by varying the Mg content. Combined analysis of radiative properties and the open circuit voltage V_{OC} in photovoltaic operation shows a clear correlation to the HCTE transition energy.

Investigation of the properties of HCTE yields valuable input for the optimization of the charge separation process at inorganic/organic semiconductor interfaces in order to fully exploit the potential of hybrid devices.

[1] M. Eyer et al., Appl. Phys. Lett. **107**, 221602 (2015).

HL 12.5 Mon 16:00 H2

VUV Pump-Probe Magneto-optical Ellipsometry at ELI Beamlines — •Shirly J. Espinoza-Herrera[1], Bastian Besner[2], Jakob Andreasson[1], and Michael A. Ruebhausen[2] — [1]ELI Beamlines Project, Institute of Physics of the ASCR, 252 41 Dolní Břežany, Czech Republic — [2]Institut fuer Nanostruktur- und Festkoerperforschung, Center for Free-Electron Laser Science, Advanced Study Group APOG, University of Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany

A new ellipsometer that is capable of measuring in one run the dielectric function of solid states samples from the IR and the VUV spectral range is being set up at ELI beamlines. ELI is a pillar of the transnational European Extreme Light Infrastructure (ELI) that will hold some of the most intense lasers in the world. The Center for Free Electron Laser in Hamburg is joining this European effort and the work presented here is the development of the pump-probe VUV ellipsometer that will allow the study of materials out of the Fermi level, testing the established tradition of condensed matter physics where most of the phenomena observed are driven the physics close to the Fermi level. Results showing the coupling between the low and high energy levels of freedoms on the case of STO and LAO will be presented.

HL 12.6 Mon 16:15 H2

Synchrotron-based spectroscopy study of the conduction band development in Cu2ZnSn(S,Se)4 with different [S]/([S]+[Se]) ratios — •Tetiana Olar[1], Iver Lauermann[1], Archana Manoharan[2], Lorenzo Pardini[2], Karsten Hannewald[2,3], Claudia Draxl[2,3], Haibing Xie[4], Edgardo Saucedo[4], Binoy Chacko[1], and Martha Lux-Steiner[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH,Albert-Einstein-Str. 15, 12489 Berlin,Germany — [2]Humboldt-Universität zu Berlin, Zum Großen Windkanal 6, 12489 Berlin, Germany — [3]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany — [4]Catalonia Institute for Energy Research- IREC, Jadinsde les Dones de Negre 1, 08930 Sant Adrià de Besòs (Barcelona), Spain

Cu2ZnSn(S,Se)4 absorber layers with different [S]/([S]+[Se]) ratios were studied using XPS, UPS, HIKE and NEXAFS. To investigate the band gap transition from the pure sulfide to the pure selenide compound, the valence band maximum (VBM) and conduction band minimum (CBM) were probed. In UPS and HIKE measurements, the relative distance between Fermi level and VBM for the pure sulfide sample was 130 meV larger than for the pure selenide. Using NEX-

AFS to probe the CBM, a systematic study of the positions of K- and L-absorption edges was done and the observed shifts are proportional to the relative shifts in the CBM. The experimental findings are further validated and analyzed by performing corresponding ab initio calculations using the full-potential all-electron code exciting.

30 min. Coffee Break

HL 12.7 Mon 17:00 H2

Role of Polar Phonons in the Photo Excited State of Metal Halide Perovskites — Menno Bokdam[1], Tobias Sander[1], Alessandro Stroppa[2], Silvia Picozzi[2], •D.D. Sarma[3], Cesare Franchini[1], and Georg Kresse[1] — [1]Faculty of Physics, Computational Materials Physics, University of Vienna, Austria — [2]Consiglio Nazionale delle Ricerche - CNR-SPIN, L'Aquila, Italy — [3]Indian Institute of Science, Bangalore, India

The development of high efficiency perovskite solar cells has sparked a multitude of measurements on the optical properties of these materials. For the most studied methylammonium(MA)PbI_3 perovskite, a large range (6-55 meV) of exciton binding energies has been reported by various experiments. The existence of excitons at room temperature is unclear. For the MAPbX_3 perovskites we report on relativistic GW-BSE calculations. This method is capable to directly calculate excitonic properties from first-principles. At low temperatures it predicts exciton binding energies in agreement with the reported 'large' values. For $MAPbI_3$, phonon modes present in this frequency range have a negligible contribution to the ionic screening. By calculating the polarisation in time from finite temperature Molecular Dynamics, we show that at room temperature this does not change. We therefore exclude ionic screening as an explanation for the experimentally observed reduction of the exciton binding energy at room temperature.

HL 12.8 Mon 17:15 H2

Stable single-phase Zn-rich $Cu_2ZnSnSe_4$ through In doping — Stefan Hartnauer[1], •Sabine Körbel[2,3], Miguel A L Marques[1,3], Silvana Botti[2,3], and Roland Scheer[1] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany — [2]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — [3]Institut Lumière Matière, UMR5306 Université Lyon 1-CNRS, F-69622 Villeurbanne Cedex, France

Alloying in the system $Cu_2ZnSnSe_4$–$CuInSe_2$–ZnSe (CZTISe) is investigated experimentally and with *ab initio* calculations. The goal is to distinguish stable (single-phase) and unstable (multi-phase) regions within the pseudo-ternary phase diagram. Thin CZTISe films are prepared by co-evaporation of the chemical elements and are investigated in real-time during growth using in-situ angle dispersive X-ray diffraction (XRD). *Ab initio* calculations with density-functional theory are performed to determine the thermodynamic stability of the alloy with respect to the formation of secondary phases. Both in experiment and calculation, we find a surprisingly large single-phase region in the phase diagram for Zn-rich $Cu_2ZnSnSe_4$ if a small amount of In is present, from which we conclude that In doping may help avoiding secondary phase formation under Zn- rich conditions and open up new possibilities for the application of CZTISe thin films in solar cells.

HL 12.9 Mon 17:30 H2

Optical characterization of Cu(In,Ga)Se2 with highly spatially, spectrally, and time resolved cathodoluminescence — •Martin Müller[1], Mathias Müller[1], Frank Bertram[1], Jürgen Christen[1], Torsten Hölscher[2], Setareh Zahedi-Azad[2], Matthias Maiberg[2], and Roland Scheer[2] — [1]Institute of Experimental Physics, Otto-von-Guericke-University, Germany — [2]Martin-Luther-University Halle-Wittenberg, Germany

Potential fluctuations and transport parameters are important factors to further improve efficiencies of Cu(In,Ga)Se2 (CIGSe)solar cells. Optical properties of CIGSe absorbers have been studied by means of highly spatially and spectrally resolved cathodoluminescence (CL) to investigate lateral fluctuations and transport parameters. The measurements were performed from low temperature (T = 4.5 K) up to room temperature. CL spectra recorded at 4.5 K, exhibit a dominant emission at 1.06 eV (1170 nm). A shoulder at 1.14 eV (1090 nm) on the low energy side and at 0.99 eV (1250 nm) on the high energy side were observable. In excitation density dependent CL measurements, a blue shift of 25 meV/decade is observed. Additionally, ps-time resolved CL was performed. A dependence of the initial lifetime of more than one order of magnitude from the emission energy could be observed, illustrating relaxation of charge carriers in potential fluctuations. Investigation of panchromatic temperature dependent initial lifetimes reveals a pronounced increase up to 50 K and a subsequent decrease caused by non-radiative recombination. A concept for optical investigations of transport parameters and first results will be presented.

HL 12.10 Mon 17:45 H2

Investigation of shallow defects in $Cu(In,Ga)Se_2$ with time-resolved photoluminescence — •Torsten Hölscher, Matthias Maiberg, Setareh Zahedi-Azad, and Roland Scheer — Martin-Luther-Universität Halle-Wittenberg, 06120 Halle(Saale), Germany

Time-resolved photoluminescence (TRPL) is a powerful method to observe the recombination kinetics of minority carriers in solar cell materials like $Cu(In,Ga)Se_2$ (CIGSe). The influence of a shallow defect (traps) close to the conduction band leads to bi-exponential and curved TRPL-transients due to trapping of minority carriers. TRPL-measurements under increased device temperatures revealed a strong reduction of the second longer decay time, which is may be attributed to the temperature enhanced restitution of the trapped carriers to the conduction band. Saturation of shallow and deep defects became observable by varying the excitation of excess carriers. With Synopsys TCAD® we simulated the recombination behavior of minority carriers in CIGSe as a function of temperature and excitation in the presence of shallow defects. In comparison with the experiments, we obtained in the simulations $E_C - E_t \approx 200$ meV for the energy level, $\sigma_n \approx 10^{-13}$ cm^2 for the electron capture cross-section and $N_t \approx 10^{16}$ cm^{-3} for the density as significant parameters of the trap-state. These trap parameters closely match the N1 admittance signature detected previously - a signature which explanation has been heavily disputed. Our findings now support the explanation of the N1 defect as due to a minority carrier trap. We will discuss the influence of this trap on the solar cell performance.

HL 12.11 Mon 18:00 H2

Plasma-enhanced atomic-layer-deposited MoO_x emitters for silicon heterojunction solar cells — •Johannes Ziegler[1], Thomas Schneider[1], Alexander N. Sprafke[1], Kai Kaufmann[3,4], and Ralf B. Wehrspohn[1,2] — [1]Martin-Luther-University Halle-Wittenberg, *μMD Group*, Institute of Physics, Heinrich-Damerow-Strasse 4, 06120 Halle, Germany — [2]Fraunhofer Institute for Mechanics of Materials IWM Halle, Walter-Hülse-Str. 1, 06120 Halle, Germany — [3]Fraunhofer Center for Silicon Photovoltaics CSP, Otto-Eißfeld-Strasse 12, 06120 Halle, Germany — [4]Hochschule Anhalt Köthen, University of Applied Sciences, Bernburger Str. 55, 06966 Köthen

A method for the deposition of molybdenum oxide (MoO_x) with high growth rates at temperatures below 200 °C based on plasma-enhanced atomic layer deposition (PE-ALD) is presented. The stoichiometry of the of the over-stoichiometric MoO_x films can be adjusted by the plasma-parameters. First results of these layers acting as hole-selective contacts in silicon heterojunction (SHJ) solar cells are presented and discussed.

HL 12.12 Mon 18:15 H2

In-Situ XRD Analysis of the structural Evolution of CZTS Nanoparticles during an Annealing Process — •Marco Brandl[1], Mohamed Sayed[2], Levent Gütay[2], and Rainer Hock[1] — [1]Chair for Crystallography and Structural Physics, Friedrich-Alexander-University of Erlangen-Nürnberg, Staudtstr. 3, 91058 Erlangen, Germany — [2]Laboratory for Chalcogenide Photovoltaics (LCP), Energy and Semiconductor Research Laboratory (EHF), Department of Physics, University of Oldenburg, Carl-von-Ossietzky-Str. 9-11, 26111 Oldenburg, Germany

A potential method for Kesterite (Cu2ZnSnS4, CZTS) based solar cell production is the synthesis of CZTS nanoparticles by a low temperature wet chemical process. Powders of nanoparticles produced by this process are analysed by X-ray powder diffraction. Initially, these particles have a cubic disordered structure with potential hexagonal stacking faults. With the method of in-situ XRD during an annealing process up to 550°C the recrystallisation to a tetragonal structure of the CZTS as well as the healing of the hexagonal defects can be observed. Furthermore, by mixing the CZTS particles with Selenium powder, the incorporation of Se into CTZS can be studied. The time and temperature resolved observation of the change in unit cell parameters can directly be connected to the Se content in the resulting CZTSSe phase via Vegard's law.

HL 13: Focus Session: Single Particle Sources for Electronic Devices II (Joint session of HL and TT, organized by HL)

Organizers: Rolf Haug (Universität Hannover) and Janine Splettstößer (Chalmers University)

Time: Monday 14:45–18:45 Location: H10

Invited Talk HL 13.1 Mon 14:45 H10

Energy- and time-resolved detection of hot single-electron wave packets — •Masaya Kataoka — National Physical Laboratory, Hampton Road, Teddington, Middlesex TW11 0LW, UK

On-demand semiconductor single-electron sources such as mesoscopic capacitors [1] have enabled an electronic analogy of quantum optics experiments. In further development of this field, the presence of a Fermi sea can present a challenge, causing decoherence due to electron-electron interactions [2]. One solution would be to set electron paths in an intrinsic region, where the conduction-band electrons are absent.

We demonstrate long-range electron transport along depleted edges of a two-dimensional system. A stream of hot electrons are emitted from a quantum-dot pump at ˜100 meV above the Fermi energy. Due to a strong magnetic field applied, these electrons travel along the edge defined by shallow etching of the surface, while the background Fermi sea along the edge is depleted by a surface gate that covers the edge.

The transport of the hot-electron wave packets is investigated with energy- and time-resolved detectors [3]. We discuss the measurements of arrival-time distribution measurements with time resolution of < 5 ps, the measurements of edge-state velocity [4], a method to extend LO-phonon scattering length to > 0.5 mm, and how the timing of two-electron emission can be tuned by the shape of pump drive signal.

[1] G. Fève et al., Science 316, 1169 (2007).
[2] V. Freulon et al., Nat. Commun. 6, 6854 (2015).
[3] J. D. Fletcher et al., Phys. Rev. Lett. 111, 216807 (2013).
[4] M. Kataoka et al., arXiv:1512.02906v1.

HL 13.2 Mon 15:15 H10

Dopant controlled single electron pumping through a metallic quantum dot in silicon — •Tobias Wenz[1], Frank Hohls[1], Xavier Jehl[2], Sylvain Barraud[3], Girts Barinovs[4], Jevgeny Klochan[4], and Vyacheslavs Kashcheyevs[4] — [1]Physikalisch-Technische Bundesanstalt (PTB), 38116 Braunschweig, Germany — [2]University Grenoble Alpes and CEA-INAC, F-38000 Grenoble, France — [3]University Grenoble Alpes and CEA-Leti-Minatec, F-38000 Grenoble, France — [4]Faculty of Physics and Mathematics, University of Latvia, LV 1002 Riga, Latvia

Single electron pumps produce a quantized current by transferring an integer number of electrons n each cycle with a high frequency f, so that the current is $I = nef$ [1], where e is the electron charge, enabling a redefinition of the ampere by fixing the value of e. Commonly, single electron pumps utilize gate-defined quantum dots to create a quantized current. In this work, we investigate a silicon nanowire produced from an industrial CMOS process and take advantage of single phosphorus dopants located in both barriers of a gate-defined quantum dot. Due to their strongly localized potential wells, single dopants have large charging energies and sharp resonances that strongly influence the coupling of the main quantum dot to source and drain. By modulating the gates with suitable RF signals to switch the coupling on and off a quantized current can be generated. The operation principle can be modeled using simple assumptions and allows the study of dynamic effects in a coupled single dopant/metallic quantum dot system.

[1] Kaestner and Kashcheyevs, Rep. Prog. Phys. **78**, 103901 (2015)

Invited Talk HL 13.3 Mon 15:30 H10

The reabsorption effect with single-electron sources — •Géraldine Haack[1] and Michael Moskalets[2] — [1]University of Geneva, Switzerland — [2]University of Kharkiv, Ukraine

In the past years, ground-breaking experiments have been realised in quantum transport in generating single-electronic states [1]. Their controlled emission enables the investigation of fundamental quantum mechanical properties such as the coherence of these single-electron states [2], useful for quantum information purposes, and the realization of fermionic analogues of quantum optics experiments such as the Hanbury-Brown and Twiss and Hong-Ou-Mandel experiments [3].

In this talk, we show that the heat current enables us to gain crucial information about the shape of the single-particle states compared to the charge current. To this end, we investigate the reabsorption effect with two single-electron sources coupled in series [4]. While the charge current nullifies, we show that the energy carried by electron-hole pairs is enhanced by a factor 2. This can be explained by the time symmetry of the single-electron state. We finally discuss the validity of the Joule-Lenz law and the fluctuation-dissipation relation, when cavities emit electron-hole pairs and particles of the same kind.

[1] G. Fève et al., Science 316, 1169 (2007); N. Maire et al. , Appl. Phys. Lett. 92, 082112 (2008); J. Dubois et al., Nature 502, 659 (2013). [2] G. Haack, Phys. Rev. B 84, 081303 (2011); G. Haack et al., Phys. Rev. B 87, 201302 (2013). [3] E. Bocquillon et al., Phys. Rev. Lett. 108, 196803 (2012); E. Bocquillon et al., Science 339, 1054 (2013). [4] M. Moskalets et al., Phys. Rev. B 87, 125429 (2013).

HL 13.4 Mon 16:00 H10

Maxwell's demon in the quantum regime — •Gernot Schaller — TU Berlin, Institut für Theoretische Physik

Feedback control can be a useful tool to change the Full Counting Statistics of charges being transferred through a microscopic device. It can be used to suppress fluctuations of the current or to revert its direction e.g., against a potential gradient. The latter case is particularly interesting from a thermodynamic perspective. For an implicit modeling of the controller, this leads to an apparent violation of the second law that may be interpreted as a modification due to a Maxwell-type demon. In contrast, when the control becomes autonomous, i.e., when the controller is included in the thermodynamic description, these apparent paradoxes can be nicely resolved. I will illustrate this viewpoint for electronic transport through quantum dots. Interestingly, these concepts from stochastic thermodynamics can be generalized to true quantum systems, where the evolution of degenerate populations and coherences in the system energy eigenbasis is coupled.

30 min. Coffee break

Invited Talk HL 13.5 Mon 16:45 H10

Electronic states in a driven quantum contact — •Mihajlo Vanevic[1], Julien Gabelli[2], Wolfgang Belzig[3], and Bertrand Reulet[4] — [1]Department of Physics, University of Belgrade, Serbia — [2]Laboratoire de Physique des Solides, Univ. Paris-Sud, France — [3]Fachbereich Physik, Universität Konstanz, Germany — [4]Département de physique, Université de Sherbrooke, Canada

Minimal excitations in a voltage-driven quantum conductor are electrons excited above the Fermi level. Generation of these minimal excitation states requires carefully tailored Lorentzian voltage pulses carrying an integer number of charge quanta. However, a general time-dependent voltage excites both electrons and electron-hole pairs whose number and probability of creation depend on the shape and the amplitude of the drive. We have studied the many-body electronic state created by a general voltage drive and expressed it manifestly in terms of single-electron and electron-hole quasiparticle excitations. We have confirmed our theoretical predictions by probing the constituent quasiparticle states in a Hong-Ou-Mandel-type experiment on a tunnel junction. The knowledge of the many-body state opens a way of engineering the required time profile or energy distribution of single-electron and electron-hole excitations. Harmonic drive with ac amplitude smaller than dc voltage offset can be used to create single-electron states with a small admixture of electron-hole pairs.

HL 13.6 Mon 17:15 H10

Lissajous Rocking Ratchet: Realization in a Semiconductor Quantum Dot — •Sergey Platonov[1,2], Bernd Kästner[3], Hans W. Schumacher[3], Sigmund Kohler[4], and Stefan Ludwig[1,2] — [1]Center for NanoScience & Fakultät für Physik, LMU-Munich, 80539 München, Germany — [2]Paul-Drude-Institut für Festkörperphysik, Hausvogteiplatz 5-7 10117 Berlin, Germany — [3]Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany — [4]Instituto de Ciencia de Materiales de Madrid, CSIC, 28049 Madrid, Spain

Symmetries are a very important concept of physics - the most famous one being the CPT symmetry. Breaking symmetries often gives

rise to interesting effects and, in particular, breaking the time-reversal symmetry is a requirement for many applications such as information processing. Here we present such a concept based on a quantum dot (QD) electrostatically defined in a AlGaAs/GaAs heterostructure. We break time-reversal symmetry by periodically modulating its barriers such that a single electron tunneling current occurs. The current direction can be controlled by introducing a phase difference between the two periodic signals. We show that our QD resembles a Lissajous rocking ratchet. A consistent theoretical model based on scattering matrix formalism describes our experimental findings. Similar devices could be realized in a large variety of systems, for instance in nanomechanical or superconducting circuits. Possible applications include noise management, filtering and signal routing.

HL 13.7 Mon 17:30 H10

A charge-driven feedback loop in the resonance fluorescence of a single quantum dot — •Benjamin Merkel[1], Annika Kurzmann[1], Jan-Hindrik Schulze[2], André Strittmatter[2], Martin Geller[1], and Axel Lorke[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany — [2]Technische Universität Berlin, Institut für Festkörperphysik, Hardenbergstrasse 36, 10623 Berlin, Germany

Generating photons with transform-limited linewidths from semiconductor quantum dots (QDs) is challenging. Charge and spin noise from the environment cause spectral fluctuations of the resonance, limiting the generation of highly coherent photons.

In our micro-patterned samples we observe an electro-optical feedback mechanism by which the QD resonance frequency follows the excitation, leading to an optical bistability of the fluorescence signal. This feedback loop can be used to stabilize the resonance and reduce the noise of the emitted photons. We investigate the effect on InGaAs/GaAs QDs by time-resolved measurements of the fluorescence under two-colour excitation and also in a magnetic field. Experiments show a purely electrical origin of the feedback which lies in the formation of a hole gas at a valence band discontinuity close to the dot. The accumulated positive charge leads to a Stark shift of the dot's resonance frequencies. The hole gas is fed by carriers that are generated by resonant excitation of excitons in the dot and that tunnel into the hole gas states at the AlGaAs/GaAs interface. We are able to quantitatively reproduce the feedback dynamics by a numerical rate-equation model.

HL 13.8 Mon 17:45 H10

Exact duality for open system time-evolution and surprises in the heat current relaxation of an interacting quantum dot — •Roman Saptsov[1,2], Jens Schulenborg[3], Federica Haupt[4], Janine Splettstoesser[3], and Maarten Wegewijs[1,2,5] — [1]Institute for Theory of Statistical Physics, RWTH Aachen University, Aachen, Germany — [2]JARA - FIT — [3]Chalmers University of Thechnology, Götenborg, Sweden — [4]JARA Institute for Quantum Information, RWTH Aachen, Aachen, Germany — [5]Peter Grünberg Institut, FZ-Jülich, Jülich, Germany

Recent progress in nanoelectronics has brought the experimental detection and manipulation of few-electron heat currents in nanodevices within reach. However, a straightforward theoretical calculation of the heat-current relaxation – already for the simplest model of an Anderson quantum dot – exhibits a surprising behavior. More precisely, the contribution to the heat-current relaxation arising from the decay of the repulsive Coulomb interaction energy exhibits signatures of electron-electron attraction, and is governed by an interaction-independent decay rate [1]. The surprising behavior of the interaction-induced dissipation mode can only be understood with the help of a new duality relating the nonunitary evolution of an open quantum system to that of dual model with inverted energies [1]. Deriving from the fermion-parity superselection postulate, this duality applies to a large class of open systems, allowing for new general insights beyond the quantum-dot heat-current problem presented here.

[1] J.Schulenborg, R. B. Saptsov, F. Haupt, J. Splettstoesser, M.R. Wegewijs, arXiv: 1508.06145

HL 13.9 Mon 18:00 H10

Energy harvester with coupled quantum dots — •Holger Thierschmann[1,2], Rafael Sánchez[3], Börn Sothmann[4], Fabian Arnold[1], Christian Heyn[5], Wolfgang Hansen[5], Hartmut Buhmann[1], and Laurens W. Molenkamp[1] — [1]Experimentelle Physik 3, Universität Würzburg, Germany — [2]Kavli Institute of Nanoscience, Faculty of Applied Sciences, Delft University of Technology, The Netherlands — [3]Instituto de Cienca de Materiales de Madrid, CISC, Spain — [4]Département de Physique Theoretique, Univeristé de Genève, Switzerland — [5]Institute of Applied Physics, University of Hamburg, Germany

Multi-terminal thermoelectrics recieve an increasing attention because they allow for ways to separate heat and charge flow, thus pointing out a new route towards highly efficient thermoelectric devices. Here we present experiments on a three-terminal energy harvester with Coulomb coupled quantum dots (QD) following a recent proposal [1]. Energy is extracted from a hot electron reservoir via occupation fluctuations of a connected QD and is converted into a directed charge current in a conductor circuit which consists of another QD and two reservoirs at a lower temperature. Heat flow is mediated only through Coulomb interaction of the dots. The key ingredient of our device is an asymmetry in tunnel-coupling of the cold reservoirs and the QD which leads to rectification of charge fluctuations. Controlling this asymmetry with gate electrodes enables us to manipulate the direction of the resulting current even without changing the direction of heat flow. [1] R.Sánchez and M. Büttiker Phys. Rev. B 83 085428 (2011)

Invited Talk HL 13.10 Mon 18:15 H10

Clocked single-electron transfer: quantized currents and electron pair partitioning — •Frank Hohls — Physikalisch-Technische Bundesanstalt (PTB), Braunschweig, Germany

The clocked transfer of single electrons or electron pairs has applications both in metrology as quantized current source and in basic physics as building block for electron quantum optics. In the future redefinition of the International System of Units (SI), expected for 2018, the unit of the electrical current will be derived from a clock frequency f and the elementary charge e, $I = nef$. A promising realization is the non-adiabatic tunable-barrier pump which allows to transfer a highly quantized number of electrons n even at GHz driving frequency [1]. We will present latest results on accuracy verification of the resulting current quantization. For a pump driven at 545 MHz we find an agreement with $I = ef$ within the measurement uncertainty of 0.2 ppm [2]. Interestingly, the same type of electron pump also allows the controlled emission of electrons and electron pairs into a one-dimensional ballistic conductor formed at the edge of a quantum Hall system, opening the route to electron quantum optics experiments. We have examined the partitioning of such electrons at an electronic beam splitter using correlation measurements which validate high fidelity pair splitting and additionally reveal interesting correlation effects for the partitioning of electron pairs [3].

[1] B. Kaestner & V. Kashcheyevs, Rep. Prog. Phys. **78**, 103901 (2015).
[2] F. Stein *et al.*, Appl. Phys. Lett. **107**, 103501 (2015).
[3] N. Ubbelohde *et al.*, Nature Nanotechnol. **10**, 46 (2015).

HL 14: Spintronics: Transport and Theory

Time: Monday 14:45–17:45 Location: H13

HL 14.1 Mon 14:45 H13

Investigation and direct mapping of the persistent spin helix in confined structures — •Markus Schwemmer, Matthias Weingartner, Roland Völkl, Martin Oltscher, Dieter Schuh, Dominique Bougeard, Tobias Korn, and Christian Schüller — Institute of Experimental and Applied Physics, Faculty of Physics, University of Regensburg, Germany

The spin-orbit field in GaAs-based quantum well (QW) structures typically consists of two different contributions: Dresselhaus and Rashba field. The geometry of the Dresselhaus field, which arises due to the bulk inversion asymmetry, is mostly determined by the growth direction of the quantum well. The Rashba field instead is caused by a structure inversion asymmetry, which can be controlled, e.g. by the modulation doping. For the specific case of a (001)-grown GaAs quantum well with equal strength of Dresselhaus and Rashba fields, the

effective spin-orbit field is oriented along the in-plane [110] direction for all k values and the spin splitting for this direction vanishes. For optically injected spins, which are initially oriented perpendicular to the QW plane, a persistent spin helix (PSH) state forms. We use a femtosecond pulsed TiSa-Laser system combined with a magneto-optical Kerr effect microscope for time- and space-resolved mapping of the PSH. With this technique, we investigate the PSH behavior in confined structures, e.g., thin channels along the helix direction. Hence we find that lateral confinement increases the effective PSH lifetime drastically. In more complex structures, we observe that PSH formation is even stable under a forced direction change.

HL 14.2 Mon 15:00 H13

Effects of lateral confinement on the spin dynamics in GaAs based two-dimensional electron systems — •Patrick Altmann[1], Makoto Kohda[2,1], Matthias P. Walser[1], Christian Reichl[3], Werner Wegscheider[3], and Gian Salis[1] — [1]IBM Research-Zurich, Saeumerstrasse 4, 8803 Rueschlikon, Switzerland — [2]Department of Materials Science, Tohoku University, Sendai, Japan — [3]Solid State Physics Laboratory, ETH Zurich, Zurich, Switzerland

In two-dimensional electron systems (2DES), the diffusive motion of the electrons leads to a precession of their spins because of spin-orbit interaction (SOI). We use time-resolved Kerr microscopy with spatial resolution below the spin-orbit length to directly visualize these precessions [1]. By this, the strength and anisotropy of the SOI are mapped out and the dominant dephasing mechanism and the diffusion constant are determined. We study the impact of lateral confinement on the spin dynamics in a GaAs based 2DES at 20 K. We observe a transition from a 2D spin mode to a quasi-1D mode in wire structures narrower than the spin-orbit length. While in the 2D case both linear and cubic terms of the SOI contribute to spin dephasing, in the 1D case only the cubic contribution remains limiting the spin dephasing time [2]. In the special case of fully anisotropic SOI, known as the persistent spin helix case, dephasing due to linear terms is already suppressed. Thus, wire confinement cannot further enhance the dephasing time, but the dilution of spins due to diffusion is reduced [3].

[1] Walser et al., Nat. Phys. 8, 757 (2012), [2] Altmann et al., accepted PRB, [3] Altmann et al., PRB 90, 201306(R) (2014)

HL 14.3 Mon 15:15 H13

Spin injection devices with a two-dimensional electron gas channel in an (Al,Ga)As/GaAs heterostructure — •Thomas Kuczmik, Dino Popp, Martin Oltscher, Josef Loher, Dieter Schuh, Dominique Bougeard, Mariusz Ciorga, and Dieter Weiss — Universität Regensburg

In recent years spin injection phenomena in bulk semiconductors have been extensively studied. However, many spintronic device concepts, like the Datta-Das spin FET, require spin transport in a two-dimensional electron gas (2DEG).

We have recently demonstrated efficient spin injection into a high mobility 2DEG confined in an inverted (Al,Ga)As/GaAs heterostructure, using (Ga,Mn)As/GaAs Esaki diodes as spin selective contacts [2]. In this contribution we discuss some issues related to the design of the employed heterostructure and to sample fabrication that are critical to preparation of working spin injection devices with a 2D channel. Particular attention has to be devoted to avoiding a parasitic 3D-like conduction channel that can be parallel to the 2DEG channel and therefore can compromise spin transport in the latter. Such a parallel channel can be formed below the active channel, on the (Al,Ga)As side of the heterojunction, in the region of the delta-doping by illuminating the device. We compare the results of nonlocal spin valve measurements on samples with and without any parasitic channel and discuss in details how the presence of such a channel affects the measured spin signal.

[1] M. Oltscher et al., Phys. Rev. Lett. 113, 236602 (2014).

HL 14.4 Mon 15:30 H13

Hanle spin precession in two-dimensional electron gas — •Martin Oltscher, Josef Loher, Dieter Schuh, Mariusz Ciorga, Dominique Bougeard, and Dieter Weiss — University of Regensburg, 93040 Regensburg, Germany

Effective electrical spin injection into two-dimensional electron systems is prerequisite for many new functionalities in possible spintronic devices, with a Datta-Das spin field effect transistor being a primary example. We have recently demonstrated efficient spin injection into high mobility 2DEG confined in the inverted (Al,Ga)As/GaAs structure. In this contribution we present the results of further investigations on that system, focusing on nonlocal Hanle measurements of spin precession in an out-of-plane magnetic field. We observe that not only the amplitude of the precession signal but also its full-width-at-half-maximum strongly changes with the bias voltage V_{3T} applied across the injector. Narrowest curves are observed in the region of the enhanced signal for negative bias. In the region of low bias -0.1 V $< V_{3T} <$ 0.1 V, on the other hand, no precession curves are observed. What is more, spin life time values extracted from the measurements ($\sim$ 23 ns for the narrowest curve) differ by orders of magnitude from the values expected for 2DEGs and from the value of 24 ps extracted earlier from spin-valve measurements. We discuss the results in connection to dynamic nuclear polarization effects in the system, which are known to narrow the experimental Hanle curves. The work has been supported by German Science Foundation (DFG) through the project SFB689.

HL 14.5 Mon 15:45 H13

Exchange coupling between soft magnetic materials and hard magnetic Dysprosium layers — •Markus Ehlert, Thomas Hupfauer, Markus Schitko, Günther Bayreuther, and Dieter Weiss — Institute of Experimental and Applied Physics, University of Regensburg, Germany

The control of the magnetic properties of thin ferromagnetic films is crucial for the functionality of spintronic devices, e.g., for the detection of the spin Hall effect [1]. The goal of our work is to improve the magnetic stability of commonly used soft ferromagnets by making use of the exchange coupling between soft and hard magnetic materials. We report on measurements of the magnetic interplay between soft magnetic Fe or Co layers and hard magnetic Dysprosium (Dy) layers. Microstructured thin films of Fe/Dy and Co/Dy multilayers were prepared by electron-beam lithography and ultra-high vacuum sputtering. The magnetic properties of the materials were determined by means of the Anisotropic Magnetoresistance (AMR) effect. By analyzing and comparing the corresponding AMR data we show that the presence of a Dy layer on top of a soft magnetic material significantly influences its magnetic properties. In our experiments we could enhance, e.g., the in-plane coercive field by one order of magnitude. We investigated the exchange coupling in the ferromagnetic (T<90 K) and antiferromagnetic (T>90 K) phase of Dy and also its dependence on the thickness of the soft magnetic material. All experimental results can consistently be explained with the model of the AMR effect.

[1] M. Ehlert *et al.*, Phys. Status Solidi B **251**, 1725-1735 (2014).

30 min. Coffee Break

HL 14.6 Mon 16:30 H13

Spin-orbit fields at semiconductor interfaces — •Martin Gmitra and Jaroslav Fabian — University of Regensburg

Solids without space inversion symmetry exhibit spin-orbit fields, which are emerging manifestations of spin-orbit coupling of the underlying atomic structure. Primary examples of spatially asymmetric systems are interfaces, which are omnipresent in electronic devices. As the device dimensions scale down, interfaces imprint their symmetries into the transport channel by proximity effects. Proximity spin-orbit fields already play important roles in anisotropic magnetoresistance of ultrathin structures such as Fe/GaAs, in the physics of Majorana fermions and Andreev reflection of semiconductor/superconductor junctions, in Skyrmion textures in ferromagnets, or in spin-orbit torques. It is thus of vital interest to gain qualitative insight and realistic quantitative description of the interfacial spin orbit fields for various materials hybrid settings. We have proposed a methodology to extract spin-orbit fields, both their magnitudes and directions, and applied it to investigate Fe/GaAs junctions. Only at low momenta the traditional description of the fields in terms of linear Rashba and Dresselhaus works. At generic momenta the fields exhibit what we call butterfly patterns, conforming to the interfacial symmetry. Remarkably, the spin-orbit fields depend rather strongly on the magnetization orientation. We will also discuss our recent results on the spin-orbit coupling in zinc-blende and wurtzite semiconductor nanostructures.

The work is supported by the DFG SFB 689.

HL 14.7 Mon 16:45 H13

Spin-orbit coupling and spin relaxation in phosphorene — •Marcin Kurpas, Martin Gmitra, and Jaroslav Fabian — Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany

We employ first principles density functional theory calculations to

study intrinsic and extrinsic spin- orbit coupling in monolayer phosphorene. We also extract the spin-mixing amplitudes of the Bloch wave functions to give realistic estimates of the Elliott-Yafet spin relaxation rate. The most remarkable result is the anisotropy in both spin-orbit coupling and spin relaxation rates, which could be tested experimentally in spin injection experiments. We also identify spin hot spots in the electronic structure of phosphorene at accidental bands anticrossings. We compare the Elliott- Yafet with Dyakonov-Perel spin relaxation times, obtained from extrinsic couplings in an applied electric field. We also compare the results in phosphorene with those of black phosphorous. This work is supported by the DFG SPP 1538, SFB 689, and by the EU Seventh Framework Programme under Grant Agreement No. 604391 Graphene Flagship.

HL 14.8 Mon 17:00 H13

Enabling spin-to-charge conversion in semiconductor spintronics through time-reversal and structure-inversion asymmetry: Fe on Ge(111) — •Ashis K. Nandy[1], Nguyen H. Long[1], Simon Oyarzun[2], Jean-Marie George[3], Henri Jaffres[3], Stefan Blügel[1], and Matthieu Jamet[2] — [1]Peter Grünberg Institute and Institute for Advanced Simulation, FZJ & JARA, D-52425 Jülich, Germany — [2]Univ. Grenoble Alpes, INAC-SP2M, F-38000 Grenoble, France — [3]Univ. Paris-Sud, F-91405 Orsay, France

One important goal of semiconductor spintronics is the realisation of the Si based spin-field-effect transistor. Its realisation is challenged by the small spin-Hall effect in bulk Si and Ge. Using first-principles theory based on DFT we show that the surface of Ge(111) introduces a large snowflake-like Rashba effect with a locking of momentum vector **k** to mostly out-of-plane spin components, whose energy dispersion shows a k^3-dependence in the vicinity of $\bar{\Gamma}$. Breaking the time-inversion symmetry by depositing Fe films on Ge(111) we exhibit a strong hybridization of Fe-*d* with Ge-*p* states, leading to a spin-splitting of the Ge Rashba states, where the majority snowflake-like Rashba states are occupied. The joint effect of exchange and Rashba spin-orbit interaction leads to an electronic structure with a lack of mirror symmetry in the plane normal to the surface and in the direction of the in-plane magnetization. Considering the asymmetry of the Fermi surface and the k^3-dependence of part of the electronic structure, we present arguments supporting experimentally observed large charge currents when generated by intrinsic spin-pumping in the interfacial electron gas.

HL 14.9 Mon 17:15 H13

Deterministic entanglement generation between spatially separated electronic spins — •Mónica Benito[1], Martin Schütz[2], Gloria Platero[1], Geza Giedke[2,3], and Ignacio Cirac[2] — [1]Insituto de Ciencia de Materiales de Madrid, CSIC, 28049 Madrid, Spain — [2]Max Planck Institut für Quantenoptik, Hans-Kopfermann Strasse I, D-85748, Garching, Germany — [3]Donostia International Physics Center DIPC, Paseo Manuel de Lardizabal 4, 20018 Donostia-San Sebastián, Spain

We propose a scheme for deterministic entanglement generation between two electronic spin qubits confined in spatially separated quantum dots. The mechanism is based on electron transport through an ancilla system driving the system spins into an entangled target steady-state. Since the entangle- ment is actively stabilized by purely dissipative dynamics, our scheme is inherently robust against noise and imperfections.

HL 14.10 Mon 17:30 H13

Proximity Anisotropic Magnetoresistance in Graphene — •Jeongsu Lee and Jaroslav Fabian — Institute for Theoretical Physics, University of Regensburg, Regensburg, Germany

We theoretically investigate charge transport in graphene that is on a ferromagnetic-insulator substrate. The substrate induces spin polarization in graphene-ferromagnetic proximity effect-as demonstrated recently experimentally [1]. We show, using realistic models [2, 3], that the presence of spin-orbit coupling in proximity ferromagnetic graphene leads to anisotropic magnetoresistance whereby graphene's resistance changes with varying magnetic field orientation (both in and out of plane). We evaluate the magnitude as well as the angular dependence of this novel effect using conventional transport models [4] and propose specific experimental schemes to measure it. This work is supported by DFG SFB 689.

[1] Z. Wang, C. Tang, R. Sachs, Y. Barlas, and J. Shi, Phys. Rev. Lett. 114, 016603, (2015)

[2] M. Gmitra, D. Kochan, and J. Fabian, Phys. Rev. Lett. 110, 246602 (2013).

[3] M. Gmitra, S. Konschuh, C. Ertler, C. Ambrosch-Draxl, and J. Fabian, Phys. Rev. B 80, 235431, (2009)

[4] S. Adam, E. H. Hwang, V. M. Galitski, and S. Das Sarma, Proc. Natl. Acad. Sci. U.S.A., 104, 18392, (2007)

HL 15: Quantum Dots and Wires: Fabrication and Devices

Time: Monday 14:45–18:45 Location: H16

HL 15.1 Mon 14:45 H16

1.3 μm low-density quantum dots for single photon emitters — •David Quandt[1], Pierce Munnelly[1], Udo Pohl[1], Stephan Reitzenstein[1], and André Strittmatter[2] — [1]Technische Universität Berlin, Institut für Festkörperphysik, Hardenbergstraße 36, D-10623 Berlin, Germany — [2]Otto-von-Guericke Universität Magdeburg, Universitätsplatz 2, D-39106 Magdeburg, Germany

The positioning of In(Ga)As quantum dots by means of a buried stressor has successfully been used to fabricate an electrically driven single photon source emitting in the wavelength range around 960 nm with a $g^{(2)}(0)$ value of 0.05 at 12.5 K. It is highly attractive to adopt this technique for the deterministic realization of practical single photons sources emitting at telecom wavelengths. Indeed it has been shown that it is possible to achieve emission wavelengths of 1.3 μm and beyond using In(Ga)As quantum dots on GaAs. Thus, a buried stressor based single photon source operating at telecommunication wavelengths is feasible. As preliminary work towards this goal, low density InGaAs quantum dots with an InGaAs strain reducing layer have been grown by MOCVD. First micro photoluminescence measurements show discrete excitonic emission lines of single quantum dots ranging from 1200 nm to 1400 nm.

HL 15.2 Mon 15:00 H16

Hybrid architecture for shallow accumulation mode AlGaAs/GaAs heterostructures with epitaxial gates — S. J. MacLeod[1], A. M. See[1], A. R. Hamilton[1], I. Farrer[2], D. A. Ritchie[2], •J. Ritzmann[3], A. Ludwig[3], and A. D. Wieck[3] — [1]School of Physics, University of New South Wales, Sydney, Australia — [2]Cavendish Laboratory, University of Cambridge, United Kingdom — [3]Angewandte Festkörperphysik, Ruhr-Universität Bochum, Germany

In accumulation-mode GaAs based heterostructures, the charge carriers are induced by a gate. Usually the top-gate spans the entire transport region and slightly overlaps the ohmic contacts in order to effectively contact and induce a continuous two dimensional conducting region. The close proximity of the contacts to the top-gate can easily cause electrical shorts. The shorting of the top-gate to the contacts is particularly problematic in shallow SISFETs in which the top-gate is an in situ, degenerately doped GaAs cap. Here, we demonstrate a hybrid device where the transport region is a SISFET. The gate recess is realized by a two dimensional electron system induced with a metal gate, insulated from an ohmic contact and the SISFET gate by a dielectric layer. Samples with spacer thicknesses of 50 nm and 160 nm are grown and processed in hybrid devices. Ohmic contact resistance, density tunability, mobiltiy and quantum Hall effect measurements are performed. We observe no shift in the bias point for different cooldown cycles. Additionally devices from different MBE setups, show identical bias point operations and nearly identical mobility.

HL 15.3 Mon 15:15 H16

In(Ga)As/GaAs quantum dots grown on GaP/Si(001) investigated on the atomic scale — •Celina S. Schulze[1], Xue Huang[2], Christopher Prohl[1], Vivien Füllert[1], Stavros Rybank[1], Scott J. Maddox[3], Stephen D. March[3], Seth R. Bank[3], Minjoo L. Lee[2], and Andrea Lenz[1,2] — [1]Technische Universität Berlin, Institut für Festkörperphysik, Germany — [2]Yale University, Department of Electrical Engineering, USA — [3]The University of Texas at Austin, Microelectronics Research Center and ECE Dept.,

USA

The epitaxial growth of III-V laser structures on Si(001) substrates is of high interest for future applications in the silicon-device technology. In this work the atomic structure, stoichiometry, and optical properties of InAs/InGaAs quantum-dot-in-a-well structures grown in a GaAs matrix on an exactly oriented GaP/Si(001) template are studied. Similar photoluminescence spectra are observed for nanostructures grown on GaP/Si(001) compared to those on GaAs(001) substrates. For a fundamental understanding of these optical properties a detailed knowledge of the atomic structure is required, which is ideally studied using cross-sectional scanning tunneling microscopy (XSTM). In detailed XSTM experiments quantum dots with lateral sizes of about 20 nm and heights up to 8 nm were observed. An inhomogeneous In concentration indicates strong segregation effects.

This project was supported by the DFG, project LE 3317/1-1, and the Air Force Office of Scientific Research (AFOSR MURI Award No. FA9550-12-1-0488).

HL 15.4 Mon 15:30 H16

Growth and structure of In0.5Ga0.5Sb quantum dots on GaP — •Elisa Maddalena Sala[1], Gernot Stracke[1], Sören Selve[2], Tore Niermann[2], Michael Lehmann[2], Andre Strittmatter[1], and Dieter Bimberg[1] — [1]Institut für Festkörperphysik, TU Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Zentraleinrichtung Elektronenmikroskopie, TU Berlin, Str. des 17. Juni 135, 10623 Berlin, Germany

III-V self-assembled QDs on GaP have recently attracted great interest for application in nanomemory cells. As demonstrated by Marent, Geller, Bimberg et al[1], such QDs can be employed as storage units in a novel type of non-volatile nanomemory, the QD-Flash. Retention times of more than 10 years for holes in In0.5Ga0.5Sb QDs embedded in a GaP matrix are predicted. Here we demonstrate for the first time the Stranski-Krastanov (S-K) growth of In0.5Ga0.5Sb QDs on GaP(001) by metalorganic vapor phase epitaxy (MOVPE). Taking advantage of the initial 2D growth of GaAs on GaP, the few GaAs layers mimic a virtual substrate for the following In0.5Ga0.5Sb deposition, playing a decisive role adjusting the surface energetics. The QD density shows a typical S-K trend, i.e. a logarithmic dependence on the amount of deposited In0.5Ga0.5Sb. High resolution cross-sectional TEM micrographs of buried QDs show a typical truncated-pyramid shape. Before supplying QD material, a short Sb-flush is used to initiate Sb incorporation. Experimental results show that Sb apparently modifies the growth kinetics by reducing the In and Ga surface diffusion length.

[1] A. Marent et al, Microelectronics Journal 40 (2009), 492-495.

HL 15.5 Mon 15:45 H16

Electrostatically defined quantum dots in undoped Si/SiGe heterostructures — •Floyd Schauer[1], Christian Neumann[1], Christian Fritsch[1], Sebastian Schwägerl[1], Simon Pfaehler[1], Dieter Weiss[1], Kentarou Sawano[2], and Dominique Bougeard[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Germany — [2]Advanced Research Laboratories, Tokio City University, Japan

Two-dimensional electron systems (2DES) in undoped heterostructures represent a promising building block for the development of electrostatically defined spin qubits. Omitting the dopants in the heterostructure eliminates fluctuating charge traps due to ionized impurities. The hyperfine interaction with the nuclear spin bath being a dominant qubit decoherence mechanism, Si/SiGe heterostructures have been receiving steadily increasing attention for building devices almost free of nuclear spin carrying isotopes.

In this contribution, we present the realization of capacitively-induced Si/SiGe Quantum Dot (QD) devices. A global top gate is used to accumulate electrons and induce a 2DES in the undoped Si quantum well via the field effect. We examine the capacitive coupling between surface gates and the 2DES as well as remaining charge noise sources in these undoped structures. A second gate layer in the devices allows to locally deplete the 2DES and to form QDs: we discuss the operation in the single QD regime.

HL 15.6 Mon 16:00 H16

Preparation of Silicon Nanocrystals in Silicon Carbide by a Multilayer Approach — •Charlotte Weiss, Andreas Reichert, and Stefan Janz — Fraunhofer Institut für Solare Energiesysteme ISE, Heidenhofstraße 2, 79110 Freiburg, Germany

The embedment of Si nanocrystals (NC) in a SiC matrix yields a promising semiconductor for tandem solar cell applications, due to its tunable bandgap by the variation of the Si NC size. The samples are prepared by plasma enhanced chemical vapour deposition (PECVD) of alternating stoichiometric SiC and Si-rich SiC (SRC) layers. During the subsequent annealing step at 1100°C phase separation into Si and SiC takes place in the SRC layers and NC form. The stochiometric SiC layer is intended to act as barrier layer for Si NC growth, which would mean that the thickness of the SRC layers define the Si NC size. It turns out that this so called multilayer (ML) approach does not control the Si NC size sufficiently, due to Si/SiC interdiffusion during annealing, accompanied with the loss of the ML structure.

Now we successfully preserved the multilayer structure by the incorporation of oxygen in the samples. This was achieved by providing CO2 during PECVD. The successful incorporation in the form of Si-O was confirmed by fourier transformed infrared spectroscopy while the preserved ML structure is observed in scanning electron micrographs. Raman measurements provide further evidence for lowered intermixing, as they show enhanced Si crystallinity in the ML with oxygen compared to samples without oxygen.

Invited Talk HL 15.7 Mon 16:15 H16

Mechanical Control of Excitonic States in Quantum Dots — Rinaldo Trotta, Javier Martín-Sánchez, and •Armando Rastelli — Institute of Semiconductor and Solid State Physics, Johannes Kepler University Linz, Austria

Several systems are under investigation for their potential use in the fields of quantum information and communication. Semiconductor quantum dots (QDs), also dubbed "artificial atoms", are one of such systems, as they can be used both as sources and hosts of "quantum bits" and can be easily integrated into compact devices and photonic structures. However, unlike natural atoms, no two QDs are identical - a major obstacle towards their actual application.

In this talk we will show how elastic strain can be used to overcome problems arising from unavoidable fluctuations during QD growth and to reshape the QD electronic structure and excitonic emission after fabrication. In particular, we will illustrate how any arbitrarily chosen QD can be employed as a wavelength-tunable source of entangled-photon pairs. This is achieved by integrating the QDs onto micro-machined piezoelectric actuators capable of controlling the in-plane strain in the QD and surrounding matrix [1-3].

[1] R. Trotta et al., Phys. Rev. Lett. 114, 150502 (2015)
[2] R. Trotta et al., Nature Comm. (in press)
[3] J. Martín-Sánchez et al., Adv. Opt. Mater. (in press)

30 min. Coffee Break

HL 15.8 Mon 17:15 H16

An electro-photo-sensitive memristor for neuromorphic and arithmetic computing applications — •Patrick Maier[1], Fabian Hartmann[1], Monika Emmerling[1], Christian Schneider[1], Martin Kamp[1], Sven Höfling[1,2], and Lukas Worschech[1] — [1]Technische Physik and Wilhelm Conrad Röntgen Research Center for Complex Material Systems, Physikalisches Institut, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]SUPA, School of Physics and Astronomy, University of St. Andrews, St. Andrews, KY16 9SS, UK

Memristors have state- and time-dependent resistances that allow the emulation of synaptic functionalities which are essential for learning and memory. We report the realization of a memristor on the mature III-V-semiconductor platform and present an electro-optical control of the conductance by tuning the amount of localized charge on a quantum dot floating gate. In analogy to synaptic strength modifications in neural networks, we show that the conductance can be increased (potentiation) or decreased (depression) by tuning the time difference between incoming voltage pulses. In addition, the localized charge on the quantum dot shifts the threshold voltages for the induction of potentiation and depression. The dependency of the threshold voltage for potentiation on the initial state in combination with the optical control of the conductance enables arithmetic computing applications of low power light pulses. Our findings may pave the way to the realization of electro-optical, memristor-based artificial neural networks with a memory-dependent ability of learning.

HL 15.9 Mon 17:30 H16

Site-Controlled MBE Growth of III/V Semiconductor Nanowires Induced by Focused Ion Beam — •Sven Scholz, Rüdiger Schott, Arne Ludwig, and Andreas D. Wieck

— Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum

Nanowires (NWs) are near one-dimensional structures that typically have a huge length-to-width ratio. This is the base of fascinating properties. Heterostructures of highly lattice mismatched materials can be combined without dislocations. Metastable phases, unattainable in bulk materials like wurtzite GaAs or InAs, are feasible. We present focused ion beam (FIB) induced molecular beam epitaxy (MBE) grown NWs from site selectively deposited Au seeds. The possibility of maskless patterning makes FIB a powerful tool and an alternative to conventional lithography based methods in semiconductor processing. By implanting distinct spots of Au ions in arbitrary distributions on GaAs substrates, we initiate GaAs and InAs NW growth in the MBE. We show, that a small amount of ions resulting in small droplets appropriate to catalyse a single NW per site with a yield of above 60%. The small size of the droplets leads to NWs with diameters of 20 nm and below, which results in high aspect ratios. Additionally to the optimization of the morphology, the crystal structure was investigated and improved to achieve defect free and single crystalline NWs. Also the bandgap modulation due to the growth of heterostructures in single NWs will be presented.

HL 15.10 Mon 17:45 H16

Selective area growth of GaAs nanowires combining high vertical yield and desirable morphology — •Hanno Küpers, Abbes Tahraoui, Ryan B. Lewis, Henning Riechert, and Lutz Geelhaar — Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5-7, 10117 Berlin

The Ga-assisted growth of GaAs nanowires (NWs) is a promising way to integrate III-V materials with Si. Toward this goal, selective area NW growth on an oxide mask by molecular beam epitaxy has been widely investigated, focusing mainly on obtaining high vertical NW yields rather than optimal NW morphologies. Key requirements for high NW yields are a high mask quality and a low V/III ratio, however, NWs grown under these conditions exhibit large diameters and a high degree of tapering, both undesired properties for applications relying on a core-shell geometry. In this study we present a two-step growth approach which results in high vertical yields with small diameters and negligible tapering: First, NWs start to grow under growth conditions optimized for a high vertical yield. Second, after some time the growth conditions are changed in order to shape the morphology of the growing NWs. Even though the V/III ratio is increased the NW growth remains stable and does not cease. This growth approach enables the growth of NW ensembles with a vertical yield of exceeding 70%, diameters of 50 nm and tapering of below 0.4%.

HL 15.11 Mon 18:00 H16

Top-down fabrication and characterization of reconfigurable silicon nanowires — •Dipjyoti Deb[1], Muhammad Bilal Khan[1], Yordan Georgiev[1], Markus Löffler[3], Walter Weber[2], Manfred Helm[1], and Artur Erbe[1] — [1]HZDR, Bautzner Landstraße 400, 01328 Dresden, Germany — [2]Namlab gGmbH, Nöthnitzer Str. 64, 01187 Dresden, Germany — [3]Center for Advancing Electronics Dresden, 01062 Dresden, Germany

The following work illustrates characterization of reconfigurable, undoped silicon nanowire field effect transistors with Schottky junctions fabricated on silicon on insulator (SOI) substrate by top-down process. The fabrication scheme is based on electron beam lithography (EBL) using hydrogen silsesquioxane (HSQ), a negative tone electron beam resist, followed by inductively coupled plasma (ICP) etching. The etch recipe was optimised in context of selectivity, sidewall roughness and anisotropy by selecting an appropriate gas chemistry (SF6/C4F8) and controlling the ICP hardware parameters like gas flow, mixed gas ratio, plasma power and chamber pressure. We produced silicon nanowires of 20 nm width and nanowire arrays with pitch of 200 nm. 50 nm thick nickel (Ni) layer was sputtered on the SiNWs at lithographically defined areas followed by lift-off and thermal annealing to create Nickel-Silicide Schottky junctions inside the nanowires. In this way, the source and drain region was formed creating silicide-silicon-silicide contacts. Transport properties of these nanowires can be modulated from P-type to N-type and vice-versa by changing polarity of the back gate.

HL 15.12 Mon 18:15 H16

Electrical characterization and modelling of p-GaAs nanowires by MT-STM — •Andreas Nägelein[1], Matthias Steidl[1], Weihong Zhao[1], Stefan Korte[2], Peter Kleinschmidt[1], and Thomas Hannappel[1] — [1]TU Ilmenau, Institut für Physik, FG Photovoltaik, 98693 Ilmenau — [2]Forschungszentrum Jülich, Peter Grünberg Institut (PGI-3), 52425 Jülich

Doped nanowires are promising candidates as components for advanced applications such as FETs or solar cells. To increase the efficiency of these upcoming applications detailed knowledge of dopant distribution along the nanowire is necessary. In this work a nondestructive method is used, where freestanding nanowires can be characterized using a multi-tip STM (MT-STM) as a prober for four-point measurements. Here, a continuous resistance profile can be recorded which is proportional to the doping profile. The nanowires were grown in the Au-catalyzed VLS growth mode on p-GaAs(111)B by metal-organic chemical vapor phase epitaxy (MOVPE) in an "AIX200" system.
Resistance profiles of p-GaAs nanowires were recorded using the MT-STM. With help of a suitable model we are able to simulate the resistances and calculate the doping of the nanowire which results in a constant doping profile. In order to establish a valid electrical model for doped nanowires we developed in the first step a simulation with resistances and diodes. We could show that a simple model is in good agreement with the measured data. Applying an extended model to nanowire measurements allows analysis of more complex dopant distributions and nanowire geometries.

HL 15.13 Mon 18:30 H16

In-situ growth of semiconductor/superconductor core-shell nanowires — •Nicholas Güsken[1,2], Torsten Rieger[1,2], Thomas Schäpers[1,2], Detlev Grützmacher[1,2], and Mihail Ion Lepsa[1,2] — [1]Peter Grünberg Institute 9, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Jülich Aachen Research Alliance for Fundamentals of Future Information Technology (JARA-FIT), Germany

Semiconductor/superconductor(SM/SC) nanowire (NW) hybrid structures are of main interest for future research as they enable to investigate a variety of quantum effects such as Andreev reflections and the proximity effect. Additionally, InAs/Nb as well as InAs/Al core-shell NWs, might pave the way for a breakthrough with regard to Majorana-fermion related research and quantum computing. For all of the experiments, a clean SM/SC interface and low SM resistivity is crucial, to circumvent unambiguous core results. In this sense, the best solution is to fabricate the SM-NW core and the SC shell in-situ. In this work, we show results of the in-situ growth and preliminary morphological and electrical characterization of InAs/Al and InAs/Nb hybrid NWs.

The InAs NWs were grown self-assisted on Si substrates, using molecular beam epitaxy. Expecting more efficient and uniform doping, Te doping was employed to tailor the electron concentration of the NWs. Electrical characterization was conducted after the NW growth to investigate the impact of Te doping on the NWs. Finally, Al or Nb, were deposited on the side facets of the NWs.

The quality of the SM/SC core-shell NWs was investigated by SEM and preliminary transport measurements at low temperatures.

HL 16: Graphene: Transport (Joint session of DS, HL and TT, organized by HL)

Time: Monday 14:45–17:45 Location: H17

Invited Talk HL 16.1 Mon 14:45 H17

Advances in Raman Spectroscopy of Graphene and Layered Materials — •Andrea C. Ferrari — Cambridge Graphene Centre, University of Cambridge, Cambridge, CB3 OFA, UK

Raman spectroscopy is an integral part of graphene research [1]. It is used to determine the number and orientation of layers, the quality and types of edges, and the effects of perturbations, such as electric and magnetic fields, strain, doping, disorder and functional groups[2,3]. I will review the state of the art, future directions and open questions in Raman spectroscopy of graphene and related materials, focussing on the effect of disorder[3,4], doping[5,6] and deep UV laser excitation[7].

I will then consider the shear [8] and layer breathing modes(LBMs)[9], due to relative motions of the planes, either perpendicular or parallel to their normal. These modes are present in all layered materials[10,11]. Their detection allows one to directly probe the interlayer interactions [10,11]. They can also be used to determine the elastic constants associated with these displacements: the shear and out-of-plane elastic moduli[12]. This paves the way to the use of Raman spectroscopy to uncover the interface coupling of two-dimensional hybrids and heterostructures[10-12].

1. A. C. Ferrari et al. Phys. Rev. Lett. 97, 187401 (2006) 2. A.C. Ferrari, D.M. Basko, Nature Nano. 8, 235 (2013) 3. A.C. Ferrari, J Robertson, Phys. Rev. B 61, 14095 (2000) 4. G. Cancado et al. Nano Lett. 11, 3190 (2011) 5. M. Bruna et al. ACS Nano 8, 7432 (2014) 6. A. Das et al. Nat. Nanotechnol. 3, 210 (2008) 7. A.C. Ferrari, S. Milana, P. H. Tan, D. M. Basko, P. Venezuela, submitted (2016) 8. P. H. Tan et al. Nature Materials 11, 294 (2012) 9. X. Zhang et al. Phys. Rev. B 87, 115413 (2013) 10. J. B. Wu et al. Nature Comms. 5, 5309 (2014) 11. J.B. Wu et al. ACS Nano, 9, 7440 (2015) 12. S. Milana et al. submitted (2016)

HL 16.2 Mon 15:15 H17

Landau Quantization in Twisted Bilayer Graphene — •Johannes C. Rode, Dmitri Smirnov, Christopher Belke, Henrik Schmidt, and Rolf J. Haug — Institut für Festkörperphysik, Leibniz Universität Hannover

The bandstructure of bilayer graphene is highly sensitive to rotational mismatch between layers. At large angles, the twisted bilayer effectively behaves like two decoupled monolayers, while the dispersions merge in low-energy van Hove singurities for small interlayer twist[1]. Whereas the regime of large rotational mismatch has been extensively studied in transport experiments[2], there have been few reports on small angle samples[3,4] and none for the transition between the two angular regimes so far. We here examine the magnetotransport behavior across this transition, closing the gap in experimental evidence. The results are discussed with respect to theory[5] and and under special consideration of gate-induced layer asymmetries.

[1] Lopes dos Santos, J. M. B., Perez, N. M. R., Castro Neto, A. H. *Phys. Rev. Lett.* **99**, 25682.
[2] Schmidt, H. *et al. Appl. Phys. Lett.* **93**, 172108.
[3] Schmidt, H., Rode, J. C., Smirnov, D., and Haug, R. J. *Nat. Commun.* **5**, 5742.
[4] Lee, D. *et al. Phys. Rev. Lett.* **107**, 216602.
[5] de Gail, R., Goerbig, M. O., Guinea, F., Montambaux, G., Castro Neto, A. H. *Phys. Rev. B* **84**, 045436.

HL 16.3 Mon 15:30 H17

Magnetic exchange coupling across a graphene layer — •Alessandro Barla[1], Valerio Bellini[2], Stefano Rusponi[3], Paolo Ferriani[4], Marina Pivetta[3], Fabio Donati[3], François Patthey[3], Luca Persichetti[5], Sanjoy K. Mahatha[1], Marco Papagno[6], Cinthia Piamonteze[7], Simon Fichtner[4], Stefan Heinze[4], Pietro Gambardella[5], Harald Brune[3], and Carlo Carbone[1] — [1]Istituto di Struttura della Materia, CNR, I-34149 Trieste, Italy — [2]S3-Istituto di Nanoscienze-CNR, I-41125 Modena, Italy — [3]Institute of Condensed Matter Physics, EPFL, CH-1015 Lausanne, Switzerland — [4]Institute of Theoretical Physics and Astrophysics, University of Kiel, D-24098 Kiel, Germany — [5]Department of Materials, ETH Zürich, CH-8093 Zürich, Switzerland — [6]Dipartimento di Fisica, Universitá della Calabria, I-87036 Arcavacata di Rende, Italy — [7]Swiss Light Source, PSI, CH-5232 Villigen PSI, Switzerland

In order to access the potential of graphene in spintronic devices, its ability to mediate magnetic exchange interactions has to be verified. We present the results of our investigations of the magnetic coupling between Co atoms and Ni(111) mediated by epitaxial graphene. Experimental and theoretical calculations reveal that individual Co atoms occupy two distinct adsorption sites, with different magnetic coupling to the underlying Ni(111) surface. We further report a transition from an antiferromagnetic to a ferromagnetic coupling with increasing Co coverage. Our results highlight the extreme sensitivity of the exchange interaction mediated by graphene to the adsorption site and to the in-plane coordination of the magnetic atoms.

HL 16.4 Mon 15:45 H17

Transport studies in laterally density-modulated graphene-boron nitride-heterostructures — •Martin Drienovsky[1], Christian Baumgartner[1], Felix Simbürger[1], Takashi Taniguchi[3], Kenji Watanabe[3], Ming-Hao Liu[2], Fedor Tkatschenko[2], Klaus Richter[2], Dieter Weiss[1], and Jonathan Eroms[1] — [1]Institut für Experimentelle und Angewandte Physik Universität Regensburg, 93053 Regensburg — [2]Institut für Theoretische Physik Universität Regensburg, 93053 Regensburg — [3]National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan

We report on ballistic transport in graphene-boron nitride heterostructures with a tunable charge carrier density profile. Employing a dry van-der-Waals stacking method, we prepare high mobility graphene devices, where the charge carrier mean free path can exceed the lattice period of the induced multibarrier system by several times. These potential barriers are generated by multiple local top gate electrodes and a global back gate, and yield a pronounced Fabry-Pérot interference pattern in the bipolar transport regime. The extended ballistic length - in comparison to former samples - gets us within reach of the superlattice effect, which we highlight by matching the experimental data to a model calculation. We additionally apply a high, perpendicular magnetic field to our multibarrier systems and observe mode-mixing in the Quantum-Hall-regime of a 4-point measurement setup. By comparing samples with different top gate periods and separately controllable top electrodes, we study adiabatic and equilibrated unipolar edge channel transmission and suppression of equilibration at bipolar junctions.

15 min. Coffee Break

Invited Talk HL 16.5 Mon 16:15 H17

Thermodynamic picture of ultrafast conduction in graphene — •Dmitry Turchinovich[1], Zoltan Mics[1], Klaas-Jan Tielrooij[1,2], Ivan Ivanov[1], Xinliang Feng[1], Klaus Müllen[1], and Mischa Bonn[1] — [1]Max Planck Institute for Polymer Research, 55128 Mainz, Germany — [2]ICFO, 08860 Barcelona, Spain

Graphene has very high steady-state conductivity, which, however, does not hold in the regime of ultrafast, sub-picosecond electric fields corresponding to the terahertz (THz) frequencies. Here we show that in graphene, the electron conduction on an ultrafast timescale is determined by a simple thermodynamic balance maintained within its electronic system acting as a thermalized electron gas [1]. The energy of ultrafast electric currents passing trough graphene is near-instantaneously converted into the thermal energy of its entire charge carrier population, thereby raising the electronic temperature and reducing the chemical potential. The interplay between electron heating and cooling dynamics in graphene ultimately defines its ultrafast conductivity. We demonstrate that this simple thermodynamic picture describes very well the THz linear, nonlinear, and photo-induced conductivity of this remarkable material [1-3].

[1] Z. Mics, K.-J. Tielrooij, K. Parvez, S. A. Jensen, I. Ivanov, X. Feng, K. Müllen, M. Bonn, and D. Turchinovich, Nat. Commun. 6, 7655 (2015). [2] S. A. Jensen, Z. Mics, I. Ivanov, H. S. Varol, D. Turchinovich, F. H. L. Koppens, M. Bonn, and K. J. Tielrooij, Nano Lett. 14, 5839 (2014). [3] I. Ivanov, M. Bonn, Z. Mics, and D. Turchinovich, EPL - Europhys. Lett. 111, 67001 (2015).

HL 16.6 Mon 16:45 H17

Magnetotransport in graphene antidot arrays: semiclassics and moiré lattices — •Andreas Sandner[1], Tobias Preis[1], Christian Schell[1], Paula Giudici[1], Kenji Watanabe[2], Takashi Taniguchi[2], Dieter Weiss[1], and Jonathan Eroms[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Germany — [2]NIMS, 1-1 Namiki, Tsukuba, Japan

Embedding graphene into a heterostructure with hexagonal boron nitride (hBN) on both sides was shown to be an efficient way of achieving a high bulk mobility. However, nanopatterning graphene can add extra damage and drastically degrade the intrinsic properties by edge disorder. But graphene encapsulated between hBN is protected during a top-down fabrication procedure. In this way, we can prepare graphene-based antidot lattices where the high mobility is preserved.

We performed magnetotransport experiments in monolayer-graphene antidot lattices with lattice periods down to 50 nm. We observe pronounced commensurability features in ρ_{xx} stemming from ballistic orbits around one or several antidots. Due to the short lattice period in our samples, we can explore the boundary between the semiclassical and the quantum transport regime, as the Fermi wavelength of the electrons approaches the smallest length scale of the artificial potential.

Additionally, we study the interplay between a moiré and the imposed antidot superlattice potential in several of our samples. There is a gradual suppression of the classical commensurability features by

approaching the satellite Dirac points of the moiré potential.

HL 16.7 Mon 17:00 H17

Influence of disordered edges on transport properties in graphene — Dmitri Smirnov[1], Galina Yu. Vasileva[1,2,3], •Christopher Belke[1], Johannes C. Rode[1], Yurij B. Vasilev[2], Yurij L. Ivanov[2], and Rolf J. Haug[1] — [1]Institut fuer Festkoerperphysik, Leibniz Universitaet Hannover — [2]Ioffe Institute, Russian Academy of Sciences, St. Petersburg — [3]Peter the Great Polytech University, St. Petersburg

The influence of plasma etched edges on electrical transport and doping on graphene devices is studied. Mono- and bilayer samples were fabricated into a specific Hall bar geometry with differing width. The fabrication was done via transfer on a Si/SiO_2 substrate and structuring and contacting via plasma oxygen etching and e-beam lithography. The specific shape allows to investigate the influence of edge disorder on the overall doping and the effective mobility.
The doping concentration, calculated from the charge neutrality point, differs for every region and an inverse dependence on the region width was observed. The sample edge was determined as a strong p-doping source, dominating the bulk doping component and the edge doping contribution and efficiency was obtained.
A further study of the mobility for different regions was used to quantify the edge scattering. We find, that for decreasing region width the mobility decreases as well. This behavior can be attributed to the samples edge, establishing it as a further scattering mechanism.

HL 16.8 Mon 17:15 H17

Acoutoelectric currents in coated graphene on SiC — •Alberto Hernández-Mínguez, Abbes Taharoui, Marcelo Lopes, and Paulo Santos — Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany

Surface acoustic waves (SAWs) provide useful mechanisms for the dynamic modulation and transport of carriers in two-dimensional semiconductor heterostructures. In the case of graphene, we have recently shown that the piezoelectric fields accompanying SAWs can induce unipolar electric currents in lithographically patterned graphene layers grown on SiC. Due to the weak piezoelectricity of SiC, however, the interaction between SAW and carriers in graphene is relatively small. Future applications of the acoustic transport require the generation of strong SAWs for their efficient coupling to graphene, as well as the control of the density and type of carriers transported by the SAW. In this contribution, we study structures for efficient generation of high frequency acoustic transport (> 1 GHz) in graphene grown on SiC that are also compatible with top gates for the electric control of the carrier density. Several Rayleigh modes with frequencies up to 7 GHz are efficiently generated in our structure, inducing acoustic currents for the fundamental frequency that are 300 times larger than the ones reported in our previous devices. These results are an important step towards the dynamic control of carriers in graphene at the sub-micrometer regime, as well as for the dynamic manipulation of the electron spin by strain-induced gauge fields.

15 min. Coffee Break

HL 17: Transport: Topological Insulators - 2D (Joint session of DS, HL, MA, O and TT, organized by TT)

Time: Monday 15:00–17:45 Location: H18

HL 17.1 Mon 15:00 H18

Probing the spin texture of generic helical edge states with an antidot — •Alexia Rod[1,2], Giacomo Dolcetto[1], Thomas L. Schmidt[1], and Stephan Rachel[2] — [1]Physics and Materials Science Research Unit, University of Luxembourg, Luxembourg — [2]Institut für Theoretische Physik, TU Dresden, Germany

Edge states of time-reversal topological insulators are generally described as helical edge states, where the spin-axis symmetry is conserved. However, this symmetry is usually not guaranteed in experimental realizations. In its absence, the most general model to describe edge states is called generic helical liquid. Using this framework, a rotation of the spin quantization axis has been predicted, independently of the microscopic model and of the considered geometry [1, 2].

Here we propose a scheme to probe the spin texture of the edge states on a transport device. We investigate the transport properties of generic helical edge states in a two-dimensional topological insulator bar with an antidot in its center. We show that the conductance is implicitly dependent of the spin texture in the case of uniform bulk or structural inversion asymmetry. We also study sequential tunneling and cotunneling in presence of Coulomb interaction due to electron confinement on the antidot.

[1] T.L. Schmidt, S. Rachel, F. von Oppen, L. Glazman, PRL **108**, 156402 (2012).
[2] A. Rod, T.L. Schmidt, S. Rachel, PRB **91**, 245112 (2015).

HL 17.2 Mon 15:15 H18

Electron quantum optics in 2d topological insulators — •Andrea Spichtinger, Sven Essert, Viktor Krückl, and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

Besides conventional quantum Hall systems [1], 2d topological insulators (TIs) are ideal systems providing ballistic channels for guiding charge carriers along edge states allowing for the study of two-particle interferometric effects. Employing wave-packet approaches we investigate correlations between indistinguishable spin pairs at opposite quantum spin Hall edges. Interconnecting opposite edges at TI constrictions or through quantum dots acting as "beam splitter" allows for realizing fermionic analogues of the famous photonic Hong-Ou-Mandel (HOM) effect. In particular, we will consider generalizations of the HOM effect since the dwell time of the quantum dot enters as a new timescale into HOM physics.

[1] E. Bocquillon et al., Ann. Phys. **526**, 1 (2014)

HL 17.3 Mon 15:30 H18

Transport in quantum spin Hall systems in parallel magnetic fields — •Michael Wimmer[1], Rafal Skolasinski[1], Dmitry Pikulin[2], and Jason Alicea[3] — [1]TU Delft, The Netherlands — [2]University of British Columbia, Canada — [3]Caltech, US

Edge states in quantum spin Hall (QSH) systems are protected by time-reversal symmetry, resulting in a qunatized conductance. A magnetic field breaks that protection, and should lead to a deviation from perfect quantization. We will discuss generic features of semiconductor-based QSH systems (such as HgTe/CdTe and InAs/GaSb) that affect the magnetic field dependence of edge state conductance, focusing on the effect of an in-plane field.

HL 17.4 Mon 15:45 H18

Spectral functions of the correlated topological insulator — •Damian Zdulski and Krzysztof Byczuk — Faculty of Physics, Institute of Theoretical Physics, University of Warsaw, ul.Pasteura 5, PL-02-093 Warsaw, Poland

In our recent paper [1], we have studied the influence of electron correlations on topological insulators (TIs) at finite temperatures. The correlated TI was represented by the Kane-Mele model with the interaction term as in the Falicov-Kimball model and it was examined within the Hartree and the Hubbard I approximations. In this talk, we will present extension of that analysis by investigating properties of the system within the dynamical mean field approximation. Our findings show that dynamical correlations yield totally new structures, which are seen in the the momentum dependent spectral functions. Namely, we see: 1) widening of Dirac nodes over finite range of **k** points in the Brillouin zone (BZ), 2) creation of almost flat subbands in a finite range of the BZ, 3) appearance of kinks, and 4) splitting of kinks with formation of overlapping bands.

[1] D. Zdulski, K. Byczuk, PRB **92**, 125102 (2015)

HL 17.5 Mon 16:00 H18

The topological Anderson insulator phase in the Kane-Mele model — Christoph P. Orth[1], •Tibor Sekera[1], Christoph Bruder[1], and Thomas L. Schmidt[2] — [1]Department of Physics,

University of Basel, Klingelbergstrasse 82, 4056 Basel, Switzerland — [2]Physics and Materials Science Research Unit, University of Luxembourg, L-1511 Luxembourg

It has been proposed that adding disorder to a topologically trivial mercury telluride/cadmium telluride (HgTe/CdTe) quantum well can induce a transition to a topologically nontrivial state. The resulting state was termed topological Anderson insulator and was found in computer simulations of the Bernevig-Hughes-Zhang model.

We show that the topological Anderson insulator is a more universal phenomenon and also appears in the Kane-Mele model of topological insulators on a honeycomb lattice. We numerically investigate the interplay between the parameters characterizing intrinsic spin-orbit coupling, extrinsic Rashba spin-orbit coupling and staggered sublattice potential. We establish the parameter regimes in which the topological Anderson insulator is found. For weak enough disorder, a calculation based on the lowest-order Born approximation reproduces the numerical data. Our results thus considerably increase the number of candidate materials for the topological Anderson insulator phase.

15 min. break

HL 17.6 Mon 16:30 H18

Interplay of topology and interactions in the quantum Hall regime of topological insulators: spontaneous symmetry breaking, tunable strongly interacting Luttinger liquid — •Stefan Jürgens, Maxim Kharitonov, and Björn Trauzettel — Institute of Theoretical Physics, University of Würzburg, Germany

We consider a class of two-dimensional topological insulators, in which the single-particle edge states are preserved in the presence of the magnetic field by a symmetry (such as crystalline) other than time-reversal, relevant to such materials as HgTe-type heterostructures.

We focus on the vicinity of the topological crossing point between two Landau levels. At half-filling, Coulomb interactions lead to the formation of the quantum Hall "ferromagnetic" many-body state with gapped charge excitations in the bulk. We derive and analyze the σ-model that describes the low-energy properties of this strongly interacting state, including the effect of the edge. We obtain the bulk phase diagram and find three phases, two with preserved and one with spontaneously broken U(1) symmetry. We study the collective edge charge excitations of these phases.

We demonstrate that in one of the phases with preserved U(1) symmetry, the edge charge excitations are gapless and described by a highly tunable, strongly interacting Luttinger liquid. When U(1) symmetry is broken in this phase, edge excitations become gapped and are described by a sine-Gordon model. Our main conclusion is that continuous U(1) symmetry is a necessary condition for the existence of the gapless edge excitations in this strongly interacting system.

HL 17.7 Mon 16:45 H18

Terahertz properties of Dirac electrons and holes in HgTe films with critical thickness — •Uladzislau Dziom[1], Alexey Shuvaev[1], Nikolai Mikhailov[2], Ze Don Kvon[2], and Andrei Pimenov[1] — [1]Institute of Solid State Physics, Vienna University of Technology, 1040 Vienna, Austria — [2]Novosibirsk State University, Novosibirsk 630090, Russia

We present and discuss properties of mercury telluride (HgTe) films with critical thickness in far-infrared (THz) spectral range. Density of charge carriers is controlled, using contact-free optical gating by visible light. Transmission measurements in applied magnetic field demonstrate switching from hole to electron-like behavior, as illumination time increases. The cyclotron mass of the electrons, extracted from the data, shows a square root dependence upon the charge concentration in a broad range of parameters. This can be interpreted as a clear proof of a linear dispersion relations, i.e. Dirac-type charge carriers.

HL 17.8 Mon 17:00 H18

Topological Edge States with Zero Hall Conductivity in a Dimerized Hofstadter Model — •Alexander Lau[1], Carmine Ortix[1,2], and Jeroen van den Brink[1,3] — [1]Institute for Theoretical Solid State Physics, IFW Dresden, Germany — [2]Institute for Theoretical Physics, Utrecht University, The Netherlands — [3]Department of Physics, TU Dresden, Germany

The Hofstadter model is one of the most celebrated models for the study of topological properties of matter and allows the study of the quantum Hall effect in a lattice system. Indeed, the Hofstadter Hamiltonian harbors the topological chiral edge states that are responsible for the quantized Hall conductivity.

Here, we show that a lattice dimerization in the Hofstadtermodel opens an energy gap at half-filling. What is more, we demonstrate that even if the ensuing insulator has a Chern number equal to zero, concomitantly a doublet of edge states appear that are pinned to specific momenta. We show that the presence of these states can be understood from the topological properties of lower dimensional cuts of the system, using a mapping of the Hofstadter Hamiltonian to a collection of one-dimensional Aubry-Andre-Harper (AAH) models. A sub-set of AAH chains in this collection preserve inversion symmetry. This guarantees the presence of topologically protected doublets of end modes to which the edge states are pinned. To explicitly prove the robustness of the emerging edge states, we define and calculate the topological invariant that protects them, which turns out to be an integer invariant for inversion-symmetric AAH models.

HL 17.9 Mon 17:15 H18

Disorder induced zero Landau level in topological insulator nanowires and its signature in conductance fluctuations — •Emmanouil Xypakis and Jens H Bardarson — Max-Planck-Institut f. Physik komplexer Systeme Noethnitzer Str. 38, 01187 Dresden, Germany

In this talk I will discuss the quantum transport properties of a disordered topological insulator in a strong magnetic field. The focus is on the case when the chemical potential is close to the Dirac point, where the transport is dominated by induced chiral modes. Disorder has a drastic role in the system electrical response by revealing a zero Landau level, which is absent for clean topological insulators. We study the dependence of the zero Landau level energy window on the system parameters, such as system size, disorder and magnetic field strength.

HL 17.10 Mon 17:30 H18

Time-resolved pure spin fractionalization and spin-charge separation in helical Luttinger liquid based devices — •Giacomo Dolcetto[1,2], Matteo Carrega[2], Alessio Calzona[2,3], and Maura Sassetti[2,3] — [1]Physics and Materials Science Research Unit, University of Luxembourg, Luxembourg — [2]SPIN-CNR, Genova, Italy — [3]Dipartimento di Fisica, Università di Genova, Italy

Helical Luttinger liquids, appearing at the edge of two-dimensional topological insulators, represent a new paradigm of one-dimensional systems, where peculiar quantum phenomena can be investigated [1]. Motivated by recent experiments on charge fractionalization [2], we propose a setup based on helical Luttinger liquids that allows one to time-resolve, in addition to charge fractionalization, also spin-charge separation and pure spin fractionalization. This is due to the combined presence of spin-momentum locking and interactions. We show that electric time-resolved measurements can reveal both charge and spin properties, avoiding the need of magnetic materials [3, 4]. Although challenging, the proposed setup could be achieved with present-day technologies, promoting helical liquids as interesting playgrounds to explore the effects of interactions in one dimension.

[1] G. Dolcetto, M. Sassetti, and T. L. Schmidt, arXiv preprint arXiv:1511.06141
[2] H. Kamata, N. Kumada, M. Hashisaka, K. Muraki, and T. Fujisawa, Nat. Nanotechnol. **9**, 177 (2014)
[3] A. Calzona, M. Carrega, G. Dolcetto, and M. Sassetti, Physica E **74**, 630 (2015)
[4] A. Calzona, M. Carrega, G. Dolcetto, and M. Sassetti, PRB **92**, 195414 (2015)

HL 18: Plasmonics and Nanooptics I: Microscopy

Time: Monday 15:00–18:00 Location: S054

Invited Talk HL 18.1 Mon 15:00 S054

Principles of plasmonic imaging — •Angela Demetriadou[1] and Alexei Kornyshev[2] — [1]Blackett Laboratory, Imperial College London, Prince Consort Road, SW7 2AZ, London, United Kingdom — [2]Department of Chemistry, Imperial College London, Prince Consort Road, SW7 2AZ, London, United Kingdom

Plasmonic imaging exploits the evanescent nature of propagating surface plasmon polariton (SPP) waves to produce real-time images of sub-wavelength objects with high-precision. It is commonly used in biological sciences to track and image organelles in cells, such as DNA, mitochondria and virus molecules. The fast dynamics of intra-cellular processes enforce to keep the cells under their native state (i.e. label-free) and to be imaged in real-time, establishing plasmonic imaging as a powerful tool for mapping and understanding cellular behaviour. Additionally, it has been widely used to map the electro-catalytic activity of single nanoparticles with high spatial resolution and sensitivity.

Our theoretical model describes the electromagnetic process that forms the plasmonic image, and accurately predicts the image properties for particles of any composition and size. The intensity and shape of the plasmonic image is dominated by the SPP-induced natural modes. Hence, through the theoretical model, spectroscopic information can be extracted from recorded plasmonic images, expanding the capabilities of current plasmonic imaging techniques.

HL 18.2 Mon 15:30 S054

Imaging the dynamics of plasmonic vortices — •Deirdre Kilbane[1], Anna-Katharina Mahro[1], Stefan Mathias[1], Grisha Spektor[2], Lior Gal[2], Meir Orenstein[2], Bettina Frank[3], Simon Ristock[3], Harald Giessen[3], Philip Kahl[4], Daniel Podbiel[4], Frank Meyer zu Heringdorf[4], and Martin Aeschlimann[1] — [1]Physics Department and Research Centre OPTIMAS, University of Kaiserslautern, Germany — [2]Department of Electrical Engineering, Technion, Haifa, Israel — [3]Fourth Physics Institute and Research Center SCoPE, University of Stuttgart, Germany — [4]Faculty of Physics and CENIDE, University of Duisburg-Essen, Germany

The formation of a plasmonic vortex (rotational flow around a phase singularity) can be achieved by selecting the spin of circularly polarized light, and the geometry of the illuminated metallic structure. We perform near-field imaging of the ultrafast dynamics of plasmonic vortices using time-resolved two photon photoemission electron microscopy (TR-PEEM). A broadband ultrashort pulse laser excites and probes surface plasmon polaritons (SPPs) with 100 as time step and 40 nm spatial resolution. Here we observe the sub-optical cycle spatiotemporal evolution of the dynamics in plasmonic Archimedes spirals (PAS) and plasmonic vortex lenses (PVL). These structures were fabricated by focused ion beam (FIB) milling into the surface of thin polycrystalline gold films and single crystalline, atomically flat gold flakes.

HL 18.3 Mon 15:45 S054

Improving the lateral near-field confinement in a nanofocusing SNOM — •Simon F. Becker[1], Martin Esmann[1], KyungWan Yoo[1,2], Petra Gross[1], Ralf Vogelgesang[1], NamkYoo Park[2], and Christoph Lienau[1] — [1]Carl von Ossietzky Universität, Oldenburg, Germany — [2]Seoul National University, Seoul, Korea

The lateral near-field confinement in apertureless scanning near-field optical microscopy (SNOM) experiments is typically governed by the tip radius of the probe used. Here, we discuss how to improve the confinement beyond this limitation using a nanofocusing SNOM taper.

We approach such a taper [1,2] to a thin, semitransparent gold film. Angle-resolved images of elastically scattered radiation transmitted through the film [3,4] show a steep increase in the detected signal over the last few nanometers. We compare the experimental results to finite element method simulations and find this steep increase to be a clear signature of gap plasmon formation in the gap between tip and sample. The lateral confinement of these fields is proportional to the geometric mean of tip-sample distance and tip radius. Hence, gap plasmons may enable decreasing the confinement to sizes typically found for interaction cross-sections of single quantum emitters. Combining this spectrally broadband effect with the background-free detection available with nanofocusing SNOM seems promising for nanospectroscopic investigations of dense and heterogeneous quantum emitter systems.

[1] M.I. Stockman, PRL 93, 137404 (2004); [2] S. Schmidt et al., ACS Nano 6, 6040 (2012); [3] M. Esmann et al., BJ Nano 4, 603 (2013); [4] S.F. Becker et al., (submitted).

HL 18.4 Mon 16:00 S054

Coherent broadband nano-spectroscopy through plasmonic nanofocusing — •M. Esmann[1], S.F. Becker[1], H. Kollmann[1], J. Witt[1], K.W. Yoo[1,2], A. Chimeh[1], P. Gross[1], R. Vogelgesang[1], N.K. Park[2], and C. Lienau[1] — [1]Carl von Ossietzky Universität, Oldenburg, Germany — [2]Seoul National University, Seoul, Korea

Plasmonic nanofocusing microscopy enables broadband coherent light scattering spectroscopy with 5 nm spatial resolution. This is used to image optical near-fields around individual metallic nanoparticles. Conceptually, surface plasmon polaritons are launched by a grating coupler on a conical metallic taper and propagate towards the taper apex where they are transformed into highly confined near-fields [1-3]. Upon optical interaction with a sample, far-fields scattered from the apex are collected almost background free. Here, we use coherent white light to excite this isolated, spectrally broadband nano-lightsource at the apex of a monocrystalline gold taper. We then investigate both the spectral and spatial characteristics of optical near-fields around chemically synthesized gold nanorods. We find dipolar plasmon resonances with comparatively high Q-factors of up to 15. These are confirmed by far-field measurements. We simultaneously also image the corresponding near-field pattern in the spatial domain and achieve spatial resolution down to 5 nm. As these measurements are fully coherent, they can be straightforwardly extended to the investigation of coherences in biological or semiconducting systems.

[1] M.I. Stockman, PRL 93, 137404 (2004); [2] S. Schmidt et al., ACS Nano 6, 6040 (2012); [3] M. Esmann et al., BJNANO 4, 603 (2013).

HL 18.5 Mon 16:15 S054

Probing and Controlling Electronic and Vibrational Coherences in Individual Carbon Nanotubes using Femtosecond Pulse Shaping Microscopy — •Veit Giegold[1,2], Richard Ciesielski[1,2], Nicolai F. Hartmann[3], Erik H. Haroz[3], Stephen K. Doorn[3], and Achim Hartschuh[1,2] — [1]Department Chemie and CeNS, LMU Munich, 81377 Munich — [2]Nanosystems Initiative Munich, 80799 Munich — [3]Los Alamos National Laboratory, New Mexico, 87545 United States

We probe and coherently manipulate the exciton population of individual semiconducting single-walled carbon nanotubes (SWCNTs) at room temperature using femtosecond laser pulse shaping microscopy [1,2]. In our experiment, the exciton state E_{11} of defect-doped (5,4)-SWCNTs is resonantly excited by a pair of phase-locked 20 fs laser pulses while the photoluminescence (PL) emission of the defect state E_{11}^D serves as reporter for the E_{11}-population. Tuning the pulse delay and relative carrier envelope phase results in damped PL intensity oscillations that can be described using the Bloch equations for a two-level system. We show that light absorption of individual SWCNTs can be controlled within their electronic dephasing time, ranging from 20 to 66 fs for different nanotubes. For longer pulse separations coherent radial breathing mode excitations with a period of 90 fs are observed.

[1] R. Hildner, D. Brinks, N.F. van Hulst, Nature Physics (2010).
[2] R. Ciesielski, V. Giegold, A. Hartschuh, et al., in prep.

HL 18.6 Mon 16:30 S054

Confocal active interference scattering microscopy: A new approach to characterize single gold nanoparticles — •Otto Hauler — Institute of Physical Chemistry — Tübingen — Germany

Gold nanoparticles and their applications have attracted considerable research interest in recent times. By using confocal interference microscopy in combination with cylindrical vector beams it is possible to directly image the orientation and to detect the shape of single metal nanoparticles, with sizes well beyond the diffraction limit [1-4]. We present a newly developed method to further investigate the properties of these promising materials, the confocal active interference scattering microscope. This novel technique allows the measurement of the phase of the elastically scattered light. It furthermore enables the control of the excitation polarization, through the use of radially- and azimuthally-polarized laser modes. [1] A.V. Failla, H. Qian, H. Qian, A. Hartschuh, A. J. Meixner, Nano Lett. (2006), 6: 1374. [2]

F. Wackenhut, A.V. Failla, A.J. Meixner, Phys. Chem. Chem. Phys. (2013),15: 5407-5414. [3] F. Wackenhut, A.V. Failla, A.J. Meixner, Anal Bioanal Chem (2015), 407: 4029-4034. [4] F. Wackenhut, A.V. Failla, T. Züchner, M. Steiner, A.J. Meixner, Appl. Phys. Lett. (2012), 100: 263102.

HL 18.7 Mon 16:45 S054

Polarization sensitive scanning near field optical microscope on polymer thin films — •Jens Brauer[1], Jinxin Zhan[1], Petra Gross[1], Christoph Lienau[1], Daniel Trefz[2], and Sabine Ludwigs[2] — [1]Carl von Ossietzky Universität, Oldenburg, Germany — [2]Institut für Polymerchemie, Stuttgart, Germany

Currently there is a high need to investigate the relationship between structure and functionality of novel, polymer-based organic solar cell materials. Specfically information about local fluctuations of their optical properties, largely affecting the charge carrier mobility is needed [1]. For this, an optical imaging method is required with a spatial resolution in the order of the domain size, typically a few nanometers, or even below.

Here we present a technique to use near field optical microscopy to fulfill these requirements. We use a Titanium:Sapphire laser focused through the sample onto a sharp gold tip and collect the scattered near-field signal from the tip in a backscattering geometry. By applying a modulation to the tip with tens of kilohertz and using a lock-in amplifier after detection to demodulate the signal at the n-th harmonic we can significantly increase the signal to noise ratio. Changing the direction of the linear laser polarization enables us to determine the molecular orientation with a resolution of about 10 nm. In this talk we present a first demonstration by applying the technique to ordered and unordered thin film polymer samples.

[1] Brinkmann, M. et al.; ACS Nano 6, pp 10319-10326 (2012)

HL 18.8 Mon 17:00 S054

Nanoscale probing of optical near-fields by ultrafast transmission electron microscopy — •Armin Feist, Katharina E. Echternkamp, Murat Sivis, Sascha Schäfer, and Claus Ropers — 4th Physical Institute, University of Göttingen, Göttingen, Germany

Ultrafast transmission electron microscopy (UTEM) allows for the study of structural and electronic dynamics on nanometer length scales [1], as well as for the local probing of optical near-fields [2].

Here, we employ the inelastic scattering of swift electrons to characterize optical near-fields in metallic nanostructures. The experiments utilize a novel short-pulsed electron gun driven by localized photoemission from a nanotip emitter, yielding electron probes with a pulse duration of 300 fs and beam diameters down to 1.5 nm.

In the interaction with optical near-fields, the energy spectra of free electrons develop into a comb of spectral sidebands representing the absorption and emission of multiple photons [2]. The quantum coherence of this process is evidenced by the observation of multilevel Rabi oscillations in the sideband populations [3]. The interaction facilitates few nanometer spatial resolution in near-field imaging, as demonstrated by raster-scanning the focused electron probe across resonantly excited plasmonic nanostructures with feature sizes down to 5 nm.

[1] A.H. Zewail, Science, **328**, 187 (2010).
[2] B. Barwick *et al.*, Nature, **462**, 902 (2009).
[3] A. Feist *et al.*, Nature, **521**, 200 (2015).

HL 18.9 Mon 17:15 S054

Coherent spectroscopy of single metallic nanostructures — •Martin Silies[1], Heiko Kollmann[1], Martin Esmann[1], Julia Witt[2], Gunther Wittstock[2], and Christoph Lienau[1] — [1]AG Ultraschnelle Nano-Optik, Institut für Physik, Carl von Ossietzky Universität Oldenburg, Germany — [2]AG Wittstock, Institut für Chemie, Carl von Ossietzky Universität Oldenburg, Germany

Metallic nanostructures exhibit strong optical resonances and enhanced optical near-fields, enabling the transfer of far-field radiation onto subwavelength scales. Even so, the mismatch of the optical absorption or scattering cross-section of a single nanostructure and the free space wavelength makes far-field spectroscopic investigations challenging. Further, single nanostructures with geometric dimensions of less than 50nm require highly sensitive and almost background-free spectroscopic methods. For this, modulation-based methods such as focus or Spatial Modulation Spectroscopy (SMS)[1] have been proven to be able to quantitatively measure the scattering and absorption cross section simultaneously [2]. Here, we present a combined approach of a commonly used confocal SMS setup and broadband VIS-IR Fourier Transform spectroscopy to measure the extinction cross section of single nanostructures in the time domain. We show polarization-resolved spectra of single chemically synthesized gold nanorods resonant in the near infrared. An extension of the approach to the study of hybrid nanostructures and to time-resolved phenomena is discussed.

[1] A. Arbouet et al., PRL 93, 127401 (2004)
[2] M. Husnik et al., PRL 109, 233902 (2012)

HL 18.10 Mon 17:30 S054

Plasmon-mediated circularly polarized luminescence of GaAs in a scanning tunneling microscope — Svenja Mühlenberend, Markus Gruyters, and •Richard Berndt — Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany

The electroluminescence from *p*-type GaAs(110) in a scanning tunneling microscope has been investigated at 6 K. Unexpectedly high degrees of circular polarization have often been observed with ferromagnetic Ni tips and also with paramagnetic W and Ag tips. The data is interpreted in terms of two distinct excitation mechanisms. Electron injection generates intense luminescence with low polarization. Plasmon-mediated generation of electron-hole pairs leads to less intense emission, which, however, is highly polarized for many tips.

HL 18.11 Mon 17:45 S054

Plasmonic Activation of Platinum Clusters for Photocatalytic Reactions Detected by STM — Sarah Wieghold[1], Lea Nienhaus[2,3], Marian D. Rötzer[1], Fabian Knoller[1], Florian F. Schweinberger[1], Joseph W. Lyding[2], Ulrich Heiz[1], Martin Grübele[2,3], and •Friedrich Esch[1] — [1]Chemistry Dept. and CRC, TU München, Lichtenbergstr. 4, 85748 Garching, Germany — [2]Beckman Institute, University of Illinois, Urbana — [3]Department of Chemistry, University of Illinois, Urbana, Illinois 61801

Their unique structural, optical and electronic properties make small metal clusters prime candidates for catalytic applications, especially under mild reaction conditions such as in photocatalysis. Due to their small cross sections for the interaction with light and due to low surface coverages, an indirect, support-mediated photoactivation mechanism is most efficient. We imaged this activation at the level of individual $Pt_{>35}$ clusters supported on a thin, structured gold film. The film shows a strong plasmonic interaction with visible light that is optimized to work in a back-illumination geometry. We used a scanning tunneling microscope to map the tunneling current modulation induced by light at 532 nm. When tunneling into unoccupied states of the film, we detect a light-induced current increase that is enhanced on the clusters. In this way, we image the plasmonic coupling of the clusters to the gold support with nanometer resolution. This activation leads indeed to an enhanced catalytic activity, as we demonstrate for the oxidative decomposition of methylene blue.

HL 19: Hybrid and Perovskite Photovoltaics I (Joint session of CPP, DS and HL, organized by CPP)

Time: Monday 15:00–17:30 Location: H38

HL 19.1 Mon 15:00 H38

Effect of phase transition on photoluminescence polarization of single perovskite nano-objects — •Daniela Täuber[1], Alexander Dobrovolsky[1], Rafael Camacho[1,2], and Ivan Scheblykin[1] — [1]Chemical Physics, Lund University, Lund, Sweden — [2]Department of Chemistry, University of Leuven, Leuven, Belgium

We use 2D polarization resolved microscopy to study the polarization of single $CH_3NH_3PbI_3$ perovskite nano-objects in excitation and emission at 295, 152 and 77 K. Depending on size and shape, polarization of up to 70% was observed at 77 K in emission, while it is in

general smaller in excitation, and it decreases with increasing temperature. For wire-shaped objects the polarization is along the long axis, which points to contributions from antenna effects and crystal growth direction in combination with asymmetric crystal structures. The difference seen in excitation and emission may be caused by the band structure and the excitation wavelength at 448 nm.

D.T. acknowledges a personal research grant DFG-TA 1049/1-1.

HL 19.2 Mon 15:15 H38

Energy Levels at Perovskite/Electron Transport Layer Interfaces — •Fengshuo Zu[1], Johannes Frisch[1], Liangsheng Liao[2], and Norbert Koch[1] — [1]Institut für Physik & IRIS Adlershof, Humboldt-Universität zu Berlin, Brook-Taylor-Str. 6, 12489 Berlin, Germany — [2]FUNSOM,Soochow University, Jiangsu 215123, China

organometal halide perovskites attract substantial attention for high-efficiency thin film solar cells. Numerous studies are focused on film processing and device configuration variation in order to further improve device efficiency, but the fundamental physics in particular regarding interfacial energy level alignment with charge transport materials (e.g., fullerene derivatives) are yet poorly understood. It is generally believed that perovskites form type-II p-n junctions with C60 or PCBM, which would favor the charge separation process at the interface. To substantiate this proposition, we performed TRPL and UPS measurements to investigate the interface energy levels and the charge separation process at perovskite/fullerene junctions. However, contrary to the common believe, our measurements show that both junctions exhibit n-n type-I level alignment. TRPL results show no different decay channels with or without fullerene layers, which indicates the perovskite/fullerene interface does not provide a driving force for charge separation. Nonetheless, our solar cells with PCBM junctions show reasonable performance, with a power conversion efficiency of 9.30%. In constrast, the perovskite/C60 solar cells show much lower efficiency, which we attribute to upward band bending within perovskite when in contact with C60.

HL 19.3 Mon 15:30 H38

The influence of hole transporting materials on the charge transport in stacked perovskite-based systems — •Kathrin Bader[1,2], Michiel Petrus[1,2], Thomas Bein[1,2], Pablo Docampo[1,2], Matthias Handloser[1,2], and Achim Hartschuh[1,2] — [1]Department of Chemistry and CeNS, LMU Munich — [2]Nanosystems Initiative Munich (NIM)

Hybrid metal halide perovskites have become a focal point of the photovoltaic community as promising candidates for next-generation solar cells. Extremely fast progress in this field has taken efficiencies to over 20 % [1] and lead to the development of a large variety of material compositions, preparation techniques and device structures [2]. Although the fabrication of the perovskite absorber itself is comparably cheap, latest device architectures incorporate the expensive hole transporting material (HTM) spiro-OMeTAD. To reduce the overall production costs for perovskite-based devices alternative organic HTMs have been developed [3]. Here we use a contact-less technique based on time-resolved laser scanning confocal microscopy [4] to visualize the influence of different HTMs on $CH_3NH_3PbI_3$ thin films. We investigate charge carrier transport properties and photoluminescence lifetimes of individual HTM layers as well as stacked perovskite/HTM systems and identify potential candidates to replace the expensive spiro-OMeTAD in the device structure. [1] Green, M. A. et al., Prog. Photovolt: Res. Appl. 2015, 23, 805-812. [2] Green, M. A. et al., Nature Photon. 2014, 8, 506-514. [3] Petrus, M. L. et al., J. Mater. Chem. A 2015, 3, 12159-12162. [4] Bader, K. et al., ACS Photonics 2015, under review.

HL 19.4 Mon 15:45 H38

Substrate-dependent electronic structure and film formation of MAPbI3 perovskites — •Selina Olthof and Klaus Meerholz — University of Cologne, Institute for Physical Chemistry, Luxemburger Straße 116, 50939 Köln, Germany

Hybrid organic / inorganic perovskite materials have attracted significant attention in the past years. However, little is known so far about the electronic structure and, more importantly, the energetic alignment at interfaces. Here, we present the investigation of the interface formation between the perovskite MAPbI3 and various substrate materials. The perovskite films are incrementally evaporated in situ while the electronic structure is evaluated using photoelectron spectroscopy (PES). The results show a deviation from the commonly assumed flat band condition, and that dipole formation and band bending dominate the interfaces. More importantly, we find a deviation from the expected perovskite stoichiometry at the interface due to a wide variety of chemical interaction taking place, which are highly dependent on the nature of the substrate material. On metal oxides the perovskite film formation is hindered and it takes up to 30 nm for the density of states of perovskite to emerge in the PES measurements. Therefore, the nature of the substrate not only changes the energetic alignment of the perovskite, but can hinder film formation and introduce gap states as well.

HL 19.5 Mon 16:00 H38

In-Situ Investigation of Optoelectronic Properties during One-Step Synthesis of $MAPbI_{3-x}Cl_x$ Perovskite — •Klara Suchan, Justus Just, Martin Kärgell, Dan R. Wargulski, Pascal Becker, and Thomas Unold — Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

Organometal halide perovskites have emerged as promising absorber materials for solid state solar cells since 2012. With the fast improvement in power conversion efficiency to over 20 %, perovskites have high prospects for low-cost, high efficiency solar cell production. $CH_3NH_3PbI_{3-x}Cl_x$ layers are prepared by a one-step solution based process using $PbCl_2$ and MAI precursors dissolved in DMF. Since solution based processes do not need cost intensive vacuum technology and no high-temperature annealing steps, they yield high potential for industrial implementation. However, little is known about the exact mechanisms during synthesis, leading to poor reproducibility. Employing in-situ photoluminescence and reflection imaging as well as spectroscopy we monitor the growth process. The evolution of optoelectronic properties for various temperature profiles and annealing durations is analysed. Additional X-ray diffraction measurements during various stages of the process are used to evaluate structural changes occurring during film formation.

HL 19.6 Mon 16:15 H38

Reversible Laser induced Amplified Spontaneous Emission from Coexisting Tetragonal and Orthorhombic Phases in Hybrid Lead Halide Perovskites — •Fabian Panzer[1,2,3], Sebastian Baderschneider[2,4], Tanaji Gujar[5], Thomas Unger[1,2], Heinz Bässler[2], Ralf Moos[3], Mukundan Thelakkat[5], Richard Hildner[2,4], and Anna Köhler[1,2] — [1]Experimental Physics II — [2]Bayreuth Institute of Macromolecular Research (BIMF) — [3]Department of Functional Materials — [4]Experimental Physics IV — [5]Applied Functional Polymers, Macromolecular Chemistry I, University of Bayreuth, 95440 Bayreuth, Germany

Organic-inorganic mixed halide perovskites received enormous attention over the last few years due to their outstanding performances when used as absorber material in solar cells or in light emitting devices, while offering the possibility for low cost production, e.g. by solution-processing. Furthermore it is known that most halide perovskite materials can exist in different crystal structures, depending on environmental conditions such as temperature. Here we show that a coexistence of tetragonal and orthorhombic phases within the same crystalline grain can be optically induced into the halide perovskite $CH_3NH_3PbI_3$ at low temperatures, leading to amplified spontaneous emission simultaneously at two distinct wavelengths. The emission feature associated with the tetragonal phase can be reproducibly written, read-out, and erased at 5 K by choosing appropriate laser fluences or raising the temperature. Finally we show to which extend our findings can be exploited for use as an all optical data storage device.

15 min. break

HL 19.7 Mon 16:45 H38

Iodine Migration and its Effect on Hysteresis in Perovskite Solar Cells — Cheng Li[1], Steffen Tscheuscher[2], Fabian Paulus[3], Paul Hopkinson[3], Johannes Kiessling[1], Anna Köhler[2], Yana Vaynzof[3], and •Sven Hüttner[1] — [1]Organic and Hybrid Electronics, Makromol. Chemie I, Universität Bayreuth — [2]Experimentalphysik II, Universität Bayreuth — [3]Centre for Advanced Materials, Universität Heidelberg

Solution-processed organic-inorganic hybrid perovskite solar cells (e.g. $CH_3NH_3PbI_3-xCl_x$) currently exhibit promising performances. However, the origin of the observed hysteresis in the current-voltage (J-V) curves, i.e. the sweeping-history-dependent electrical current, is still not sufficiently understood. To investigate its origin we employ electroabsorption (EA) spectroscopy to explore the built-in potential in

working photovoltaic devices. Furthermore, we study the temperature dependent dynamic processes in perovskite solar cells by characterizing their current-voltage behavior at different temperatures. The electrical current relaxation process during temperature dependent J-V measurements provides the evidence of the migration of ions. In order to investigate the nature of these ions, we further present X-ray photoemission spectroscopy (XPS) experiments which shows the elemental redistribution after applying an electrical bias. The results give a concise picture that mainly iodide ions can be driven by an external electrical field and then accumulate at the respective perovskite/electrode interfaces. The migration and accumulation of iodide ions create a modulation of the respective interfacial barriers which is the origin of the hysteresis.

HL 19.8 Mon 17:00 H38

The Importance of Hydrogen Defect Migration in Organic-Inorganic Perovskites — •David A. Egger[1], Leeor Kronik[1], and Andrew M. Rappe[2] — [1]Department of Materials and Interfaces, Weizmann Institute of Science, Rehovoth 76100, Israel — [2]The Makineni Theoretical Laboratories, Department of Chemistry, University of Pennsylvania, Philadelphia, PA 19104-6323, USA

Solar cells based on organic-inorganic perovskites have been proven to be remarkably efficient in recent years. However, they exhibit hysteresis in the current-voltage curves, and their stability properties, especially in the presence of water, are problematic. Both issues are possibly related to ionic diffusion phenomena occurring in the hybrid perovskite material. Using first-principles calculations based on density functional theory, we study the properties of an important defect in hybrid perovskites - interstitial hydrogen.[1] We show that differently charged defects occupy different sites in the hybrid perovskite crystal, which allows for an ionization-enhanced defect migration following the Bourgoin-Corbett mechanism. Our analysis further highlights the structural flexibility of organic-inorganic perovskites, where successive displacements of iodide combined with hydrogen bonding enables proton diffusion with low migration barriers. These findings indicate that hydrogen species can be highly mobile in hybrid perovskite solar cells and thus relevant for their performance.

[1] Angew. Chem. Int. Ed. 54, 12437 (2015)

HL 19.9 Mon 17:15 H38

Humidity-induced hydration of methylammonium lead iodide perovskite: Understanding and prevention — •Yinghong Hu[1], Pablo Docampo[1], Aurélien Leguy[2], and Piers Barnes[2] — [1]Department of Chemistry, Ludwig-Maximilians-Universität, 81377 München, Germany — [2]Physics Department, Imperial College, London, SW7 2AZ, United Kingdom

The long-term stability of hybrid metal halide perovskite solar cells is of paramount importance for the future of this emerging technology. In particular, solar cells composed of methylammonium lead iodide (MAPI) are notorious for their sensitivity to moisture. Here, we elucidate the humidity-induced degradation mechanisms occurring within the perovskite material and report on the development of a novel interlayer which improves the moisture stability of perovskite solar cells. Our results show that MAPI undergoes a stepwise transformation into two species of hydrated MAPI crystal phases upon exposure to moist air at room temperature. However, we show that this hydration process can be reversed when the material is subsequently dried in nitrogen. In contrast to water vapor, the presence of liquid water directly leads to the irreversible decomposition of MAPI to form lead iodide. Our developed functional moisture barrier significantly enhances the stability of the perovskite solar cells towards cycles of hydration and dehydration. We believe that our results open new possibilities for the design of moisture resistant, highly efficient perovskite solar cells.

HL 20: Frontiers of Electronic Structure Theory: Focus on Topology and Transport

Time: Monday 15:45–17:45 Location: H51

HL 20.1 Mon 15:45 H51

Mechanism of Li intercalation/deintercalation into/from the surface of $LiCoO_2$ — •Ashkan Moradabadi and Payam Kaghazchi — Institut für Chemie und Biochemie, Freie Universität Berlin, Takustr. 3, 14195 Berlin, Germany

$LiCoO_2$ is the most commonly used cathode material in Li-ion batteries. In this work, we have investigated atomic and electronic structures, magnetic properties, formation energies, and energy barriers for the diffusion of Li in single vacancies, divacancies, and missing rows in bulk and surface of $LiCoO_2$. Our GGA-PBE results indicate that there is almost no energy barrier for the Li-ion deintercalation from the surface layer. Energy barrier for the Li-ion intercalation is also very small. However, we find that Li hopping in PBE+U is accompanied by electron hopping between nearby transition metal ions. Therefore a PBE+U barrier, which is for both Li hopping and charge hopping, is higher than the corresponding PBE barrier [1]. This study has implications in understanding the role of the surface in the rate capability of nanostructured $LiCoO_2$ cathodes of Li-ion batteries.

[1] Ashkan Moradabadi and Payam Kaghazchi, Mechanism of Li intercalation/deintercalation into/from the surface of $LiCoO_2$, Phys. Chem. Chem. Phys., 2015, 17, 22917-22922.

HL 20.2 Mon 16:00 H51

Potential-dependent mechanism of Li diffusion in Li_2S — •Ashkan Moradabadi[1,2] and Payam Kaghazchi[1] — [1]Institut für Chemie und Biochemie, Freie Universität Berlin, Takustr. 3, 14195 Berlin, Germany — [2]Institut für Materialwissenschaft, Fachgebiet Materialmodellierung, Technische Universitat Darmstadt, Jovanka-Bontschits-Str. 2, 64287 Darmstadt, Germany

Li-S batteries are promising candidates for large-scale applications such as electrical vehicles. However, the measured discharge capacity is often less than the theoretical one [1,2]. This is mainly due to the slow diffusion of Li through Li_2S shells formed on S_8 cores, which leads to an incomplete conversion of S_8 cores to Li_2S (the final product of lithiation of S_8). In the present work, using density functional calculation, we have investigated mechanism of Li diffusion in Li_2S. At low cell voltages (< 0.93 V), Li diffusion occurs via an exchange mechanism with a high energy barrier of 0.45 eV. However at higher cell voltages, Li diffusion takes place via a vacancy mechanism with a lower energy barrier of 0.27 eV. Our findings can explain the capacity fading in Li-S batteries at high operation rates.

[1] Liang, X.; Hart, C.; Pang, Q.; Garsuch, A.; Weiss, T.; Nazar, L. F.; A highly efficient polysulfide mediator for lithium-sulfur batteries. Nature Communications, 2015, 6, 5682.

[2] Wang, L.; Wang, Y.; Xia, Y.; A high performance lithium-ion sulfur battery based on a Li_2S cathode using a dual-phase electrolyte. Energy Environ. Sci. 2015, 8, 1551.

HL 20.3 Mon 16:15 H51

Extremely high magnetoresistance in topological insulator candidate LaBi — •Nitesh Kumar, Chandra Shekhar, and Claudia Felser — Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany.

Lanthanum monopnictides (LaX, X=N, P, As, Sb, Bi) have recently been predicted to be topological insulators, except LaN which is a topological semimetal. Inspired from this report we have studied the transport properties of LaBi. It has a simple rock salt-type structure with alternate La and Bi atoms arranged in all three directions. Temperature variation of resistivity at different magnetic fields follows Kohler's rule. Resistivity follows almost a parabolic relation with magnetic field without saturation, exhibiting a huge magnetoresistance (1.5×10^5% at 2 K and 9 T). By employing two band model we calculate carrier density and mobility of electrons and holes which suggests that LaBi is a compensated system. We believe this to be responsible for high unsaturated MR in LaBi. We observe excellent Shubnikov-de Haas (SdH) oscillations starting from around 3T. We also analyse the angle and temperature dependence of these oscillations.

HL 20.4 Mon 16:30 H51

VOTCA-STP - Multi Scale Modeling of Spin Transport in Organic Semiconductors — •Erik R. McNellis, Shayan Hematiyan, Amaury Melo Souza, Sebastian Müller, and Jairo Sinova — Johannes Gutenberg University, Mainz, Germany

Organic molecules present a range of unique and highly attractive properties in solid state technology applications. So also in spintronics, where the weak but highly tailorable spin-orbit coupling in light elements offers spin lifetimes of unparalleled length and controllability.

1st-principles theoretical modeling stands to provide a crucial perspective on the emerging field of spin transport in organic semiconductors. Comprehensive modeling of relevant systems is challenging, with several of the spin transport mechanisms in traditional solid state materials non-existent or strongly modified in organics.

We are developing a multi-scale modeling framework for spin transport in bulk organic materials, based on the VOTCA toolkit for charge transport in the same. The core component is a semi-classical kinetic Monte-Carlo model, with input parameters calculated using 1st-principles theory.

The scope, capabilities of and particular challenges for this development will be presented along with possible extensions to e.g. 'spinterfaces', where spin currents are manipulated by tailoring of an inorganic / organic solid interface, as well as a perspective on the potential ramifications for experimental work in the field.

15 min. coffee break

HL 20.5 Mon 17:00 H51

High-pressure and nonlinear elastic response of solids: Example of carbon allotropes — •Pasquale Pavone, Rostam Golesorkhtabar, Stefan Kontur, and Claudia Draxl — Humboldt-Universität zu Berlin, Physics Department and IRIS Adlershof, 12489 Berlin, Germany

As prototype materials showing strong nonlinear elastic behaviour, diamond and, more recently, layered carbon allotropes have attracted much attention. However, even the nonlinear elasticity of diamond is not completely clarified: Experimentally, nonlinear elastic constants of diamond were investigated only recently [1], showing significant discrepancies with theoretical results. Furthermore, the standard ab-initio reference calculation for diamond [2] is nowadays about 30 years old and needs to be updated in the light of current development of theory, numerical algorithms, and available computer power. Using the full-potential all-electron package `exciting` [3], we perform a systematic ab-initio investigation of the nonlinear elastic properties of diamond, graphene monolayers, as well as simple-hexagonal and hexagonal graphite. We develope an extension of the `ElaStic` tool [4] for the determination of third-order elastic constants. From these results the pressure dependence of linear elastic constants is obtained and connected to dynamical quantities like the mode Grüneisen parameters.

[1] J.M. Lang *et al.*, Phys. Rev. Lett. **106**, 125502 (2011).
[2] O.H. Nielsen, Phys. Rev. B **34**, 5808 (1986).
[3] A. Gulans *et al.*, J. Phys.: Condens. Matter **26**, 363202 (2014).
[4] R. Golesorkhtabar *et al.*, Comp. Phys. Commun. **184**, 1861 (2013).

HL 20.6 Mon 17:15 H51

Calculations of temperature dependent resistivity for transition metals from the first principles — •David Wagenknecht[1,2], Ilja Turek[1,2], and Karel Carva[1] — [1]Department of Condensed Matter Physics, Faculty of Mathematics and Physics, Charles University in Prague; Ke Karlovu 3, 12116 Prague 2, Czech Republic — [2]Institute of Physics of Materials, Academy of Sciences of the Czech Republic; Žižkova 22, 61662 Brno, Czech Republic

The temperature dependence of electrical resistivity is studied from the first principles. Properties of late transition metals have been calculated using the linear muffin-tin orbital (LMTO) method with the coherent potential approximation (CPA). The influence of non-zero temperature has been described by a frozen lattice disorder – atoms were moved from the positions on an ideal lattice and different temperatures are then given by the magnitudes of the random displacement vectors. Dependence of the physical quantities on the parameters of the displacements (like random and non-random directions of the displacement vectors) has been observed and taken into account during discussion of the results. Special attention has been paid to an influence of spin-orbit interaction on the final resistivity, as well as to comparison with other *ab initio* calculations and experimental data; the obtained results agree reasonably well with those of other authors. Derived analytical modifications of the LMTO potential functions and the numerical codes can be now used to calculate relevant physical properties of different materials.

HL 20.7 Mon 17:30 H51

Ab Initio Molecular Dynamics Study of Conjugated Polymer Systems: The Elusive Localization of the Polaron — •Håkan W. Hugosson[1], Amina Mirsakiyeva[1], and Anna Delin[1,2] — [1]Department of Materials och Nano Physics, KTH Royal Institute of Technology, Stockholm, Sweden. — [2]Ångstrom Laboratory, Uppsala University, Uppsala, Sweden.

The thermoelectric conjugated polymer poly(3,4-ethylenedioxythiophene), or PEDOT, contains a carbon backbone consisting of alternating short and long carbon bonds. Therefore there are two isomeric states: aromatic and quinoid. Charge injection or the presence of charged doping agents leads to the formation of localized charge in the conjugated polymer - a so-called polaron. This polaron induces a localized structural distortion (a shift from the aromatic form towards the quinoid) in the conjugated carbon backbone.

Self-localized polarons in conjugated carbon systems have been found using semi-empirical or HF-theory, but formerly never using DFT with local or gradient corrected functionals (e.g. LDA/BLYP). Self-localization has been seen using DFT and long range hybrid functionals with partial exact exchange included.

Using modern ab initio molecular dynamics methods based on DFT we have studied PEDOT and its charge carrying polarons. A localized polaron is now found when studying the time-averaged changes in bond-distances and also in snap-shots for the frontier orbitals for long oligomers (12 monomers).

HL 21: Graphene: Fabrication (Joint session of DS, HL and TT, organized by HL)

Time: Monday 17:45–18:45 Location: H17

HL 21.1 Mon 17:45 H17

Growth and characterization of mono- and bilayer graphene nanoribbons grown on SiC(0001) — •Lauren Aranha Galves, Joseph Wofford, Uwe Jahn, João Marcelo J. Lopes, and Henning Riechert — Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5-7, 10117 Berlin, Germany

Graphene Nanoribbons (GNRs) are promising for applications in nanoelectronics due to their unique properties. Unlike graphene sheets, GNRs possess a bandgap and the gap is inversely proportional to their width [1]. Additionally, bilayer GNRs offer the possibility to further tune their bandgap via the application of an external electric field [2]. The thermal decomposition of SiC surfaces is a suitable synthesis method for GNRs due to the control it offers over their size [3].

In this report we present the structural characterization of mono- and bilayer GNRs grown on SiC(0001) by surface graphitization. Bilayer GNRs were obtained via a post-growth air-annealing process [4]. The width of the ribbons were determined via atomic force microscopy (AFM) height and phase imaging as well as scanning electron microscopy (SEM), while the number of layers (i.e. mono or bilayer GNRs) were examined by Raman spectroscopy. Based on these measurements it was possible to identify an activation energy for the formation of the nanostructures and a lateral etching effect in the bilayer GNRs due to the air-annealing process.

[1] Barone et al., Nano Lett. 6, 2748 (2006); [2] Li et al., Eur. Phys. J. 64, 73 (2008); [3] Sprinkle et al. Nat. Nanotechnol. 5, 727 (2010); [4] Oliveira Jr. et al., Nat. Comm. 6, 7632 (2015).

HL 21.2 Mon 18:00 H17

Optoelectronic Properties of Graphene Nano-Ribbons Patterned By Helium Ion Beam Lithography — •Akshay Kumar Mahadev Arabhavi[1], Andreas Brenneis[1,2], Simon Drieschner[1,2], Marcus Altzschner[1], Helmut Karl[3], Jose Garrido[1,2], and Alexander Holleitner[1,2] — [1]Walter Schottky Institut and Physics-Department, Technical University Munich, Am Coulombwall 4a, 85748 Garching, Germany. — [2]Nanosystems Initiative Munich (NIM), Schellingstr. 4, 80799 Munich, Germany. — [3]Institute of Physics, University of Augsburg, 86135 Augsburg, Germany.

High electron mobility, excellent thermal conductivity and uniform absorption in the visible range makes graphene an outstanding material for high-frequency optoelectronic applications. However, the lack of

a band gap limits graphene in switching applications. A quantization energy can be introduced by confining graphene to one-dimensional ribbons of widths below 20 nm, for instance, using Helium Ion Beam Lithography (HIBL) [1-2]. We have optimized the parameters to pattern graphene nano-ribbons on sapphire substrates using HIBL, such as dose, beam current, spot control and dwell time. Moreover, we apply an ultrafast photocurrent spectroscopy [3] to investigate the optoelectronic properties of the patterned graphene nano-ribbons with respect to their high-frequency properties. References: [1] M. Han et al., Phys. Rev. Lett. 98, 206805, (2007). [2] Bell DC et al., Nanotechnology 20, 455301, (2009). [3] A. Brenneis, et al., Nature Nanotech, 10, 135, (2015).

HL 21.3 Mon 18:15 H17

High quality bilayer graphene from chemical vapor deposition on reusable copper — •Michael Schmitz[1], Stephan Engels[1,2], Luca Banszerus[1], Kenji Watanabe[3], Takashi Taniguchi[3], Bernd Beschoten[1], and Christoph Stampfer[1,2] — [1]JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, 52074 Aachen, Germany — [2]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany — [3]National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan

We recently introduced a dry transfer method for single-layer graphene grown by chemical vapor deposition (CVD) yielding ultra high quality graphene comparable to the best exfoliated samples [1]. Here, we demonstrate that this method can be extended to bilayer graphene. In particular, we show the fabrication and characterization of bilayer graphene/hexagonal boron nitride heterostructures using high quality CVD bilayer graphene grown on reusable copper foils. Raman measurements reveal a high structural quality [2]. We achieve carrier mobilities up to 45,000 $cm^2/(Vs)$ at 1.8 K and up to 17,000 $cm^2/(Vs)$ at room temperature outperforming all state-of-the-art CVD bilayer graphene devices. Finally, we show dual-gated transport measurements to investigate band-gap opening in our CVD grown bilayer graphene.

[1] L. Banszerus, M. Schmitz, S. Engels *et al.*, Science Advances **1**, e1500222 (2015)
[2] C. Neumann, S. Reichardt, P. Venezuela *et al.*, Nature Communications **6**, 8429 (2015)

HL 21.4 Mon 18:30 H17

Graphene-based fast hot-electron bolometer with bandwidth from THz to VIS — Martin Mittendorff[1,2], Josef Kamann[3], Jonathan Eroms[3], Dieter Weiss[3], Christoph Drexler[3], Sergey D. Ganichev[3], Jochen Kerbusch[2], Artur Erbe[2], Ryan J. Suess[1], Thomas E. Murphy[1], Jacob C. König-Otto[2,4], Harald Schneider[2], Manfred Helm[2,4], and •Stephan Winnerl[2] — [1]University of Maryland, College Park, USA — [2]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [3]Universität Regensburg, Regensburg, Germany — [4]Technische Universität Dresden, Dresden, Germany

We present a fast detector (rise time 40 ps) operating at room temperature that is capable to detect radiation from the THz to visible spectral range (demonstrated wavelengths 500 μm - 780 nm) [1]. The detector consists of a CVD-grown graphene flake contacted by a broadband logarithmic periodic antenna. SiC acts as a substrate material that does not interfere with the detection mechanism in the desired frequency range, even within the Reststrahlen band of SiC (6 - 12 μm). The detector is ideal for timing purposes. Near infrared (mid- and far infrared) pulse energies of the order of 10 pJ (1 nJ) are sufficient to obtain good signal-to-noise ratios. We suggest that the bandwidth is limited by the antenna dimensions (typically several mm) on the long wavelength side and by the bandgap of SiC (380 nm) on the short wavelength side.

[1] M. Mittendorff et al., Opt. Express 23, 28728 (2015).

HL 22: Ultrafast Phenomena I (Joint session of HL and O, organized by HL)

Time: Tuesday 9:30–13:15 Location: H10

HL 22.1 Tue 9:30 H10

Sub-cycle quantum interference in solid-state high-harmonic generation — •Matthias Hohenleutner[1], Fabian Langer[1], Olaf Schubert[1], Matthias Knorr[1], Christoph Lange[1], Ulrich Huttner[2], Stephan W. Koch[2], Mackillo Kira[2], and Rupert Huber[1] — [1]University of Regensburg, 93040 Regensburg, Germany — [2]University of Marburg, 35032 Marburg, Germany

Utilizing intense light pulses to control electron motion in atoms and molecules has opened up spectacular new routes in ultrafast and attosecond photonics such as high-harmonic generation (HHG). The recent discovery of HHG in solids combines ultrafast quantum control with complex condensed matter systems. We employ intense, phase-controlled multi-THz waveforms to drive HHG in bulk gallium selenide. Non-resonantly driven interband polarization and simultaneous intraband carrier acceleration throughout the entire Brillouin zone result in the emission of extremely broadband, phase-locked high-harmonics (HH). More importantly yet, sub-cycle time- and field-resolution allows us to directly trace the underlying electron dynamics with precise temporal correlation to the driving waveform. Remarkably, the HH are emitted as a unipolar train of ultrashort, nearly unchirped few-femtosecond bursts, which coincide precisely with the driving field maxima. These features unravel a novel quantum interference of multiple interband excitation paths during HHG, as explained by our microscopic quantum theory. The first direct time domain study of HH from solids paves the way towards a full quantum picture of the underlying mechanisms and sparks hope for solid-state sub-femtosecond sources.

HL 22.2 Tue 9:45 H10

Lattice dynamics of optically excited few-layer graphite — Christian Gerbig, Silvio Morgenstern, Marlene Adrian, Cristian Sarpe, •Arne Senftleben, and Thomas Baumert — Institut für Physik und CINSaT, Universität Kassel, Heinrich-Plett-Straße 40, 34132 Kassel

Time-resolved diffraction with femtosecond electron pulses has become a promising technique to directly provide insights into photo induced primary dynamics at the atomic level in molecules and solids. Ultrashort pulse duration as well as extensive spatial coherence are desired, however, space charge effects complicate the bunching of multiple electrons in a single pulse. We experimentally investigate the interplay between spatial and temporal aspects of resolution limits in ultrafast electron diffraction (UED) on our highly compact transmission electron diffractometer. To that end, the initial source size and charge density of electron bunches are systematically manipulated and the resulting bunch properties at the sample position are fully characterized in terms of lateral coherence, temporal width and diffracted intensity. We obtain electron pulse durations down to 120 fs and transversal coherence lengths up to 20 nm. Instrumental impacts on the effective signal yield in diffraction and electron pulse brightness are discussed as well. The performance of our compact UED setup at selected electron pulse conditions is finally demonstrated in a time-resolved study of lattice heating in few-layer graphite after optical excitation. During the heating process, we observe shearing modes and acoustic breathing modes.

HL 22.3 Tue 10:00 H10

Ultrafast carrier dynamics in bulk MoS_2 studied by transient absorption spectroscopy — •Tim Völzer, Matthias Lütgens, Franziska Fennel, and Stefan Lochbrunner — Institut für Physik, Universität Rostock, Albert-Einstein-Str. 23, 18059 Rostock

Transistion metal dichalcogenides feature unique electronic and optical properties. In addition, they are characterised by a layered structure, allowing the preparation of atomically thin crystals. As a representative of those materials, molybdenum disulfide is suggested as a promising candidate for optoelectronic and photocatalytic applications. To characterise the optical excitation and its dynamics we performed both static transmission and time-resolved pump-probe spectroscopy.

Two absorption bands, labelled A and B, are observed in the static absorption spectrum which are attributed to direct transitions at the K point of the Brillouin zone. The lower electronic transition is excited within the femtosecond absorption measurements and the dynamics is followed by a white light continuum covering the whole visible range. A decrease of absorption for the A and B transition is observed whereas

an increase of absorption is present for lower energies. This signature is indicative for a band renormalization induced by the population in the first excited band. The subsequent signal decay shows two distinct time dependencies, an exponential sub picosecond contribution caused by carrier-carrier and carrier-phonon scattering and a strongly non-exponential component for longer times. The latter is attributed to electron-hole recombination via defect states and shows an acceleration with increasing excitation density.

HL 22.4 Tue 10:15 H10

Internal structure and ultrafast dynamics of excitons in monolayer WSe_2 — •Christoph Pöllmann[1], Philipp Steinleitner[1], Ursula Leierseder[1], Philipp Nagler[1], Gerd Plechinger[1], Michael Porer[1], Rudolph Bratschitsch[2], Christian Schüller[1], Tobias Korn[1], and Rupert Huber[1] — [1]Department of Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Institute of Physics, University of Münster, 48149 Münster, Germany

Atomically thin transition metal dichalcogenides (TMDCs) promise groundbreaking optoelectronic applications and devices due to their direct bandgap in the optical range. As a consequence of the layered structure, unusually strongly bound excitons can exist even at room temperature, dominating the optical and electronical properties. In order to exploit the full potential of this new material system, key open questions regarding the excitons in TMDC monolayers have to be answered. Here we report the first direct observation of the intraexcitonic 1s-2p transition via time resolved pump/THz probe studies, tracing both optically bright and dark exciton states. Beside quantitative information about transition energies, oscillator strengths, linewidths and many-body effects a record fast radiative decay of bright excitons with a time constant of only 150 fs can be revealed.

HL 22.5 Tue 10:30 H10

Auger Recombination and Charge Transfer of CdSe/CdS Core/Shell Quantum Dot/Quantum Rods — •Mona Rafipoor[1,2], Jan Niehaus[3], Holger Lange[1,2], and Horst Weller[1,2,3] — [1]Universität Hamburg, Institut für Physikalische Chemie, Grindelallee 117, 20146 Hamburg — [2]The Hamburg Centre for Ultrafast Imaging, Luruper Chaussee 149, 22761 Hamburg, Germany — [3]CAN GmbH Grindelallee 117 20146 Hamburg

We investigated clustered CdSe/CdS quantum dots/quantum rods (QDQRs) by time-resolved optical spectroscopy.

Power dependent measurements were conducted by excitation with different intensities and recording time traces of the photoluminescence (PL) decay simultaneously with the PL intensity. Increasing the excitation power generally increases the average exciton population per QDQR. We observe signatures of exciton-exciton interactions starting with exciton populations of one. This is tentatively assigned to an interaction between the excitons across the QDQRs. The non-monotonic increase of the PL intensity with excitation power in this regime supports the idea of a new, non-radiative multiexciton decay across the cluster.

To get more Information about this kind of interaction we apply Transient Absorption spectroscopy. By varying the pump wavelength, we are able to specifically excite core and shell and follow the subsequent relaxation.

HL 22.6 Tue 10:45 H10

The role of intervalley scattering and phonon softening in the ultrafast carrier dynamics of PbTe — Prashant Padmanabhan, Kestutis Budzinauskas, Kiran H. Prabhakara, and •Paul H. M. van Loosdrecht — Physics Institute 2, University of Cologne, 50937 Cologne, Germany

PbTe is a leading thermoelectric material, notable for its low thermal conductivity and unusually large carrier mobility at very low doping levels. Here, we report on ultrafast pump-probe experiments on PbTe that shed light on the ultrafast relaxation of highly excited carriers. By employing time-resolved differential reflectivity measurements, we probe the dynamics of electron-electron and electron-phonon interactions on the femtosecond time-scale. Additionally, the use of a super-continuum probe pulse allows us to investigate the wavelength dependence of the carrier relaxation dynamics. Our results suggest that phonon mediated intervalley scattering involving the band gap between the Γ and K points plays a significant role in carrier cooling. Further, the temperature dependence of these dynamics point to anomalous behavior that may be the result of phonon softening, recently reported to be a key element in the unique thermal properties of PbTe.

HL 22.7 Tue 11:00 H10

Theory of the coherent A_{1g} phonon decay in antimony — •Sergej Krylow, Eeuwe S. Zijlstra, and Martin E. Garcia — Universität Kassel, Theoretische Physik II, Heinrich-Plett-Straße 40, 34132 Kassel,Germany

The fluence-dependent decay paths of the femtosecond laser-excited coherent A_{1g} phonon mode in antimony are investigated by means of electronic-temperature-dependent density-functional-theory molecular-dynamics simulations, which yield an exponentially decaying coherent phonon, comparable to experiments. Additional calculations of the phonon dispersion indicate that third order decay processes occur mainly within the acoustic and fourth order processes within the optical phonon branches. This can also be seen in the subsequent analysis of the molecular dynamics simulations, which reveal that the third and fourth order phonon contributions to the decay can be influenced by means of the applied fluence.

30 min. Coffee Break

Invited Talk HL 22.8 Tue 11:45 H10

Coherent Quantum Dynamics of Excitons in Atomically Thin Semiconductors — •xiaoqin li — Univ. of Texas-Austin, Austin, USA

The transitional metal dichalcogenides (TMDs) are an emerging class of atomically thin semiconductors with tightly-bound excitons and charged excitons (i.e. trions). A fundamental property of these quasiparticles is quantum decoherence time, which reflects irreversible quantum dissipation arising from system (excitons) and bath (vacuum and other quasiparticles) interaction and determines the timescale during which excitons can be coherently manipulated. Dephasing time is also equivalent to the intrinsic homogeneous linewidth of exciton resonances. In addition, excitons in TMDs are localized at the corners of the Brillouin zone and provide a convenient way to optically manipulate the valley degree of freedom. Direct measurement of valley coherence time is challenging because it corresponds to non-radiative coherence between two degenerate states. Using ultrafast multi-dimensional optical spectroscopy, we investigate the intrinsic homogeneous linewidth of excitons, exciton valley coherence as well as coupling between excitons and trions. Our studies reveal coherent exciton dynamics on the order of ~ 100 fs in monolayer TMDs. Decoherence time is not only an important parameter for characterizing fundamental properties of excitons, but also serves as a sensitive probe for exciton-exciton and exciton-phonon interaction.

HL 22.9 Tue 12:15 H10

Ultrafast Pump-Probe Analysis of Exciton-Polariton Propagation — Jan Lohrenz[1], Stephan Melzer[1], Claudia Ruppert[1], Ilya Akimov[1], •Matthias Reichelt[2], Alexander Trautmann[2], Torsten Meier[2], and Markus Betz[1] — [1]Experimentelle Physik 2, TU Dortmund, Otto-Hahn-Str. 4, 44221 Dortmund, Germany — [2]Department of Physics and CeOPP, University of Paderborn, Warburger Str. 100, D-33098 Paderborn, Germany

In bulk CdZnTe light is significantly slowed down in a spectral range close to the lower exciton-polariton branch. [1] Here, we investigate nonlinear optical signatures in a pump-probe experiment with femtosecond laser pulses. Experimental data and model simulations for the optical response of a nonlinearly driven two-level system suggest that the excitation induced dephasing [2] and slow light propagation lead to unexpected features in the differential transmission spectra. [3]

[1] T. Godde, I. A. Akimov, D. R. Yakovlev, H. Mariette, and M. Bayer, Phys. Rev. B **82**, 115332 (2010).
[2] H. Wang, K. Ferrio, D.G. Steel, Y.Z. Hu, R. Binder, and S.W. Koch, Phys. Rev. Lett. **71**, 1261 (1993).
[3] J. Lohrenz, S. Melzer, C. Ruppert, I.A. Akimov, M. Reichelt, A. Trautmann, T. Meier, M. Betz, to be published.

HL 22.10 Tue 12:30 H10

Dynamics of exciton-polariton condensates in semiconductor microcavities with periodic potentials — •Xuekai Ma[1], Stefan Schumacher[1], and Oleg Egorov[2] — [1]Physics Department, Universität Paderborn, Warburger Strasse 100, 33098 Paderborn, Germany — [2]Institute of Condensed Matter Theory and Solid State Optics, Abbe Center of Photonics, Friedrich-Schiller-Universität Jena, Max-

Wien-Platz 1, 07743 Jena, Germany

Exciton-polaritons are quasi-particles made of quantum well (QW) excitons coupled to cavity photons. They have very small effective mass ($10^{-4}m_e$) and lifetimes on the tens of picoseconds scale. Due to their photonic properties, they can be excited by light and probed, respectively. Due to their excitonic properties, nonlinearity is introduced into this system at elevated densities. Polaritons, which are composite bosons, can undergo a condensation process (with similarities to Bose-Einstein condensation) under incoherent excitation. Many features in the dynamics of polariton condensates can be described by a modified Gross-Piteavskii equation (GPE). Here, we study the nonlinear dynamics of polariton condensates in periodic potentials. In the presence of a periodic potential, a band structure including a band-gap can be obtained. We show that polariton condensates can occupy and switch between different energy states by changing the pump excitation intensity and shape. Our simulation results agree very well with recent experimental results.

HL 22.11 Tue 12:45 H10

Nonlinear terahertz quantum control of Landau-quantized electrons — •Thomas Maag[1], Andreas Bayer[1], Sebastian Baierl[1], Matthias Hohenleutner[1], Tobias Korn[1], Christian Schüller[1], Dominique Bougeard[1], Christoph Lange[1], Rupert Huber[1], Martin Mootz[2], Stephan W. Koch[2], and Mackillo Kira[2] — [1]Department of Physics, University of Regensburg, 93053 Regensburg, Germany — [2]Department of Physics, Philipps-University Marburg, 35032 Marburg, Germany

Controlling superpositions of many-body electronic quantum states in solids is impeded by rapid dephasing through inter-particle scattering. However, Walter Kohn found in 1961 that the cyclotron resonance of Landau-quantized electrons in a two-dimensional electron gas (2DEG) is immune to Coulomb forces. This protection warrants long coherence times and makes the system interesting for quantum control, but explicitly excludes nonlinearities. Here, we demonstrate how intense light pulses in the terahertz (THz) spectral range can induce well-controlled electronic many-body correlations in a magnetically biased 2DEG and tailor a distinctly anharmonic response. Coherent ladder climbing up to the 6th rung yields population inversion and abruptly increases dephasing. Strikingly, 2D THz spectroscopy reveals distinct multi-wave mixing signatures, which our quantum theory explains through Coulomb interactions between electrons and the positively charged ionic background. These many-body dynamics demonstrate how internal degrees of freedom of solid state quantum systems enable coherent nonlinear interactions for future ultrafast quantum information processing.

HL 22.12 Tue 13:00 H10

Ultrafast nonlinear response of GaAs under high pressures — •Johannes M. Braun[1,2], Jan F. Schmidt[3], Denis V. Seletskiy[3], Harald Schneider[1], Manfred Helm[1,2], and Alexej Pashkin[1,3] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]TU Dresden, Germany — [3]Department of Physics and Center for Applied Photonics, University of Konstanz, Germany

Applying hydrostatic pressure leads to dramatic changes in the band structure of semiconductors. In particular, it enables a continuous tuning of the bandgap energy. Here we study the nonlinear response of bulk gallium arsenide (GaAs) in the vicinity of its bandgap. The optical pump-probe experiment is performed in a non-collinear reflection geometry at pressures up to 3 GPa generated inside a diamond anvil cell. By increasing pressure we observe pronounced slowing down of the relaxation dynamics of photoexcited charge carriers: the time constant of the dominating relaxation process increases from about 10 ps at ambient pressure to 35 ps above 0.7 GPa. These time scales are by an order of magnitude shorter than the recombination time determined using optical pump - THz probe spectroscopy. Thus, the fast dynamics observed in the optical pump-probe measurements is governed by the cooling of hot electron distribution and not by the recombination process. Furthermore, at pressures above 2 GPa the bandgap energy of GaAs is above the excitation spectrum of our experiment. The sample becomes transparent for the femtosecond pulses leading to a transient pump-probe signal with a negative sign due to the third order nonlinear response of GaAs.

HL 23: Oxide Semiconductors I

Oxide Semiconductors except for ZnO

Time: Tuesday 9:30–13:00 Location: H13

HL 23.1 Tue 9:30 H13

Method of choice for the fabrication of Schottky contacts for unipolar devices on heteroepitaxial Ga_2O_3 — •Daniel Splith, Stefan Müller, Florian Schmidt, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Leipzig, Germany

Ga_2O_3 is a promising material for a new generation of high-power devices. For the fabrication of devices like unipolar diodes or metal-semiconductor field-effect-transistors (MESFETs), the optimization of the fabrication of Schottky contacts (SCs) is crucial.

In this contribution we compare different methods for the fabrication of Pt-Schottky contacts on heteroepitaxial Ga_2O_3 thin films: While the rectification of SCs fabricated by standard dc-sputtering remains poor, contacts fabricated by thermal evaporation and long-throw (LT) sputtering show rectification ratios above 6 orders of magnitude and ideality factors of about 1.3 for the best contacts. Using a reactive atmosphere during the sputtering process additionally increases the barrier height from about 1 eV to values of 1.4 eV for the best contacts. Contacts comparable to those fabricated with LT sputtering can be achieved in a standard sputtering chamber by positioning the sample out of the axis of the plasma, thereby reducing the kinetic energy of the impinging particles.

We used the latter method to fabricate circular MESFETs [1] on heteroepitaxial Ga_2O_3 thin films. Although the channel resistances are high, on/off ratios of up to 5 orders of magnitude were achieved.
[1] M. Higashiwaki *et al.*, Appl. Phys. Lett. 100.1, 013504 (2012)

HL 23.2 Tue 9:45 H13

Cu deficient, nanocrystalline $CuCrO_2$ — Leo Farrell, Emma Norton, Christopher Smith, David Caffrey, Igor Shvets, and •Karsten Fleischer — School of Physics and Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN), Trinity College, University of Dublin, Dublin 2, Ireland

The delafossite structured $CuCrO_2$ system is well known as one of the best performing p-type transparent conducting oxides. In this paper the details of a low temperature facile growth method for highly copper deficient Cu_xCrO_2 by spray pyrolysis is described. The dependence of the growth on the precursors, the temperature and oxygen partial pressure are examined. The decomposition routes are critical to obtain the best performing films. The thermopower and electrical measurements indicate p-type films with conductivity ranging from 1-12 Scm^{-1} depending on the growth conditions. This p-type conductivity is retained despite the nanocrystallinity and Copper deficiency of the films ($x \approx 0.4$). The figure of merit of these films can be as high as 350 μS, which is the best performing p-type TCO by solution methods to date. The optical properties are also investigated using ellipsometry and UV-Vis spectrophotometry.

HL 23.3 Tue 10:00 H13

Nitrogen incorporation in SnO2 thin films grown by chemical vapor deposition — •Jie Jiang, Yinmei Lu, Benedikt Kramm, Fabian Michel, Christian T. Reindl, Max Kracht, Bruno K. Meyer, Detlev M. Hofmann, and Martin Eickhoff — I. Physikalisches Institut, Justus-Liebig-Universität Gießen, Gießen, Germany

As a transparent conducting oxide film, SnO2 have great technological potential for the application in opto-electronic devices, due to its large band gap of 3.6 eV, and high carrier mobility of about 250 cm2/Vs at room temperature. Nitrogen is proposed to be an excellent anion dopant in SnO2 owing to its suitable electronegativity and ion size, high solubility limit, and non-toxicity. Here we study the characteristics of SnO2 films with high concentrations of incorporated nitrogen.

We deposited SnO2-xNx thin films on c-sapphire substrates via chemical vapor deposition (CVD), using SnI2 powder and O2 and NH3 gas as source materials. The crystal structure, electrical properties and optical properties of the films were measured and investigated. The N atomic concentration in SnO2-xNx film increases from 0 to 7.9 at.% (XPS) without phase separation with increasing NH3 flow rate during the deposition. The substitutional lattice location in this concentration range was confirmed. The carrier concentration increases from 4.1E18 to 3.9E19 cm-3 and the absorption edge shifts from 4.26 to 4.08 eV. The effect of annealing on the structural, optical and electrical properties is also analyzed.

HL 23.4 Tue 10:15 H13

Doped and Undoped β-Ga_2O_3 Structures Prepared by Ultrasonic Nebulization and Spray Pyrolysis — •Constance Schmidt, Axel Fechner, and Dietrich R. T. Zahn — TU Chemnitz, Insitut für Physik, Reichenhainerstr. 70, 09126 Chemnitz

With its wide band gap of around 4.9 eV, β-Ga_2O_3 is a promising semiconductor for many applications like optoelectronic devices. Besides the established techniques for the preparation of β-Ga2O3 layers,for instance chemical vapor deposition, electron beam deposition, molecular beam epitaxy, and pulsed laser deposition, low cost techniques such as ultrasonic nebulization and spray pyrolysis are also of great interest. With the latter we obtained different types of microstructures of β-Ga_2O_3 (from 3D structures to thin films) on silicon substrates.

For the preparation of β-Ga_2O_3 a solution of $Ga(NO_3)_3$ in water, or in a water/ethanol mixture was employed. Rare earths, like Er^+, Sm^+ and Gd^+, were used as dopants. The different β-Ga_2O_3 microstructures were confirmed by SEM, and investigated with XRD, Raman spectroscopy, and microscopic ellipsometry. In all cases β-Ga_2O_3 was clearly identified. Since the structures have dimensions in the micrometer range, Raman spectroscopy (325 nm, 514.7 nm) was used to investigate individual β-Ga_2O_3 structures and determine their composition and other effects like strain in detail.

The experimental results demonstate that even with the low cost techniques it is possible to produce high quality doped and undoped β-Ga_2O_3 thin films and other structures, which are interesting for potential applications.

HL 23.5 Tue 10:30 H13

Temperature-dependent anisotropic thermal properties of β-Ga_2O_3 bulk-crystals — •Martin Handwerg[1,2], Rüdiger Mitdank[1], Zbigniew Galazka[3], and and Saskia F. Fischer[1] — [1]AG Neue Materialien, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, 14109 Berlin, Germany — [3]Leibniz Institute for Crystal Growth, 12489 Berlin, Germany

Transparent semiconducting oxides like Ga_2O_3 are important materials for high power electronics and optoelectronics. Here, we investigate the crystallographic anisotropy of the thermal conductivity and the thermal diffusivity for a β-Ga_2O_3 single crystal. The thermal conductivity, thermal diffusivity and specific heat capacity is measured by applying multiple electrical AC-heating methods on Czochralski-grown[1] β-Ga_2O_3 bulk crystals. At room temperature the thermal conductivity along the [100]-direction in Mg-doped electrical insulating and undoped semiconducting β-Ga_2O_3 is confirmed as 13 ± 1 $Wm^{-1}K^{-1}$[2]. Additionally a value for the [001]-direction of 15 ± 1 $Wm^{-1}K^{-1}$[3] is detected. The observed function $\lambda(T)$ is in accord with phonon-phonon-Umklapp scattering and the Debye-model for 50 K $< T <$ 300 K. Here a detailed discussion of the phonon-phonon-Umklapp scattering for $T < \theta_D$ is carried out.

[1] Z. Galazka *et al.* J. Cryst. Growth **404**, 184 (2014)
[2] M. Handwerg *et al.* Semcond. Sci. Technol. **30**, 024006 (2015)
[3] M. Handwerg *et al.* arXiv 1506.05294 (2015)

HL 23.6 Tue 10:45 H13

Influence of thermal and oxidative treatments on the electronic surface properties of In_2O_3 films — •Theresa Berthold[1], Thomas Stauden[1], Stefan Krischok[1], Marcel Himmerlich[1], Markus Mischo[2], Volker Cimalla[2], Julius Rombach[3], and Oliver Bierwagen[3] — [1]Institut für Mikro- und Nanotechnologien, Technische Universität Ilmenau — [2]Fraunhofer-Institut für Angewandte Festkörperphysik, Freiburg — [3]Paul-Drude-Institut für Festkörperelektronik, Berlin

In_2O_3 is widely used as sensitive gas sensor material. As grown films typically exhibit a high surface electron concentration, which can be modified by an oxygen plasma treatment [1]. In this study, the surface composition and electronic properties of undoped and Mg-doped In_2O_3 films grown by MBE or MOCVD are characterized by photoelectron spectroscopy to investigate the underlying mechanisms. We analyze the influence of different surface preparation methods, like thermal annealing in vacuum or O_2, oxygen plasma treatment as well as exposure to O_3, on formation of adsorbates, oxygen vacancies and defects as well as on variation in band bending, electron concentration and electric dipoles at the In_2O_3 surface. Oxygen plasma and other oxidative surface treatments induce attachment of negative O adsorbates forming an effective negative dipole at the surface that increases the barrier for electron emission and induces depletion of the surface electron layer via charge transfer, which can be reversed by adsorbate desorption. [1] O. Bierwagen, et al., Appl. Phys. Lett. 98, 172101 (2011)

30 min. Coffee Break

HL 23.7 Tue 11:30 H13

Influence of incoherent twin boundaries on the electrical properties of homoepitaxial β-Ga_2O_3 layers grown by metal organic vapor phase epitaxy — •Andreas Fiedler, Klaus Irmscher, Robert Schewski, Martin Albrecht, Michele Baldini, and Günter Wagner — Leibniz-Institute for Crystal Growth, Max-Born-Str. 2, 12489 Berlin, Germany

Doped β-Ga_2O_3 layers have been grown homoepitaxially on (100) orientated substrates by metal organic vapor phase epitaxy (MOVPE) using either the shallow donor impurity Sn or Si. Conductivity and Hall effect measurements at room temperature show n-type conductivity. However, the measured electron concentrations between 5×10^{17} cm^{-3} and 2×10^{19} cm^{-3} indicate a strong electrical compensation and the electron mobilities of up to 30 $cm^2V^{-1}s^{-1}$ unexpectedly decline for low carrier densities. A possible explanation for this behavior comes from a structural analysis by transmission electron microscopy (TEM). It reveals that the layers contain a high density of planar defects consisting of twin lamellas and stacking faults. The lateral twin boundaries are incoherent and contain dangling bonds that trap charge carriers. This leads to charge accumulation and hinders lateral charge carrier transport. This behavior is in analogy to that of dislocation walls treated in [1]. Based on this model, we explain the observed steep decline in electron mobility at low carrier concentrations. Furthermore, the strong compensation of the donor dopants can, at least partly, be ascribed to the acceptor effect of the incoherent twin boundaries.
[1] Farvacque *et al.*, *Physical Review B* **63** 115202 (2001).

HL 23.8 Tue 11:45 H13

Influence of cation stoichiometry on performance of unipolar and bipolar zinc-tin-oxide diodes — •Sofie Bitter, Peter Schlupp, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Institut für Exp. Physik II, Germany

Amorphous zinc-tin-oxide (ZTO) consists of naturally abundant, nontoxic elements only and can be deposited at room temperature with an electron density and a mobility as high as 10^{19} cm^{-3} and 10 cm^2/Vs, respectively [1]. Therefore, ZTO is a suitable material for low-cost, transparent transistors and thus low-cost, transparent electronic applications.

We present our results on the influence of the Zn/Sn ratio on the electrical properties of thin films grown by pulsed laser deposition on glass substrates using a continuous composition spread method (CCS) [2]. Furthermore we discuss the performance of diodes fabricated thereon. Opposite to previous reports on only a limited number of discrete Zn/Sn ratios [3], we obtained a comprehensive data set for almost the entire composition range. Using energy dispersive X-ray analysis the spatial dependence of the Zn/Sn ratio was mapped. Charge carrier concentration and resistivity were determined in dependence on the composition. Further, the properties of Schottky diodes and all-amorphous *pn*-heterojunctions using $ZnCo_2O_4$ as *p*-type electrode will be discussed in dependence on the thin film stoichiometry.

[1] Jayaraj et al., J. Vac. Sci. & Technol. B, **26**, 2, 2008
[2] von Wenckstern et al., CrystEngComm, **15**, 10020, 2013
[3] Görrn et al., Applied Physics Letters, **91**, 193504, 2007

HL 23.9 Tue 12:00 H13

Dielectric and Raman tensor of monoclinic Ga_2O_3 — •Chris Sturm[1], Christian Kranert[1], Jürgen Furthmüller[2], Friedhelm Bechstedt[2], Rüdiger Schmidt-Grund[1], and Marius Grundmann[1] — [1]Institut für Experimentelle Physik II, Universität Leipzig, Linnéstr. 5, 04103 Leipzig, Germany — [2]Institut für Festkör-

pertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

Ga_2O_3 is a promising material for deep UV applications due to its band-gap energy of about 4.8 eV. At ambient conditions it crystalizes in a monoclinic structure and the dielectric function is a tensor consisting of 4 independent elements. The magnitude and dispersion of these elements were not known previously. We determined the full dielectric tensor in the spectral range of $0.5-8.5$ eV by using generalized spectroscopic ellipsometry. The obtained DF is in excellent agreement with that obtained by many-body perturbation theory including quasiparticle and excitonic effects. This analysis yield that the off-diagonal element cannot be neglected in the entire investigated spectral range. Although this element seems to be negligible small in the transparent spectral range ($|\varepsilon_{xz}| \leq 0.02$), it causes a rotation of the dielectric axis of about 20°. Using this DF we applied a new formalism for Raman scattering in anisotropic crystals to model the dependency of the Raman intensities on the scattering geometry for most phonon modes and determined the Raman tensor elements for these modes.

[1] C. Sturm *et al.*, APL Mater. **3**, 106106 (2015).

HL 23.10 Tue 12:15 H13

An *ab initio* study of defect complexes in Fe- and Gd-doped MgO co-doped with Li — •Sergey V. Levchenko, Sebastian Alarcon Villaseca, and Matthias Scheffler — Fritz-Haber-Institut der MPG, Berlin, DE

Li/Fe- and Li/Gd-co-doped MgO have recently attracted attention due to their potential applications in catalysis and dosimetry [1,2]. In this work, we calculate formation energies of defect complexes in these materials using DFT with the hybrid PBE0 functional, and estimate their relative concentrations at realistic temperatures and oxygen pressures using the *ab initio* atomistic thermodynamics. We find that the Fe_{Mg}-Li_{Mg} defect pairs are bound weaker than Gd_{Mg}-Li_{Mg} pairs, and the dissociated Fe_{Mg}-Li_{Mg} pairs are favored at elevated temperatures due to the increased configurational entropy. This explains why experimental EPR spectra of Gd^{3+} showed apparent changes upon Li-doping of Gd-MgO, while no changes have been detected in Li/Fe-MgO samples [3]. This qualitative result is found to be insensitive to the fraction of the exact exchange α in the hybrid functional for $0<\alpha<0.5$. – [1] U. Simon *et al.*, Catal. Comm. 18, 132 (2012); [2] L.C. Oliveira, B.A. Doull, E.G. Yukihara, J. Luminescence 137, 282 (2013); [3] U. Simon, S. Arndt, T. Otremba, S. Alarcon Villaseca, S.V. Levchenko, M. Wollgarten, J.D. Epping, A. Kwasniewski, A. Berthold, F. Schmidt, O. Gorke, M. Scheffler, R. Schomacker, K.P. Dinse, in preparation.

HL 23.11 Tue 12:30 H13

Electronic band structure and infrared lattice dynamics of single-crystal nickel oxide (NiO) — •Stefan Zollner, Cayla M. Nelson, Travis I. Willett-Gies, Ayana Ghosh, and Lina S. Abdallah — New Mexico State University, Las Cruces, NM, USA

Using spectroscopic ellipsometry, we determined the dielectric function of bulk NiO from 25 meV to 6 eV to study its lattice dynamics and electronic structure. In the visible and UV, NiO looks remarkably similar to Si: Both materials are transparent in the near-infrared. A slow rise of the absorption throughout the visible is followed by a sharp peak at 3.4 eV (Si) and 3.8 eV (NiO). In Si, this peak is caused by transitions from the highest valence band to the lowest conduction band along the (111) direction of the BZ. In NiO, it is associated with the charge-transfer (Hubbard) gap. In both materials, the peaks broaden and redshift with increasing temperature, due to electron phonon interactions. Many recent band structure calculations for NiO focus on the charge-transfer absorption peak (3.8 eV) and ignore the absorption below the main peak. Our data show a direct band gap of NiO at 0.85 eV, which we attribute to interband transitions from the Ni+O valence band to the Ni(4s) conduction band at the zone center. We also find strong TO phonon absorption in infrared ellipsometry spectra, which is modified by two-phonon absorption.

HL 23.12 Tue 12:45 H13

Lattice dynamics of EuO: an evidence for giant spin-phonon coupling — •Ramu Pradip[1,2], Przemysław Piekarz[3], Alexei Bosak[4], Dániel Géza Merkel[4], Olga Waller[1,2], Anja Seiler[1,2], Alexander I. Chumakov[4], Rudolf Rüffer[4], Andrzej M. Oleś[5,6], Krzysztof Parlinski[3], Michael Krisch[4], Tilo Baumbach[1,2,7], and Svetoslav Stankov[2,1] — [1]Laboratory for Applications of Synchrotron Radiation, Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany — [2]Institute for Photon Science and Synchrotron Radiation, KIT, Eggenstein-Leopoldshafen, Germany — [3]Institute of Nuclear Physics, Polish Academy of Sciences, Kraków, Poland — [4]European Synchrotron Radiation Facility, Grenoble, France — [5]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [6]Marian Smoluchowski Institute of Physics, Jagiellonian University, Kraków, Poland — [7]ANKA, KIT, Eggenstein-Leopoldshafen, Germany

Europium monoxide is a semiconducting ferromagnet recently proposed as a spin-filter in the emerging field of spintronics. Using inelastic x-ray scattering and nuclear inelastic scattering combined with ab initio calculations we determined the lattice dynamics of EuO. The results revealed a giant momentum and temperature dependent spin-phonon coupling above and well below the Curie temperature. Acknowledgement: KIT-VHNG-625; NCN 2011/01/M/ST3/00738 and 2012/04/A/ST3/00331

HL 24: Carbon-based Nanostructures

Time: Tuesday 9:30–12:00 Location: H14

HL 24.1 Tue 9:30 H14

High-frequency optically detected magnetic resonance of nitrogen-related centers in diamond — •Dion Braukmann[1], Jörg Debus[1], Vitalii Yu. Ivanov[2], Dariya Savchenko[3], Dmitri R. Yakovlev[1,4], Marek Godlewski[2], and Manfred Bayer[1,4] — [1]Experimentelle Physik 2, Technische Universität Dortmund, 44227 Dortmund, Germany — [2]Institute of Physics, Polish Academy of Sciences, 02668 Warsaw, Poland — [3]Institute of Physics, AS CR, 18221 Prague, Czech Republic — [4]Ioffe Institute, Russian Academy of Sciences, 194021 St. Petersburg, Russia

Impurities in diamond have been studied in recent years on account of possible applications in quantum information processing, spin-electronics and, e.g., biophotonics. The most promising impurity is the negatively charged nitrogen-vacancy (NV^-) center. Particular focus has been drawn on its optical and magnetic properties. The majority of studies neglects however the interplay between the NV^- center and other, mainly nitrogen-related, impurities giving rise to extraordinary changes in the magneto-optical characteristics.
In that context, we report on spectrally resolved optically detected magnetic resonance of nitrogen-related centers in diamond crystals. The application of microwaves with 65 GHz and low power allows us to reveal resonant microwave amplification.

HL 24.2 Tue 9:45 H14

Electronic transport properties of diamondoids within a gold nanojunction — Bibek Adhikari, •Ganesh Sivaraman, and Maria Fyta — Institute for Computational Physics , University of Stuttgart, Germany

Diamondoids are tiny hydrogen terminated diamond-like cages with tunable optoelectronic properties. These nanometer sized nanostructures, as well as their derivatives have been proposed as potential candidates for molecular electronics. For such an application, it is essential for diamondoids, when placed between electrodes, to facilitate electronic transport. In this work, we aim to shed light to this direction and reveal the electronic transport properties of diamondoids in a Au(111) nanojunction. The diamondoids need to be modified on either ends with functional groups in order to efficiently attach on the gold electrodes. Accordingly, the diamondoids will be attached through functional units to Au(111) electrodes. We will begin with diamantane and continue up to tetramantane. Two functional groups are chosen for grafting the diamondoid on the gold electrodes of the break junction: (a) a thiol group, and (b) a carbene molecule. Our work is based on quantum-mechanical simulations within the density functional theory (DFT) approach. The quantum transport calculations are carried out using the DFT approach together with the non-equilibrium Greens functions formalism. The electronic and transport properties of the gold electrodes including the functionalized diamon-

doids are presented based on this approach. Our results are highly relevant to molecular electronics and sensing devices.

HL 24.3 Tue 10:00 H14

Picosecond photocurrents in single-walled carbon nanotubes — •Maximilian Engl, Christoph Karnetzky, and Alexander W. Holleitner — Walter-Schottky-Institute and Physics-Department, Technical University of Munich, Germany

The exciton dynamics in carbon nanotubes are typically detected in a time-resolved way by optical techniques such as the transient absorption technique and the time-resolved photoluminescence spectroscopy. Both methods focus mainly on the dynamics of localized charge carriers within the carbon nanotubes. Many questions remain concerning the separation and the transport of photogenerated charge carriers to source and drain leads in an optoelectronic device structure. We address these questions by an ultrafast photocurrent spectroscopy, which is based on an on-chip THz time domain spectroscopy [1]. We find a combination of an optically induced ultrafast displacement current and interband charge-carrier recombination processes to dominate the ultrafast photocurrent of the single-walled carbon nanotubes [2]. We further discuss inter-subband relaxation processes after the optical excitation [3].

We acknowledge financial support from the ERC-grant "NanoREAL" and the DFG excellence cluster "Nanosystems Initiative Munich" (NIM).

[1] L. Prechtel et al., Nature Communications, 3, 646, (2012).
[2] L. Prechtel et al., Nano Letters, 10, 1021, (2011).
[3] C. Karnetzky et al. (2016).

HL 24.4 Tue 10:15 H14

Do clathrate structures exist at carbon? — •Conrad Schuster and Miguel Marques — Martin-Luther-Universität Halle-Wittenberg

For doped carbon clathrates many interesting properties have been proposed like super conductivity, super hardness or application as a semiconductor. Although this interest and the ability of silicon to form clathrate structures, no such material could have been produced yet.

Via DFT calculations with DFTB+ and VASP and minima hopping code we performed ab initio calculations on the stability of clathrates of carbon to show why they could not be found in experiments yet.

30 min. Coffee Break

HL 24.5 Tue 11:00 H14

Magnetotransport properties of a disordered graphite microwire produced by He^+ bombardment and embedded in a diamond crystal — •Jose Barzola-Quiquia[1], Tobias Lühmann[2], Ralf Wunderlich[1], Mahsa Zoraghi[1], Jan Meijer[1], and Pablo Esquinazi[1] — [1]Institute for Experimental Physics II, University of Leipzig, 04103 Leipzig, Germany — [2]Institute for Medicine Physics and Biophysics, University of Leipzig, 04107 Leipzig, Germany

We have investigated the magnetotransport properties of a graphite-like microwire (GLM) embedded in a diamond crystal in the temperature range of 2 K to 300 K and magnetic field to ± 8 T. The GLM was produced at ≈ 3 μm below the surface of a diamond crystal through the implantation of He^+ ions of 1.8 MeV energy using a microbeam. The initial wire was amorphous and was crystallised after heat treatment at $T \approx 1475$ K. After a first annealing treatment the electrical transport at low temperatures is well described by a fluctuation-induced tunneling conductance model. The tunneling process occurs between the partially graphitized grains separated by nearly insulating thin amorphous regions. After a second annealing the transport mechanism changes to variable range hopping conduction. A finite magnetoresistance (MR) was observed at temperatures $T < 250$ K, which can be well described by a semi-empirical model that takes into account a spin dependent scattering process. The magnetic properties indicate the existence of magnetic order in the GLM. The appearance of the graphitic structure after annealing treatment was confirmed by confocal Raman spectroscopy.

HL 24.6 Tue 11:15 H14

States of antiferromagnetic molecules detected with a carbon nanotube quantum dot — •Christian Lurz[1], Michael Schnee[1], Robert Frielinghaus[1], Claire Besson[1,2,3], Paul Kögerler[1,3], Claus M. Schneider[1,4], and Carola Meyer[1,5] — [1]Peter Grünberg Institut, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Department of Chemistry, The George Washington University, Washington, DC 20052, United States — [3]Institut für Anorganische Chemie, RWTH Aachen, 52074 Aachen, Germany — [4]Fakultät für Physik, Universität Duisburg-Essen, 47057 Duisburg, Germany — [5]Department of Physics, Universität Osnabrück, 49069 Osnabrück, Germany

Some of the most outstanding properties of carbon nanotubes (CNTs) are displayed in their sensitiveness towards changes in the environment and their spin-dependent conductivity. Thus, they are ideal devices to investigate the states of antiferromagnetic molecules via electronic transport experiments on functionalized CNTs. In this work, we present experimental data on quantum transport through CNTs covalently functionalized with antiferromagnetic tetramanganese coordination complexes. The experiments reveal a random telegraph signal (RTS), which is presumably caused by interactions between electron spin and the antiferromagnetic spin system. Furthermore, the statistics of the RTS indicate the relevant time and energy scales for transitions in this regime.

HL 24.7 Tue 11:30 H14

Effects of driving in carbon nanotube quantum dots — •Patrick Haughian — Université du Luxembourg

The field of nanomechanics has been seen to provide a toolbox to investigate non-classical states of matter. In particular, past work has explored the interplay between photonic and vibronic degrees of freedom in engineering interesting photon states. More recently, the transport properties of quantum dots with additional electron-vibron interaction have been investigated. The case of strong interaction features significant suppression of the conductance through those systems in what is known as Franck-Condon blockade.

Our present efforts consist of analyzing such an electromechanical system, making use of theoretical techniques familiar from the treatment of optomechanical settings. Here, we want to profit from recent developments in engineering carbon nanotubes as quantum dots to control the parameters of the system. This undertaking provides a novel interface between electronic and vibronic systems, allowing us to exhibit non-classical vibron states, with possible uses in measurement setups and in exploring the quantum behavior of macroscopic systems.

HL 24.8 Tue 11:45 H14

A Fully Tuneable Fabry-Perot Microcavity for Diamond-Based Photonics — •Daniel Riedel, Brendan Shields, Sebastian Starosielec, Patrick Maletinsky, and Richard J. Warburton — Department of Physics University of Basel, Basel, Switzerland

Coupling between solid-state quantum emitters and photonic channels is a critical challenge for many applications in quantum sciences. A key requirement is a high fluence of indistinguishable photons, the generation of which requires photonic engineering and high quality, solid-state hosts. Here, we present an approach to this problem in the form of a fully tuneable Fabry-Perot micro cavity. The goal is to enhance the emission rate and zero-phonon line (ZPL) collection efficiency of nitrogen vacancy (NV) centers in diamond. At the core of the device, there is a high-quality, nano-fabricated, single-crystalline diamond membrane, bonded to a highly reflective Bragg mirror; the cavity is completed by a second, concave mirror. As a result, we achieve full spectral and spatial tunability and freedom in selecting NVs with favourable emission properties. We present first results showing how the finesse, limited to a few thousand by the reflectivity of the mirrors, is not degraded by the presence of the diamond membrane, and that the linewidth of the NV centers in the membrane can be sub-GHz. Our experimentally determined key device characteristics suggest that a 100-fold Purcell enhancement of the ZPL can be achieved in the future. Our results may thereby pave the way for highly efficient NV entanglement generation and ultraprecise quantum metrology applications.

HL 25: Quantum Information Systems (Joint session of HL and TT, organized by HL)

Time: Tuesday 9:30–12:30 Location: H15

HL 25.1 Tue 9:30 H15

Nuclear spins as quantum memories for quantum networks and repeaters — •Andreas Reiserer[1,2], Norbert Kalb[1,2], Machiel Blok[1,2], Koen van Bemmelen[1,2], Tim Taminiau[1,2], and Ronald Hanson[1,2] — [1]Kavli Institute of Nanoscience, TU Delft, The Netherlands — [2]QuTech, TU Delft, The Netherlands

A future quantum network will consist of quantum processors that are connected by quantum channels, just like conventional computers are wired up to form the Internet. To realize such network, we plan to use spin qubits in diamond, which combine access to few-qubit nuclear-spin registers with exceptional coherence properties. However, preserving the coherence of the register while generating entanglement between remote spins is an open challenge.

Here, we investigate the coherence of single ^{13}C spins that occur in an otherwise spin-free diamond sample of natural isotope abundance. Five individual nuclear spins are controlled via the weak hyperfine interaction with the electronic spin of a nitrogen vacancy (NV) center in a strong magnetic field. We encode quantum bits in the nuclear spins and investigate the loss of coherence caused by repeated electron spin initialization, which is required for any quantum protocol that is subject to errors. Encoding the qubits in a decoherence-protected subspace of two rather than one nuclear spin increases the robustness of the protocol and enables the investigation of a large parameter space with a single sample. Our results open perspectives for the realization of large scale quantum networks and quantum repeaters using NV centers with weakly coupled nuclear spins.

HL 25.2 Tue 9:45 H15

Long distance coupling of resonant exchange qubits — •Maximilian Russ and Guido Burkard — Department of Physics, University of Konstanz, D-78457 Konstanz, Germany

We investigate the effectiveness of a microwave cavity as a mediator of interactions between two resonant exchange (RX) qubits [1,2] in semiconductor quantum dots (QDs) over long distances [3], limited only by the extension of the cavity. Our interaction model includes the orthonormalized Wannier orbitals constructed from Fock-Darwin states under the assumption of a harmonic QD confinement potential. We calculate the qubit-cavity coupling strength g_r in a Jaynes Cummings Hamiltonian, and find that dipole transitions between two states with an asymmetric charge configuration constitute the relevant RX qubit-cavity coupling mechanism. The effective coupling between two RX qubits in a shared cavity yields a universal two-qubit iSWAP-gate with gate times on the order of nanoseconds over distances on the order of up to a millimeter.

[1] J. Medford et al., Phys. Rev. Lett. **111**, 050501 (2013).
[2] J. M. Taylor, V. Srinivasa, and J. Medford, Phys. Rev. Lett. **111**, 050502 (2013).
[3] M. Russ and G. Burkard, arXiv: 1508.07122 (2015)

HL 25.3 Tue 10:00 H15

Higher Order Spin Correlation in Semi-Conductor Quantum Dots — •Nina Fröhling, Jan Böker, and Frithjof Anders — Fakultät Physik, TU Dortmund, 44227 Dortmund, Deutschland

We study higher order auto-correlation functions of electron spin decay in an isolated semi-conductor quantum dot described by the central spin model. The electronic central spin is coupled to a bath of nuclear spins via hyperfine interaction, which dominates the short time regime. In a mean field approach the nuclear spin field is assumed to be frozen, since the precession frequency of the electron in the nuclear hyperfine field is much greater than the precession frequency of the nuclei in the hyperfine field of the electron. Since the higher order cumulants of this mean-field approximation vanish, these functions can serve as a tool to reveal the entanglement between the electron spin and the nuclear spin bath. We also evaluate analytically the symmetries exhibited by third order correlation functions in the high-temperature limit. It can be shown that the third order correlation function is constrained to a small subspace of all possible frequencies. Furthermore, we calculate the third order correlation function using the Lanczos-algorithm and statistic trace evaluation. The viability of this method is benchmarked by the analysis of the established spin noise spectrum given by the second order correlation function.

HL 25.4 Tue 10:15 H15

Spin Decoherence in a Pulsed Quantum Dot System — •Natalie Jäschke and Frithjof Anders — Fakultät Physik, TU Dortmund, 44227 Dortmund, Deutschland

In pump-probe experiments electron spin polarization in a semiconductor quantum dot is generated by periodic optical excitations. The decoherence of this polarization is dominated by the hyperfine interaction with a bath of nuclear spins in the short time regime. We aim for a theory that combines the effect of the periodic laser pulses and the nuclear spin bath on the electron spin polarization. Since the laser pulses occur on the shortest time scale of the system, and the electronic decay times are small compared to those of the nuclear spin bath, we treat the laser pumping quantum-mechanically using a Lindblad approach and keep the nuclear spins as frozen during that time. Then a classical simulation of the Overhauserfield bridges the time until the next laser pulse. We analyze the stability of different non-equilibrium nuclear spin bath distribution functions as well as the magnetic field dependent build up of a laser-induced nuclear spin polarization.

HL 25.5 Tue 10:30 H15

A model for slow decoherence in semiconductor quantum dots — •Wouter Beugeling, Frithjof B. Anders, and Götz S. Uhrig — Lehrstuhl für Theoretische Physik I/II, Technische Universität Dortmund, 44221 Dortmund, Germany

Quantum dots on semiconductor materials have been proposed as candidates for quantum computational applications. The information is carried by a single electron spin, which interacts with the substrate nuclei with a hyperfine coupling. The electron spin is manipulated with excitation by periodic laser pulses and by an external magnetic field. The nuclear spins can be polarized indirectly, due to the hyperfine coupling, an effect known as dynamical nuclear polarization.

The leading contribution in the dynamics is the Larmor precession, which dephases due to small frequency shifts from the hyperfine coupling. Typically, the dephasing causes almost complete decoherence at the time scale of the pulse interval. Thus, a different mechanism must be responsible for the finite coherence observed in experiments.

In this presentation, we propose a mechanism explaining the experimental findings. We study the dynamics using the Lindblad equation, which includes the non-unitarity from the decay of the excited state. We separate the time scales of the Larmor precession (fast) and the nuclear-spin dynamics (slow) by treating the hyperfine couplings in a perturbative fashion. We find low-frequency contributions that dephase at a much slower rate, providing a plausible explanation for the finite coherence at the pulse interval time. We support this claim with analytical derivations and numerical results.

30 min. Coffee Break

HL 25.6 Tue 11:15 H15

Force sensing via individual nitrogen-vacancy spins in diamond mechanical resonator — Phani Peddibhotla[1], Michael Barson[2], Kumar Ganesan[3], Preeti Ovartchaiyapong[5], Berndt Koslowski[4], Ania Jayich[5], Steven Prawer[3], Neil Manson[2], Marcus Doherty[2], and •Fedor Jelezko[1] — [1]Institute for Quantum Optics, University of Ulm, 89081 Ulm, Germany — [2]Laser Physics Centre, Australian National University, Canberra, Australia — [3]School of Physics, University of Melbourne, Victoria 3100, Australia — [4]Institute for Solid State Physics, University of Ulm, 89081 Ulm, Germany — [5]Department of Physics University of California, Santa Barbara

We propose to use the embedded nitrogen-vacancy (NV) defect states in single-crystal diamond cantilever for measuring external forces. In order to experimentally demonstrate the force sensing capabilities, we employed an atomic force microscope (AFM) tip to apply a force on the non-clamped end of the diamond cantilever, which in turn induces lattice strain to a NV center close to the clamping point of a cantilever. The strain-mediated coupling between NV spin and diamond mechanics is observable via clear signatures in the optically detected electron spin resonance (ESR) spectrum of the NV center [1, 2].

[1] J. Teissier et al., PRL 113, 020503 (2014). [2] P. Ovartchaiyapong, et al., Nat. Commun. 5:4429 (2014).

HL 25.7 Tue 11:30 H15

Identification of the positively charge Nitrogen Vacancy center in diamond — Helmut Fedder[1], •Sina Burk[1], Mathias Pfender[1], Nabeel Aslam[1], Sebastian Zaiser[1], Philipp Neumann[1], Andrej Denisenko[1], Patrick Simon[2], José Garrido[2], Martin Stutzmann[2], Marcus Doherty[3], Neil Manson[3], Audrius Alkauskas[4], and Jörg Wrachtrup[1] — [1]3. Physikalisches Institut, Uni Stuttgart — [2]Walter Schottky Institut, TU München — [3]Australian National University, Canberra, Australia — [4]Center for Physical Sciences and Technology, Lithuania

Electron and nuclear spins associated with point defects in semiconductors are promising systems for solid state quantum technologies with applications in quantum information processing and quantum sensing. In a typical quantum register architecture, an electron spin is used as an ancilla for readout and control, whereas nuclear spins serve as register qubits [1-2]. Flip-flop processes of the electron spin limit the nuclear spin coherence time. This limitation can be overcome by controlling the defect's ionization state. Here we increase the coherence time of the ^{14}N nuclear spin associated with the Nitrogen-Vacancy center in diamond by controlling its charge state. We exploit planar double junction diodes fabricated by surface transfer doping with hydrogen [3] to rapidly switch the charge state from NV^- (S=1) to NV^+ (S=0). We verify the NV^+ state by nuclear magnetic resonance and demonstrate the enhancement of the ^{14}N coherence time. [1] Saeedi et al., Science 342, 830 (2013). [2] P.C. Maurer et al., Science 336, 1283 (2012). [3] M. Hauf et al., Nano Lett. 14, 2359 (2014)

HL 25.8 Tue 11:45 H15

Electrical Charge State Control of Single Defects in Silicon Carbide — •Matthias Widmann[1], Sang-Yun Lee[1], Matthias Niethammer[1], Ian Booker[2], Takeshi Ohshima[3], Nguyen Tien-Son[2], Adam Gali[4], Erik Janzén[2], and Jörg Wrachtrup[1] — [1]3.Phys. Institut, Stuttgart — [2]Dep. of Phys., Linköping — [3]Japan AEA, Takasaki — [4]Wigner Res.C f.Phys., Budapest

Atomic scale defects in solids attracted a lot of interest over the last decade, because their spins can be used to detect magnetic- and electric fields and temperature with high sensitivity. They are also promising candidates as qubits and used for quantum information processing. Mostly color centers in diamond, e.g. NV centers, and impurities in silicon are used in the past. A single NV spin can be read out optically at room temperature. Electrical readout is possible, but remains challenging. Spins in silicon can be driven and read out electrically very well, however require low temperatures. Spins in silicon carbide (SiC) can overcome these drawbacks. Their spins can be driven and detected both optically[1] and electrically at ambient conditions. SiC electrical properties are promising since integrated single spins in modern electronic devices will allow manipulation of spins in various manners. Here we extend our single defect studies[1] towards electrical manipulation of its charge state in order to get better insight about creation of isolated defects with desired spin quantum number. We will also present how the charge state control affects spin control, and discuss possible applications. 1. M. Widmann et al.,Nat. Mat. 14 (2015)

HL 25.9 Tue 12:00 H15

Spin Coherence Time of Si Vacancies in Silicon Carbide Exceeding One Millisecond — •D. Simin[1], H. Kraus[1,2], A. Sperlich[1], T. Ohshima[2], G. V. Astakhov[1], and V. Dyakonov[1,3] — [1]Experimental Physics VI, Julius Maximilian University of Wuerzburg, 97074 Wuerzburg — [2]Japan Atomic Energy Agency (JAEA), 370-1292 Takasaki, Japan — [3]ZAE Bayern, 97074 Wuerzburg

Quantum information processing has been the hot topic in the field of information theory for several decades. While great progress was achieved, both on the theoretical and experimental field, to recognize and to employ the most suitable material and information carrier from the vast amount of possibilities is still the main goal of ongoing research activities all over the world. Whereas a wide availability and easy handling are crucial for a functioning device, long-preserving spin coherence is also essential for such a system. Therefore, we investigate the coherence time properties of the Si-vacancies in a 4H-SiC wafer using the pulsed-ODMR technique. Implementing the common Rabi-, Ramsey-, Spin-Echo- and CPMG-sequences, we can precisely measure spin-lattice (T_1) and spin-spin (T_2) relaxation times. The measurements are not only conducted at ambient conditions, but also at different temperatures and in different magnetic fields. In particular, the coherent spin properties of the V_{Si} defect are investigated in the temperature range from 10K to 300K and at magnetic field strengths of up to 30mT. Using dynamic decoupling protocols we achieve spin coherence time exceeding 1ms, demonstrating the high potential of SiC for various quantum applications.

HL 25.10 Tue 12:15 H15

Controlled Implantation of Silicon Vacancy Layers for Quantum Applications in Bulk Silicon Carbide — •H. Kraus[1,2], C. Kasper[2], S.-I. Sato[1], M. Haruyama[1], S. Onoda[1], T. Makino[1], T. Ohshima[1], G. Astakhov[2], and V. Dyakonov[2,3] — [1]Japan Atomic Energy Agency, Takasaki, Gunma, Japan — [2]Exp. Physics VI, Julius Maximilian University of Würzburg — [3]ZAE Bayern, Würzburg

Quantum centers in silicon carbide (SiC) have already transcended their former reputation as mere performance-hampering defects. Their long spin lifetime, unique spin-preserving optical pumping mechanism[1], and the possibility of downscaling to single-photon source level[2,3] makes them viable candidates for a plethora of quantum applications in sensing, rf devices, and quantum computing.

One quantum center species, the silicon vacancy (V_{Si}), can be reliably and homogeneously produced in the bulk by electron or neutron[3] irradiation. In contrast, a method to implant defects at a specific depth would be very interesting, especially when aiming for spatially separated centers for single photon sources. We present a study on proton irradiation to create a layer of V_{Si} in an irradiation-energy-tunable depth in bulk SiC. We discuss the spectroscopic response of this layer, and compare the V_{Si} depth profile—measured by confocal microscopy—with the H^+ stopping power of silicon carbide. Finally, we extend this study on the effects of high energy heavy ion damage.

[1] H. Kraus et al., Nature Phys. **10**, 157 (2014)
[2] M. Widmann et al., Nature Mater. **14**, 164 (2015)
[3] F. Fuchs et al., Nature Commun. **6**, 7578 (2015)

HL 26: Quantum Dots and Wires: Quantum Optics I

Time: Tuesday 9:30–11:00 Location: H16

Invited Talk HL 26.1 Tue 9:30 H16

Exploring spin quantum state decoherence in optically active quantum dots — •Jonathan Finley — Walter Schottky Institut and Physik Department, Technische Universität München, Am Coulombwall 4, 85748 Garching, Germany

For spin qubits in optically active quantum dots (QDs) considerable progress has been made in uncovering the qubit dynamics in external magnetic fields ($\mathbf{B}_{ext} \geq 50$ mT). In contrast, decoherence at $\mathbf{B}_{ext} \sim 0$T and specifically the role of quadrupolar coupling of nuclear spins is comparatively poorly understood. Phenomenological models of decoherence typically include *two* basic types of spin relaxation: fast dephasing due to static but randomly distributed hyperfine fields (~ 2ns) and a much slower process ($\geq 1\mu$s) of irreversible monotonic relaxation due either to nuclear spin co-flips or many-body interaction effects. Our results show that electron spin relaxation is determined by *three* rather than two distinct stages (1). The additional stage corresponds to the effect of coherent precession processes that occur in the nuclear spin bath itself, leading to a relatively fast but incomplete non-monotonic relaxation at intermediate timescales and vanishing exernal magnetic fields (~ 750 ns). The interplay between field induced electron spin motion and the quadrupolar induced dynamics of the nuclear field are probed using spin echo. Moreover, we show how new information about spin dynamics can be obtained from direct measurements of two-time spin time correlators ($g^3(\tau_1, \tau_2)$).(2,3) - Refs: (1) A. Bachtold et al., Nature Physics (2015). DOI: 10.1038/nphys3470, (2) A. Bechtold et al. arXiv:1511.03684, (3) R. B. Liu et al, New. J. Phys, 12 013018, (2010)

HL 26.2 Tue 10:00 H16

Dependency of semiconductor quantum dot shape on absorption and pump probe spectra in negatively charged quan-

tum dots — •Matthias Holtkemper, Doris Reiter, and Tilmann Kuhn — Institut für Festkörpertheorie, Universität Münster, 48149 Münster, Germany

Optically operated semiconductor quantum dots (QDs) are promising structures for quantum information, single photon sources and spintronics. In single QD experiments the geometric properties of the QD often play a vital role, however this is experimentally hard to access. Therefore simulations are essential to gain a detailed understanding of the electronic structure and dynamics in QDs in dependence of the QD geometry. We present a systematic analysis of absorption and pump-probe spectra for negatively charged QDs. To be specific, we model a negatively charged CdSe QD using a configuration interaction approach with a harmonic confining potential and include the direct Coulomb interaction as well as the short-range Coulomb exchange interaction (SRE). We calculate trion and charged biexciton states and compute the dynamics after a pump pulse using a Lindblad model. We discuss trends in the spectra caused by a variation of QD volume, asymmetry and height but also of the SRE strength and the difference between electron and hole confinement length. Our results enable us to extract geometric information about a QD from its absorption spectrum.

HL 26.3 Tue 10:15 H16

Transfer of a quantum state from a photonic qubit to a gate defined quantum dot — •Benjamin Jöcker[1], Pascal Cerfontaine[1], Beata Kardynal[2], and Hendrik Bluhm[1] — [1]JARA-Institute for Quantum Information, RWTH Aachen University, D-52056 Aachen, Germany — [2]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, D-52425 Jülich, Germany

An interface between a well-functioning, scalable stationary and a photonic qubit could substantially advance quantum communication applications and serve as an interconnect between future quantum processors. Qubits consisting of gate-defined quantum dots in GaAs are electrically controllable with high fidelity, whereas self-assembled quantum dots are established as an optical interface.
Here, we discuss a procedure to transfer the state of a photonic qubit to a quantum dot spin qubit. In the device under consideration a gate-defined quantum dot is tunnel-coupled to an optically addressable self-assembled quantum dot. When a photon is absorbed in the latter, an exciton is created whose spin configuration depends on the polarization of the photon. By applying an in-plane magnetic field, one can optically address exciton states with identical hole spin. As a result, no quantum information remains in the self-assembled quantum dot when the electron is transferred adiabatically to the gate-defined quantum dot. Using experimentally realistic parameters, we find that this transfer can be completed within the coherence time. We also consider an extension of the protocol to two-electron spin qubits, which have the advantage of being controllable via the exchange interaction.

30 min. Coffee Break

HL 27: Zinc Oxide and Zinc Selenide

Time: Tuesday 9:30–13:00 Location: H17

HL 27.1 Tue 9:30 H17

Self-compensation in Al and Ga doped (Mg,Zn)O PLD thin films — •Abdurashid Mavlonov, Steffen Richter, Holger von Wenckstern, Rüdiger Schmidt-Grund, Michael Lorenz, and Marius Grundmann — Universität Leipzig, Leipzig, Germany

The Al and Ga doping efficiency of transparent conductive (Mg,Zn)O thin films has been investigated in dependence on growth and annealing parameters. For this purpose, the samples have been prepared on glass substrates at RT, 200 °C, and 300 °C by pulsed-laser deposition (PLD) using a continuous composition spread method (CCS) [1, 2]. Further, post-annealing was performed at 400 °C in vacuum in order to analyze the stability of the films. It has been found that growth and annealing conditions have an impact on structural, electrical, and optical properties of the films. With increasing growth temperature, crystallographic quality of the films improved. However, at high temperature, i.e. after post-annealing at 400 °C, the free charge carrier density saturated and optical bandgap decreased. That can be explained by self-compensation of free charge carriers by intrinsic defects [2, 3].

[1] H. von Wenckstern *et al.*, CrystEngComm **15**, 10020 (2013).
[2] A. Mavlonov *et al.*, PSS-A 2015, DOI:10.1002/pssa.201431932.
[3] A. Zakutayev *et al.*, APL **103**, 212306 (2013).

HL 27.2 Tue 9:45 H17

Hybrid top gate transistors based on solution processed Zinc Tin Oxide and organic dielectrics — •Benedikt Sykora and Heinz von Seggern — TU Darmstadt, Materialwissenschaften, Elektronische Materialeigenschaften, Alarich-Weiss-Straße 2, 64287 Darmstadt, Germany

Metal oxide semiconductors like Zinc Tin Oxide (ZTO) are extensively studied because of their solution processability, transparency and cost efficiency. Transistors with top contact configuration are widely reported in literature. Top gate transistors on the contrary have several advantages e.g. protection of semiconducting layer, switching speed.

Here we present hybrid inorganic-organic top-gate transistors based on solution processed ZTO and organic dielectrics. An ethanol based precursor solution route for ZTO was developed that is environmental friendly, cost efficient, simple to process and long term stable. Thin films are investigated by TEM, SEM, XPS, XRD and absorption measurements. Transparent, top gate transistors exhibiting electron mobility values of up to 2.8 $cm^2/(Vs)$ and high on/off ratios exceeding 10^6 were realized.

HL 27.3 Tue 10:00 H17

CMOS-compatible PLD-growth of ultrathin ZnO nanowires — •Alexander Shkurmanov, Chris Sturm, Holger Hochmuth, and Marius Grundmann — Universität Leipzig, Inst. for Exp. Phys. II, Linnéstr. 5, 04103 Leipzig, Germany

An interesting feature of ZnO is self-organized growth of micro- and nanowires (NWs) with high crystalline quality. Comparing to microwires, quantum confinement effects appear in NWs with diameter less than 10 nm. This makes them interesting for quantum effects researches such as topological quibits [1].

Here we present the growth of an array of well oriented ZnO NWs by pulsed laser deposition (PLD). For the NWs growth we used ZnO seed layers which are doped with Al or rather Ga. In dependence on the concentration of these metals in the seed layer we were able to change the diameter of these wires, by two orders of magnitude, i.e from d $\geq$ 550 nm down to 10nm. The aspect ratio for all wires is typically 70. Beside the shape of the wire, the seed layer has also an impact on the optimum growth temperature of the NWs which can be reduced down to 400°C, making them compatible with CMOS technology.

[1] S. Nadj-Perge, et al, Nature 468 (7327),1084, 2010.

HL 27.4 Tue 10:15 H17

Self-consistent hybrid functional calculations: Implications for structural and electronic properties of oxide semiconductors — •Daniel Fritsch, Benjamin Morgan, and Aron Walsh — Department of Chemistry, University of Bath, Claverton Down, BA2 7AY Bath, UK

Density functional theory has proven hugely successful in the calculation of structural properties of condensed matter systems and the electronic properties of simple metals. Band gaps of semiconductors and insulators, however, are often severely underestimated due to the limitations of existing approximate exchange-correlation functionals. Considerable improvements are possible by including a fraction of Hartree-Fock exchange, constructing a so-called "hybrid" functional. The precise proportion of Hartree-Fock exchange is typically treated as an empirical parameter chosen from intuition and experimental calibration.

This empirism can be removed with a recent self-consistent hybrid functional for condensed systems [1], which offers a new approach for parameter-free hybrid functional investigations. Using this approach, we report on the implications for structural and electronic properties of oxide semiconductors, with ZnO, SnO_2, and MgO as specific examples. Structural and electronic properties will be compared to theoretical and experimental data, showing considerable improvement with respect to previous approaches.

[1] J. H. Skone *et al.*, Phys. Rev. B **89**, 195112 (2014).

HL 27.5 Tue 10:30 H17

Mechanisms for p-type conduction in ZnO, (Zn,Mg)O, and related oxide semiconductors — •Daniel F. Urban, Wolfgang Körner, and Christian Elsässer — Fraunhofer Institute for Mechanics of Materials IWM, Wöhlerstr. 11, 79108 Freiburg, Germany

Intrinsically n-type oxide semiconductors like ZnO and (Zn,Mg)O can be turned into p-type materials if a sufficient amount of shallow acceptor defect levels in the band gap is created and a depletion of the net electron concentration which activates the acceptor levels is achieved. Motivated by recent experiments [1,2] on (Zn,Mg)O doped with nitrogen we analyze the defect levels of substitutional nitrogen (N_O), zinc vacancies (v_Zn) and their combination by means of self-interaction-corrected density functional theory calculations. We show how the interplay of defects can lead to the favoured shallow acceptor defect levels, although the levels of isolated point defects N_O lie too deep in the band gap for being responsible for p-conduction. We relate our results to p-type channels seen in polycrystalline ZnO containing grain boundaries [3] which allows us to develop an understanding of p-type mechanisms in ZnO, (Zn,Mg)O, and related materials.

[1] L. Liu, J. Xu, et al, Phys. Rev. Lett. 108, 215501 (2012).
[2] M. N. Amini, et al, Phys. Chem. 17, 5485 (2015).
[3] W. Körner and C. Elsässer, Phys. Rev. B 81, 085324 (2010).

HL 27.6 Tue 10:45 H17

Optimization of seed layer thickness to grow ZnO nanowires for hybrid solar cell applications — •Emily Tansey[1], Alejandra Castro-Carranza[1], Stephanie Bley[1], Jairo C. Nolasco[2], Tobias Voss[3], and Jürgen Gutowski[1] — [1]Institute of Solid State Physics, Semiconductor Optics, University of Bremen, 28359 Bremen — [2]Energy and Semiconductor Research Laboratory, Carl von Ossietzky University of Oldenburg, 26129 Oldenburg — [3]Institute of Semiconductor Technology, TU Braunschweig University of Technology, 38092 Braunschweig

An interesting application of ZnO nanowires is the formation of hybrid junctions with other materials, e.g. polymers, to create solar cells. Wet chemical growth of ZnO nanowires is a low-cost method that implements zinc acetate hexahydrate in solution as a seed layer to form ordered nanostructures on metal oxide substrates. The current-voltage characteristics of this junction, however, show the formation of an unwanted potential barrier at the interface between the ordered nanowires and bottom oxide electrode, which must be considered to get efficient cells. To better understand the impact of the seed layer on this junction, its thickness is modified. Our results indicate that a thicker seed layer yields a higher potential barrier formed at the ZnO nanowires-metal interface. An optimal seed layer thickness for solar cell applications is proposed accordingly.

30 min. Coffee Break

HL 27.7 Tue 11:30 H17

Inversion of absorption anisotropy in wurtzite MgZnO — •Maciej Neumann[1], Martin Feneberg[2], Rüdiger Goldhahn[2], Jean-Michel Chauveau[3], and Norbert Esser[1] — [1]Leibniz-Institut für Analytische Wissenschaften - ISAS - e.V., 12489 Berlin, Germany — [2]Otto-von-Guericke-Universität Magdeburg, 39106 Magdeburg, Germany — [3]University of Nice Sophia-Antipolis, 06103 Nice, France

ZnO and its ternary alloy MgZnO are considered promising candidates for optoelectronic devices operating in the violet and ultraviolet regime. Therefore, the precise knowledge of its optical properties is mandatory. They are characterized by the dielectric function (DF) perpendicular and parallel to the optical axis, respectively.

Using spectroscopic ellipsometry the DFs were obtained from m-plane MgZnO thin films with Mg contents up to 45 %, grown on ZnO substrates by plasma-assisted molecular beam epitaxy. With increasing Mg content the absorption edges of the DFs shift to higher energies, whereas the splitting between the perpendicular and the parallel DF decreases. This results in an inversion of the absorption anisotropy above approximately 24 % Mg content. In order to gain insight this behavior a line shape analysis of the DFs in the vicinity of the bandgap is performed. It considers free excitons, exciton-phonon complexes, and Coulomb enhanced interband transitions, yielding characteristic transitions energies. Using these transition energies the inversion is explained in terms of valence band ordering and oscillator strength.

HL 27.8 Tue 11:45 H17

Schottky barrier diodes on amorphous zinc tin oxide — •Peter Schlupp, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Leipzig, Germany

Amorphous zinc tin oxide (ZTO) can be fabricated at room temperature and exhibits electron mobilities of more than $10\,cm^2V^{-1}s^{-1}$ [1]. This makes its use interesting for channel layers in pixel driving thin film transistors for active matrix displays. Schottky barrier diodes acting as gate are a viable option. They can additionally be employed for material characterization by space charge spectroscopy.

We present Schottky barrier diodes on ZTO using platinum contacts. The semiconducting films are grown by pulsed laser deposition, the Schottky contacts by reactive direct current sputtering. Diodes exhibit rectification ratios of more than 5 orders of magnitude. Temperature dependent current voltage characteristics were obtained and modelled using thermionic emission model. Additionally, capacitance-voltage and thermal admittance spectroscopy were performed. We found two defect levels in a-ZTO, one deep level at about 200 meV and one shallow level near the conduction band minimum who's properties are discussed following the method of Pautrat et al. [2].

[1] Jayaraj et al., J. Vac. Sci. Technol. B **26**, 495 (2008)
[2] Pautrat et al., Solid-State Electron. **23**, 1159 (1980)

HL 27.9 Tue 12:00 H17

Electron-hole recombination dynamics in CdS nanocrystals: limiting steps of photocatalytic H2 generation — •Thomas Simon, Michael Carlson, Jacek Stolarczyk, and Jochen Feldmann — Chair for Photonics and Optoelectronics Ludwig-Maximilians-Universität, Amalienstr. 54, 80799 Munich, Germany

Semiconductors functionalized with additional noble metal clusters are well-known materials for photocatalytic fuel generation. The generation of elemental hydrogen from aqueous solution with cadmium sulfide nanorods decorated with platinum particles is of particular interest. Here the photoexcited electron is efficiently transfered from the semiconductor to the metal where it in turn reduces water molecules to elemental hydrogen. However, the photohole is not able to oxidize the water molecules but has to be removed by a sacrificial reducing agent to prevent the crystal from oxidation [1]. We studied the relaxation and recombination pathways of photoexcited carriers by femtosecond transient absorption spectroscopy. We found that a non-perfect or unstable charge separation finally leads to enhanced electron-hole recombination diminishing the photocatalytic quantum yield. Proper deposition techniques of the co-catalyst particles can bypass this problem.

[1] T. Simon, N. Bouchonville, M.J. Berr, A. Vaneski, A. Adrović, D. Volbers, R. Wyrwich, M. Döblinger, A.S. Susha, A.L. Rogach, F. Jäckel, J.K. Stolarczyk and J. Feldmann Nat. Mat. 13, 1013-1018 (2014)

HL 27.10 Tue 12:15 H17

Magnetic-Field-Induced Second-Harmonic Generation in ZnSe — •Johannes Mund[1], Walter Warkentin[1], and Dmitri Yakovlev[1,2] — [1]Experimentelle Physik 2, Technische Universität Dortmund, 44221 Dortmund, Germany — [2]Ioffe Physical-Technical Institute, Russian Academy of Sciences, 194021 St. Petersburg, Russia

We apply femtosecond laser pulses to ZnSe bulk material to investigate exciton resonances. The non-linear technique of optical second harmonic generation (SHG) allows us to test other excitation rules than in linear optics. Despite the broad bandwidth of the laser pulses we succeed to measure narrow exciton resonances. We present measurements in different crystal directions without and in magnetic fields in voigt and faraday configuration. The polarisation dependency of the SHG intensity is analysed as well. Especially incident light in (100)-direction is of interest as the process of SHG is forbidden in this geometry in the electric-dipole approximation without magnetic field. The application of a magnetic field up to 10 T leads to a rich spectrum of exciton resonances which can be assigned to envelope-hole coupling of the 2P exciton and to landau-levels of the 2P and 3P exciton by comparison with calculations.

HL 27.11 Tue 12:30 H17

ODNMR studies of selenium nuclei in a flourine-doped ZnSe epilayer — •Erik Kirstein[1], Fabian Heisterkamp[1], Alexander Greilich[1], Evgeny A. Zhukov[1], Tomasz Kazimerczuk[1], Dmitri R. Yakovlev[1,2], Alexander Pawlis[3], and Manfred Bayer[1] — [1]Experimentelle Physik 2, Technische Universität Dortmund, 44221

Dortmund, Germany — [2]Ioffe Physical-Technical Institute, Russian Academy of Sciences, 194021 St. Petersburg, Russia — [3]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany

A longitudinal (T_1) and transverse (T_2) relaxation times of selenium nuclei present in a fluorine-doped ZnSe epilayer are studied by optically detected nuclear magnetic resonance. Circularly polarized laser pulses optically orient the electron spins, which in its turn polarize the nuclei. The nuclear polarization of selenium reveals itself as an Overhauser field, affecting, in its turn, the electron Larmor frequency in tranverse magnetic field, measured by Kerr rotation [1]. The changes of the Larmor frequency are then analized in timescale to measure: the time needed for a complete polarization of the nulcear system under the optical excitation (T_{pol}), and the time needed for a system to come back to equilibrium in a complete darkness, T_1. Furthermore, radio frequency pulses are applied to measure the inhomogeneous T_2^* and homogeneous T_2 nuclear spin coherence using Ramsey and Hahn-Echo pulse sequences. Finally, we found that the spin temperature approach is fully justified for that system, as $T_1 \gg T_2$. [1] F. Heisterkamp, *et al.*, arXiv:1508.05295 [cond-mat.mes-hall]

HL 27.12 Tue 12:45 H17

Thermal annealing of GaAs nanowires studied by in-situ time-resolved x-ray diffraction — •Seyed M M Kashani[1], Philipp Schroth[1,2,3], Julian Jakob[2], Jonas Vogel[1], Martin Köhl[3], Tilo Baumbach[2,3,4], and Ullrich Pietsch[1] — [1]University of Siegen, Solid State Physics, Siegen, Germany — [2]Laboratory for Application of Synchrotron Radiation (LAS), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany — [3]Institute for Photon Science and Synchrotron Radiation (IPS), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany — [4]Synchrotron Facility ANKA, Karlsruhe Institute of Technology, Karlsruhe, Germany

In this contribution, we present a first attempt in studying the evolution of sublimation kinetics and polytypism during after-growth annealing of GaAs nanowires by in-situ X-ray diffraction and using a portable MBE chamber. The experiment has been performed at the beamline P09 of PETRA III (DESY) synchrotron using a wavelength of ~0.83 Å. Prior to annealing GaAs NWs were grown by self-catalyzed MBE onto Si(111). In a second step, the characteristic Bragg reflections of zinc-blende (ZB) (220) and (311), and wurtzite (WZ) (10.3) were simultaneously and repeatedly monitored during annealing at nine different temperatures ranging from 270°C to 670°C in steps of 50°C. The decomposition rate of ZB and WZ portions and NW diameters were determined from the evolution of integrated intensity and reflection shape, respectively. Whereas the intensity of WZ reflection decreases continuously, there is a discontinuity of ZB intensity at about 445+-25°C.

HL 28: Transport: Quantum Coherence and Quantum Information Systems - Theory 1 (Joint session of HL, MA and TT, organized by TT)

Time: Tuesday 9:30–12:45 Location: H22

HL 28.1 Tue 9:30 H22

Measurement-induced entanglement of two transmon qubits by a single photon — Christoph Ohm and •Fabian Hassler — JARA Institute for Quantum Information, RWTH Aachen University, 52056 Aachen

On-demand creation of entanglement between distant qubits is desirable for quantum communication devices but so far not available for superconducting qubits. We propose an entanglement scheme that allows for single-shot deterministic entanglement creation by detecting a single photon passing through a Mach-Zehnder interferometer with one transmon qubit in each arm. The entanglement production essentially relies on the fact that superconducting microwave structures allow to achieve strong coupling between the qubit and the photon. By detecting the photon via a photon counter, a parity measurement is implemented and the wave function of the two qubits is projected onto a maximally entangled state. Moreover, due to the indivisible nature of single photons, our scheme promises full security for entanglement-based quantum key distribution.

HL 28.2 Tue 9:45 H22

Quantum Chemistry on a Superconducting Quantum Processor — •Michael P. Kaicher[1], Frank K. Wilhelm[1], and Peter J. Love[2] — [1]Theoretical Physics, Saarland University, 66123 Saarbruecken, Germany — [2]Department of Physics and Astronomy, Tufts University, Medford, MA 02155, USA

Quantum chemistry is the most promising civilian application for quantum processors to date. We study its adaptation to superconducting (sc) quantum systems, computing the ground state energy of LiH through a variational hybrid quantum classical algorithm. We demonstrate how interactions native to sc qubits further reduce the amount of quantum resources needed, pushing sc architectures as a near-term candidate for simulations of more complex atoms/molecules.

HL 28.3 Tue 10:00 H22

Optimization of Quantum Microwave Photodetection for circuit QED applications — •Marius Schöndorf[1], Luke C. Govia[1,3], Maxim Vavilov[2], Robert McDermott[2], and Frank K. Wilhelm[1] — [1]Universität des Saarlandes, Saarbrücken, Deutschland — [2]University of Wisconsin, Madison, USA — [3]McGill University, Montreal, Canada

Superconducting qubits are a promising candidate architecture for quantum computing and information. Readout of the qubit state is an important step that has to be taken for realising quantum algorithms in experiment. Recently we presented a qubit readout scheme [1] using a device called Jospehson Photomultiplier (JPM) [2]. One main step in this architecture is to read out a light state of a transmission line with the JPM. In this work we present a guide how to tune the different parameters in the experiment to optimize the measurement efficiency. We use Input-Output Theory to look at a continuous driven transmission line as well as various pulse states. Using analytical and numerical mehtods, we calculate conditions on the different parameters to optimize the respective measurement.

[1] L. C. G. Govia et al., PRA **92**, 022335 (2015)
[2] Y.-F. Chen et al., PRL **107**, 217401 (2012)

HL 28.4 Tue 10:15 H22

Theory and practice of dressed coherent states in circuit QED — •Frank Wilhelm[1] and Luke C. G. Govia[1,2] — [1]Theoretical Physics, Saarland University, Campus E 2.6, 66123 Saarbrücken, Germany — [2]Department of Physics, McGill University, Montreal, Canada

In the dispersive regime of qubit-cavity coupling, classical cavity drive populates the cavity, but leaves the qubit state unaffected. However, the dispersive Hamiltonian is derived after both a frame transformation and an approximation. Therefore, to connect to external experimental devices, the inverse frame transformation from the dispersive frame back to the lab frame is necessary. We show that in the lab frame the system is best described by an entangled state known as the dressed coherent state, and thus even in the dispersive regime, entanglement is generated between the qubit and the cavity. Also, we show that further qubit evolution depends on both the amplitude and phase of the dressed coherent state. This provides a limitation to readout in the dispersive regime. We show that only in the limit of infinite measurement time is this protocol QND, as the formation of a dressed coherent state in the qubit-cavity system applies an effective rotation to the qubit state. We show how this rotation can be corrected by a unitary operation, leading to improved qubit initialization by measurement and unitary feedback.

[1] L. C. G. Govia and F.K. Wllhelm,
Phys. Rev. Appl. **4**, 054001 (2015)
[2] L. C.G. Govia and F.K. Wilhelm, arXiv: 1506.04997

HL 28.5 Tue 10:30 H22

Gradient optimization for analytic controls — •Elie Assémat[1], Shai Machnes[2], David Tannor[2], and Frank Wilhelm-Mauch[1] — [1]Saarland University, Saarbrücken, Germany — [2]Weizmann Institute of Science, Rehovot, Israël

Quantum optimal control becomes a necessary step in a growing num-

ber of studies in the quantum realm. Recent experimental advances showed that superconducting qubits can be controlled with an impressive accuracy. However, most of the standard optimal control algorithms are not designed to manage such high accuracy. To tackle this issue, a novel quantum optimal control algorithm have been introduced: the Gradient Optimization for Analytic conTrols (GOAT). It avoids the piecewise constant approximation of the control pulse used by standard algorithms. This allows an efficient implementation of very high accuracy optimization. It also includes a novel method to compute the gradient that provides many advantages, e.g. the absence of backpropagation or the natural route to optimize the robustness of the control pulses. This talk will present the GOAT algorithm and a few applications to transmons systems.

HL 28.6 Tue 10:45 H22

Optimal control of single flux quantum (SFQ) pulse sequences — •Per J. Liebermann and Frank K. Wilhelm — Universität des Saarlandes, Saarbrücken

Single flux quantum (SFQ) pulses are a natural candidate for on-chip control of superconducting qubits [1]. High accuracy quantum gates are accessible with quantum optimal control methods. We apply trains of SFQ pulses to operate single qubit gates, under the constraint of fixed amplitude and duration of each pulse. Timing of the control pulses is optimized using genetic algorithms and simulated annealing, decreasing the average fidelity error by several orders of magnitude. Furthermore we are able to reduce the gate time to the quantum speed limit. Leakage out of the qubit subspace as well as timing errors of the pulses are considered, exploring the robustness of our optimized sequence. This takes us one step further to a scalable quantum processor.

[1] R. McDermott, M.G. Vavilov, Phys. Rev. Appl. **2**, 014007 (2014)

HL 28.7 Tue 11:00 H22

Nonlinearities in Josephson-Photonics — •Björn Kubala and Joachim Ankerhold — Institute for Complex Quantum Systems and IQST, Ulm University, Ulm, Germany

Embedding a voltage-biased Josephson junction within a high-Q superconducting microwave cavity provides a new way to explore the interplay of the tunneling transfer of charges and the emission and absorption of light. While for weak driving the system can be reduced to simple cases, such as a (damped) harmonic or parametric oscillator, the inherent nonlinearity of the Josephson junction allows to access regimes of strongly non-linear quantum dynamics.

Classically, dynamical phenomena such as thresholds for higher-order resonances, other bifurcations, and up- and down-conversion have been found [1]. Here, we will investigate how and to which extent these features appear in the deep quantum regime, where charge quantization effects are crucial. Theory allows to employ phase-space quantities, such as the Wigner-density of the cavity mode(s) [2], but also observables amenable to more immediate experimental access, such as correlations in light emission and charge transport, to probe these novel non-equilibrium transitions.

[1] S. Meister, M. Mecklenburg, V. Gramich, J. T. Stockburger, J. Ankerhold, B. Kubala, PRB **92**, 174532 (2015).
[2] A. D. Armour, B. Kubala, J. Ankerhold, PRB **91**, 184508 (2015).

15 min. break

HL 28.8 Tue 11:30 H22

Normal-metal quasiparticle traps for superconducting qubits — •Amin Hosseinkhani — Peter Grunberg Institute (PGI-2), Forschungszentrum Julich, D-52425 Julich, Germany — JARA-Institute for Quantum Information, RWTH Aachen University, D-52056 Aachen, Germany

Superconducting qubits are promising candidates to implement quantum computation, and have been a subject of intensive research in the past decade. Excitations of a superconductor, known as quasiparticles, can reduce the qubit performance by causing relaxation; the relaxation rate is proportional to the density of quasiparticles tunneling through Josephson junction. Here, we consider engineering quasiparticle traps by covering parts of a superconducting device with normal-metal islands. We utilize a phenomenological quasiparticle diffusion model to study both the decay rate of excess quasiparticles and the steady-state profile of the quasiparticle density in the device. We apply the model to various realistic configurations to explore the role of geometry and location of the traps.

HL 28.9 Tue 11:45 H22

Decoherence and Decay of Two-level Systems due to Non-equilibrium Quasiparticles — •Sebastian Zanker, Michael Marthaler, and Gerd Schön — Karlsruher Institut für Technologie, Institut für Theoretische Festkörperpgysik, Karlsruhe, Deutschland

It is frequently observed that even at very low temperatures the number of quasiparticles in superconducting materials is higher than predicted by standard BCS-theory. These quasiparticles can interact with two-level systems, such as superconducting qubits or two-level systems (TLS) in the amorphous oxide layer of a Josephson junction. This interaction leads to decay and decoherence of the TLS, with specific results, such as the time dependence, depending on the distribution of quasiparticles and the form of the interaction. We study the resulting decay laws for different experimentally relevant protocols.

HL 28.10 Tue 12:00 H22

Theory of the double Quantum-dot Maser — •Clemens Müller and Thomas M. Stace — ARC Centre of Excellence for Engineered Quantum Systems, The University of Queensland, Brisbane, Australia

We consider a voltage-biased double quantum-dot (DQD) in the transport regime, dipole-coupled to a superconducting microwave cavity [1, 2]. We explore the effect of dissipative coupling of the DQD to a phononic environment and its influence on microwave gain and loss observed in the resonator. To this end, we develop a rate equation based on fourth-order perturbation theory in the dissipative and coherent DQD interactions. We compare our findings with the recent paper Ref.[3], where a different technique based on the Polaron transformation was used.

[1] Y.-Y. Liu, K. D. Petersson, J. Stehlik, J. M. Taylor, and J. R. Petta, PRL **113**, 036801 (2014)
[2] Y.-Y. Liu, J. Stehlik, C. Eichler, M. J. Gullans, J. M. Taylor, J. R. Petta, Science **347**, 285 (2015)
[3] M. J. Gullans, Y.-Y. Liu, J. Stehlik, J. R. Petta, J. M. Taylor, PRL **114**, 196802 (2015)

HL 28.11 Tue 12:15 H22

Upper bound for SL-invariant entanglement measures for mixed states of arbitrary rank — •Andreas Osterloh — Universität Duisburg-Essen, Lotharstr. 1, 47048 Duisburg, Germany.

I present an algorithm that calculates an SL-invariant entanglement measure E as the threetangle of a mixed state of arbitrary rank. It is an alternative algorithm to ref. [1] and exploits the knowledge obtained for the rank-two case [2,3]. Whereas the known algorithm has an advantage of taking into consideration the whole range of the density matrix ρ, it on the other hand has the disadvantage of searching in a high-dimensional Hilbert space. Here, I only consider ensembles of two states each time but then calculate the upper bound obtained by the method presented in [2,3]. I discuss examples where the advantage of the new algorithm is obvious, but also highlight the obvious disadvantage of only considering rank two parts of ρ.

[1] S. Rodriques, N. Datta, and P. Love, PRA **90**, 012340 (2014)
[2] R. Lohmayer, A. Osterloh, J. Siewert, and A. Uhlmann, PRL **97**, 260502 (2006)
[3] A. Osterloh, J. Siewert, and A. Uhlmann, PRA **77**, 032310 (2008).

HL 28.12 Tue 12:30 H22

Occupation number entanglement in mesoscopic conductors — •David Dasenbrook[1] and Christian Flindt[2] — [1]Université de Genève, Genève, Switzerland — [2]Aalto University, Finland

The controlled entanglement of electrons in mesoscopic conductors has been theoretically investigated before using the spin- and orbital degrees of freedom. By contrast, entanglement of two spatially separated electronic channels using the fermionic occupation number has mostly been considered inaccessible due to the charge superselection rule. However, using non-local measurements or combining several copies of occupation number entangled states, the superselection rules can be lifted and the entanglement can be detected using current and noise measurements. We present the theory for an interferometric setup to detect entanglement in the electron-hole degree of freedom of electronic excitations[1] as well as a mesoscopic setup that demonstrates entanglement and nonlocality of a single electron[2].

[1] D. Dasenbrook and C. Flindt, PRB **92**, 161412(R) (2015)
[2] D. Dasenbrook, J. Bowles, J. Bohr Brask, P. P. Hofer, C. Flindt, and N. Brunner, arXiv:1511.04450 (2015)

HL 29: Hybrid and Perovskite Photovoltaics II (Joint session of CPP, DS and HL, organized by CPP)

Time: Tuesday 10:45–13:00 Location: H37

HL 29.1 Tue 10:45 H37

Charge Carrier Recombination Dynamics in Perovskite and Polymer Solar Cells probed by Time-Delayed Collection Field (TDCF) Experiments — •Andreas Paulke[1], Samuel D. Stranks[2], Juliane Kniepert[1], Jona Kupiers[1], Christian M. Wolff[1], Natalie Schön[1], Henry J. Snaith[2], Thomas J.K. Brenner[1], and Dieter Neher[1] — [1]Institut für Physik und Astronomie, Universität Potsdam, Karl-Liebknecht-Str.24-25, 14476 Potsdam — [2]Department of Physics, University of Oxford, Clarendon Laboratory, Parks Road, Oxford OX1 3PU, United Kingdom

Time-Delayed Collection Field (TDCF) experiments are applied to organometal halide perovskite ($CH_3NH_3PbI_3$) based solar cells to investigate charge carrier recombination in a working solar cell at the nanosecond to microsecond timescale. Planar perovskite solar cells ($ITO/PEDOT:PSS/Perovskite/PCBM/C_{60}/BCP/Al$) display a second-order recombination process with a slow-down of the apparent recombination coefficient over several tens of nanoseconds. In contrast, recombination in the $ITO/TiO_2/mesoporous-TiO_2/Perovskite/Spiro-OMeTAD/Au$ device is governed by a slow first order process, but again with an apparent time-dependence of the recombination coefficient. We also conclude that organometal halide perovskite solar cells differ significantly from prototypical organic bulk heterojunction devices with regard to the mechanism and time-scale of free carrier recombination.

HL 29.2 Tue 11:00 H37

Recombination of photogenerated charge carriers in planar methylammonium lead halide perovskite solar cells — •David Kiermasch[1], Stefan Väth[1], Kristofer Tvingstedt[1], Andreas Baumann[2], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Bavarian Center for Applied Energy Research (ZAE Bayern) Bayern, 97074 Würzburg

In the last years, solar cells based on organo-metal halide perovskites gained a lot of attention. The efficiency of solar cells with a perovskite absorber nowadays reaches more than 20%. With charge carrier mobilities up to tens of $cm^2V^{-1}s^{-1}$ and diffusion lengths exceeding 1 μm transport doesn't seem to be a limiting issue in this new kind of photovoltaic technology. However, recombination of the photgenerated charge carriers is an important factor defining e.g. the open circuit voltage of the solar cell. We prepared different methylammonium lead halide perovskite solar cells in planar configuration. Adressing the recombination dynamics, lifetime and concentration of photogenerated charge carriers are studied by transient photovoltage, charge extraction experiments as well as by the technique of open circuit voltage decay. We measured charge carrier lifetimes in the sub-μs-range for high illumination intensities ($\geq$ 1 sun), which is lower than in state of the art bulk heterojunction cells like P3HT:PCBM. Furthermore we discuss our results for different device morphologies and light-absorbing materials.

HL 29.3 Tue 11:15 H37

Correlating charge carrier mobility, morphology and efficiency in hybrid halide perovskite photovoltaic devices — •Irene Grill[1,2], Michiel Petrus[1,2], Nadja Giesbrecht[1,2], Thomas Bein[1,2], Pablo Docampo[1,2], Matthias Handloser[1,2], and Achim Hartschuh[1,2] — [1]Department of Chemistry and CeNS, LMU Munich — [2]Nanosystems Initiative Munich (NIM)

Hybrid perovskites currently represent one of the most promising material systems for incorporation in future solar cell devices since their efficiencies increased enormously in the last few years [1,2]. To date, fundamental physical properties including charge carrier dynamics and transport in these materials are not completely understood and are therefore at the focus of intense research. Here we extract the mobility of charge carriers in working thin film solar cells based on perovskite absorber layers and correlate it to the efficiency of the respective devices. To this end we performed Time-of-flight (ToF) studies on different perovskite thin films serving as photoactive layers. Further, in order to analyze the influence of contacts and other interfaces on charge transport and to identify possible optimization steps in the stacked architecture we carried out additional ToF measurements on each of the individual layers. Our results are discussed in terms of respective device efficiencies, morphologies and optical properties, allowing for a detailed investigation and identification of the limiting factors for the mobility and the efficiency in perovskite based thin film devices.

[1] M.A. Green and T. Bein, Nature Mater. 2015, 14, 559-561.
[2] N. Jeon et al., Nature 2015, 517, 476-480.

HL 29.4 Tue 11:30 H37

Analysis of electronic trap states in methylammonium lead halide perovskite solar cells via thermally stimulated current — •Philipp Rieder[1], Andreas Baumann[1,2], Stefan Väth[1], Kristofer Tvingstedt[1], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Bavarian Center for Applied Energy Research ZAE, 97074 Würzburg

Organolead halide perovskite solar cells have emerged as one of the most promising technologies in thin-film photovoltaics due to their extraordinary increase in performance in only six years. Yet, the working principles of this material class still lack fundamental understanding. To address the possible influence of electronic traps on device performance, we probed solution processed methylammonium lead halide perovskite solar cells via thermally stimulated current (TSC) analysis.[1] Thereby, the sample is heated from 10 K to 300 K, while monitoring the current flow. This current is attributed to charge carriers being released from previously filled trap states in the semiconductor, allowing drawing conclusions about their distribution and energetic depth. Signals detected at low as well as at high temperatures can be attributed to shallow and deep traps, accordingly. Furthermore, a peak at around T=162 K can be assigned to the reported structural phase transition of the perovskite crystal from orthorhombic to tetragonal crystal lattice structure.

[1] A. Baumann et al., *J. Phys. Chem. Lett.* ***6****, 2350 (2015)*

15 min. break

HL 29.5 Tue 12:00 H37

Tunable ferroelectric polarization and its interplay with spin-orbit coupling in tin iodide perovskite — Alessandro Stroppa[1], •Domenico Di Sante[2], Paolo Barone[1], Menno Bokdam[3], Georg Kresse[3], Cesare Franchini[3], Myung-Hwan Whangbo[4], and Silvia Picozzi[1] — [1]CNR-SPIN L'aquila, Italy — [2]CNR-SPIN L'aquila, Italy and Wuerzburg University — [3]Faculty of Physics, Center for Computational Materials Science, University of Vienna, Wien, Austria — [4]Department of Chemistry, North Carolina State University, USA

Ferroelectricity is a potentially crucial issue in halide perovskites, breakthrough materials in photovoltaic research. Using density functional theory simulations and symmetry analysis, we show that the lead-free perovskite iodide (FA)SnI_3, containing the planar formamidinium cation FA, $(NH2CHNH2)^+$, is ferroelectric. In fact, the perpendicular arrangment of FA planes, leading to a weak polarization, is energetically more stable than parallel arrangements of FA planes, being either antiferroelectric or strong ferroelectric. Moreover, we show that the weak and strong ferroelectric states with the polar axis along different crystallographic directions are energetically competing. Intriguingly, the relatively strong spin-orbit couling in noncentrosymmetric (FA)SnI_3 gives rise to a co-existence of Rashba and Dresselhaus effects and to a spin texture that can be induced, tuned and switched by an electric field controlling the ferroelectric state.

A. Stroppa, D. Di Sante et al., Nature Commun. 5, 5900 (2014)

HL 29.6 Tue 12:15 H37

Mixed Pb:Sn methyl-ammonium halide perovskites: Thermodynamic stability and optoelectronic properties — •Lars Winterfeld, Ksenia Korshunova, Wichard J.D. Beenken, and Erich Runge — Institut für Physik, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Using density functional theory, we investigate systematically mixed $MA(Pb:Sn)X_3$ perovskites, where MA is $CH_3NH_3^+$, and X is Cl, Br or I. Our results cover optoelectronic properties, structural and thermodynamic stability. Ab initio calculations of the orthorhombic,

tetragonal and cubic perovskite phases show that the substitution of lead by tin has a much weaker influence on both structure and cohesive energies than the substitution of the halogen. The thermodynamic stability of the $MA(Pb:Sn)X_3$ mixtures at finite, non-zero temperatures is studied within the Regular Solution Model. We predict that it will be possible to create iodide mixtures at any temperature. Mixing is unlikely for the low-temperature phase of bromide and chloride compounds, where instead local clusters are more likely to form. We further predict that in the high-temperature cubic phase, Pb and Sn compounds will mix for both $MA(Pb:Sn)Br_3$ and $MA(Pb:Sn)Cl_3$ due to the entropy contribution to the Helmholtz free energy. We calculated optoelectronic properties using both DFT and post-DFT methods (including self-consistent GW) with and without spin orbit coupling. Interestingly, the optoelectronic properties are not just a linear combination of the non-mixed parent structures and are not limited by the non-mixed values, which allows band gap engineering.

HL 29.7 Tue 12:30 H37

A model Hamiltonian for perovskite solar cells — •Martin Schlipf, Marina R. Filip, Miguel A. Pérez-Osorio, and Feliciano Giustino — Department of Materials, University of Oxford, Parks Road, Oxford OX1 3PH, United Kingdom

Hybrid organic-inorganic halide perovskites emerge as one of most promising materials for new solar cells based on their high energy-conversion efficiency. The most commonly investigated materials include a large spin-orbit coupling, which may give rise to Rashba and Dresselhaus effects and makes them suitable for spintronic applications. In this contribution, we develop a simple model Hamiltonian that allows to study the impact of the spin-orbit coupling on the band structure. In particular, we focus on the physics near the bottom of the conduction band. Using group-theoretical considerations, we can reduce the number of parameters that the model exhibits. We apply this model to the prototype material $MAPbI_3$ ($MA = CH_3NH_3$) and show how different parameters of the model can be obtained from first-principles density functional theory (DFT) calculations. We discuss how the model can assist in designing improved perovskite solar cells.

HL 29.8 Tue 12:45 H37

Stability and electronic properties of novel perovskites for photovoltaics from high-throughput ab initio calculations — •Sabine Körbel[1,2], Miguel A L Marques[2,3], and Silvana Botti[1,2] — [1]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — [2]Institut Lumière Matière, UMR5306 Université Lyon 1-CNRS, F-69622 Villeurbanne Cedex, France — [3]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany

Using a high-throughput approach based on density functional theory, we perform an extensive search for stable ABX_3 perovskites, where X is a non-metallic anion and A and B are cations spanning the largest portion of the periodic table. Our search is motivated by the necessity to improve the thermodynamic stability of hybrid organo-metal halide perovskite absorbers. We calculate the ternary phase diagram for each composition and we discuss the thermodynamic stability of the perovskite phases. We find a large number of ABX_3 perovskites which are still absent from databases, and which are stable with respect to decomposition into known ternary, binary or elementary phases. For these structures, we then calculate electronic band gaps, hole effective masses, and the spontaneous ferroelectric polarization as relevant material properties for an application as photovoltaic absorbers. We find several novel perovskites which exhibit promising properties for photovoltaic applications. Based on our findings, we discuss possible strategies to improve the thermodynamic stability of perovskite absorbers.

HL 30: Focus Session: On-Chip Quantum Photonics I

Organizers: Simone Portalupi and Peter Michler (Universität Stuttgart)

Time: Tuesday 11:00–13:15 Location: H16

Invited Talk HL 30.1 Tue 11:00 H16

On-chip quantum photonics with integrated quantum dot emitters — •Mark Fox — Department of Physics & Astronomy, University of Sheffield, Sheffield S3 7RH, U.K.

On-chip quantum photonics relies on the integration of efficient single-photon sources with advanced quantum-optical circuits. In this presentation I will review progress at the University of Sheffield on a chip-compatible III-V semiconductor platform in which quantum-dot (QD) single-photon sources are integrated into GaAs photonic circuits. I will first describe work demonstrating a monolithic on-chip Hanbury Brown-Twiss interferometer, a resonantly-excited QD source emitting high coherence single photons into a single-mode waveguide, and an on-chip single-photon router [1]. I will then discuss experiments investigating the coupling of the spin of single QD excitons to circularly-polarized photonic modes on chip [2], focusing on very recent results demonstrating chiral emission from quantum dots embedded in nano-photonic waveguides [3]. These results lay the foundations for more complex photonic integration, opening the route to multi-qubit circuits with advanced quantum-optical functionality.

[1] N. Prtljaga et al., Appl. Phys. Lett. 23, 231107 (2014); M.N. Makhonin, et al. Nano Letters, 14, 6997-7002 (2014); C. Bentham, et al. Appl. Phys. Lett., 106, 221101 (2015)

[2] I.J. Luxmoore, et al. Phys. Rev. Lett., 110, 037402 (2013); R.J. Coles, et al., Optics Express, 22, 2376-2385 (2014)

[3] R. J. Coles et al., arXiv:1506.02266

Invited Talk HL 30.2 Tue 11:30 H16

Quantum photonics with quantum dot single photons in silicon oxynitride waveguide circuits — •Anthony Bennett[1], James Lee[1,2], David Ellis[1], Eoin Murray[1,3], Frederik Floether[1,3], Jonathon Griffiths[3], Thomas Meany[1], Ian Farrer[3], David Ritchie[3], and Andrew Shields[1] — [1]Toshiba Research Europe Limited, Cambridge Research Laboratory, 208 Science Park, Milton Road, Cambridge, CB4 OGZ, United Kingdom. — [2]Engineering Department, University of Cambridge, 9 J. J. Thomson Avenue, Cambridge, CB3 0FA,United Kingdom. — [3]Cavendish Laboratory, Cambridge University, J. J. Thomson Avenue, Cambridge, CB3 0HE, United Kingdom.

The interferometric stability and scalability of silicon oxynitride circuits makes them well suited to quantum optics experiments. Waveguides, phase shifters and couplers can be combined with a semiconductor light source to create an attractive and compact source of few-photon quantum states.

We report our experiments where resonant pi-pulse excitation of quantum dots in micro-pillars creates highly indistinguishable photons. We overlap these photons in a SiON circuit to create a two-photon N00N state, and show its phase super-resolving ability (A. J. Bennett et al, arxiv.org/abs/1508.01637 (2015)). We also report a device where the semiconductor light source is directly bonded to the end facet of the SiON circuit. The photonic circuit is then used to measure the quantum nature of the emitted light and create path-encoded qubits (E. Murray et al, Appl. Phys. Lett. 107, 171108 (2015)).

15 min. Coffee break

Invited Talk HL 30.3 Tue 12:15 H16

GaAs integrated quantum photonics — •S. Höfling[1], C. P. Dietrich[1], A. Fiore[2], M. Thompson[3], and M. Kamp[1] — [1]Technische Physik, Würzburg University, Germany — [2]TU Eindhoven, The Netherlands — [3]University of Bristol, UK

Quantum information processing is a rapidly developing research field. The exploitation of quantum bits instead of classical bits offers key advantages for future technologies including secure communication and ultra-fast computation. Lab-size experiments on quantum information processes have already proven the validity of its concepts. However, any wide spread utilization will require dense integration of functionalities. This requires the realization of semiconductor integrated quantum photonic circuits on a single semiconductor chip with embedded sources, photon processing units and detectors on the single photon level. Among the different material platforms currently being investigated, direct-bandgap semiconductors and particularly gallium ar-

senide (GaAs) offer the widest range of functionalities, including single- and entangled-photon generation by radiative recombination, low-loss routing, electro-optic modulation and single-photon detection. We review recent achievements in quantum integrated photonic components and circuits based on the GaAs technology platform. All key functionalities, including single-photon sources and single-photon detectors, integrated auto-correlators and tuneable Mach-Zehnder interferometers have been realized and tested. These results lay the foundation for a fully-functional and densely integrated quantum photonic technology based on GaAs components.

Invited Talk HL 30.4 Tue 12:45 H16

Photonic integrated circuits with on-chip single-photon emitters based on III-V semiconductors — •Mario Schwartz, Ulrich Rengstl, Thomas Herzog, Matthias Paul, Jan Kettler, Simone Luca Portalupi, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen, Research Center SCoPE and IQST, University of Stuttgart, Allmandring 3, 70569 Stuttgart, Germany

In quantum photonics the full on-chip integration of major optical components, like beamsplitters, single-photon sources and detectors are currently one of the main goals. Here, we present our progress on the implementation of InAs quantum dots as single photon sources in on-chip rib GaAs/AlGaAs waveguide structures. An on-chip evanescent field coupler is shown to act as a 50:50 beamsplitter for single photons, generated by pumping an integrated quantum dot quasi-resonantly and resonantly in order to improve the coherent properties of the emitted photons. The purity of the single photon emission is verified under quasi-resonant and resonant continues wave excitation, by directly measuring the photon correlations at the output arms of the on-chip beamsplitter. Especially for pulsed resonant excitation, we demonstrate that the hurdle of strong laser stray light can be overcome by carefully adjusted laser excitation pulses enabling nearly background free, triggered single-photon emission. This manifests in the observation of clear Rabi oscillations over two periods of the quantum dot emission as a function of laser excitation power. The present results open exciting new perspectives for fully integrated quantum circuits.

HL 31: Silicon-based Semiconductors I

Time: Tuesday 12:15–13:00 Location: H14

HL 31.1 Tue 12:15 H14

Ultrahigh Sensitivity Chemical and Biological Sensors Based on Silicon Junctionless Nanowire Transistors — •Yordan M. Georgiev[1], Ran Yu[2], Elizabeth Buitrago[3], Adrian M. Nightingale[4], Olan Lotty[2], Nikolay Petkov[2], and Justin D. Holmes[2] — [1]Institute of Ion Beam Physics & Materials Research, HZDR, Dresden, Germany — [2]Materials Chemistry and Analysis Group, Department of Chemistry and Tyndall National Institute, UCC, Cork, Ireland — [3]Nanoelectronic Devices Laboratory, EPFL, Lausanne, Switzerland — [4]Nanostructured Materials & Devices Group, Department of Chemistry, Imperial College London, UK

Junctionless nanowire transistors (JNTs) are very promising as chemobiosensors due to their simple structure, easy fabrication and potential for ultrahigh sensitivity. Therefore, JNT sensors with various numbers, lengths, and widths (down to 10 nm) of the nanowires were fabricated by a top-down process on positively doped SOI wafers. The nanowires were functionalised either with 3-aminopropyltriethoxysilane (APTES) or with APTES and biotin. Polydimethylsiloxane (PDMS) stamps with microfluidic channels were then attached to the chip surface and buffer solutions containing different analytes were flowed over the sensors by a syringe pump. In this way, series of experiments for sensing ionic strength, pH value, and the protein streptavidin were performed. The JNT sensors demonstrated the highest sensitivity reported to date towards streptavidin, corresponding to a detection of only few protein molecules.

HL 31.2 Tue 12:30 H14

A microscopic theory of valley dependent g-factors in Si/SiGe quantum dots — •Marko Rancic and Guido Burkard — University of Konstanz, 78464 Konstanz, Germany

In this theoretical study we model a Si/SiGe quantum dot with a micromagnet embedded on top. The micromagnet is present in order to achieve two-axis control of the electron spin states by oscillating it in real space (EDSR). The two-axis control of the electron spin is a necessary prerequisite for implementing a spin-based quantum bit. When both valley-orbit mixing and an in-plane magnetic field gradient are present the electronic g-factor can become valley dependent. The tilted Si/SiGe interface causes the valley and orbit degrees of freedom to mix, while the in-plane magnetic field gradient comes from the micromagnet. The formalism treats step-like interface defects as a continuous tilt of the Si/SiGe quantum well. Our findings suggest that the valley g-factor becomes valley dependent for a large parameter regime of the electrostatic confinement potential. Furthermore, by knowing the measured difference of valley dependent g-factors we are able to predict the valley splitting in a Si/SiGe quantum dot.

HL 31.3 Tue 12:45 H14

Lattice location of Se in hyperdoped Si — •Fang Liu[1,2], Slawomir Prucnal[1], Kun Gao[1,2], René Heller[1], Lars Rebohle[1], Wolfgang Skorupa[1], Manfred Helm[1,2], and Shengqiang Zhou[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Dresden, Germany — [2]Technische Universität Dresden, Dresden, Germany

Se implanted Si wafers with very high doping concentrations exceeding the solid solubility limit have been formed by ion implantation and subsequently by flash lamp annealing. Rutherford backscattering spectrometry/channeling and Raman scattering have been used to determine the recrystallization and lattice location of Se in implanted Si layers after flash lamp annealing. It is found that the crystal order of the implanted sample can be recovered with a high quality after optimal annealing [1]. In order to study the incorporation site of Se, angular maps across planes {100} and {110} were carried out. Prominent channeling effects are observed, which is strong evidence that most of Se atoms are located on substitutional lattice sites. The detailed angular scans along [001] and [110] reveal a small displacement of Se impurities from the substitutional lattice sites.

[1] S. Zhou, F. Liu, S. Prucnal, K. Gao, M. Khalid, W. Skorupa and M. Helm, Scientific Report 5, 8329 (2015).

HL 32: Transport: Quantum Coherence and Quantum Information Systems - Theory 2 (Joint session of HL, MA and TT, organized by TT)

Time: Tuesday 14:00–15:00 Location: H22

HL 32.1 Tue 14:00 H22

Emulating the 1-Dimensional Fermi-Hubbard Model with Superconducting Qubits — •Jan-Michael Reiner, Michael Marthaler, and Gerd Schön — Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany

A chain of qubits with both ZZ and XX couplings is described by a Hamiltonian which coincides with the Fermi-Hubbard model in one dimension. The qubit system can thus be used to study the quantum properties of this model. We investigate the specific implementation of such an analog quantum simulator by a chain of tunable Transmon qubits, where the ZZ interaction arises due to an inductive coupling and the XX interaction due to a capacitive coupling.

HL 32.2 Tue 14:15 H22

A method to efficiently simulate the thermodynamic proper-

ties of the Fermi-Hubbard model on a quantum computer — •Pierre-Luc Dallaire-Demers and Frank K. Wilhelm — Saarland University, Saarbrücken, Germany

Many phenomena of strongly correlated materials are encapsulated in the Fermi-Hubbard model whose thermodynamic properties can be computed from its grand canonical potential. In general, there is no closed form expression of the grand canonical potential for lattices of more than one spatial dimension, but solutions can be numerically approximated using cluster methods. To model long-range effects such as order parameters, a powerful method to compute the cluster's Green's function consists in finding its self-energy through a variational principle. This allows the possibility of studying various phase transitions at finite temperature in the Fermi-Hubbard model. However, a classical cluster solver quickly hits an exponential wall in the memory (or computation time) required to store the computation variables. Here it is shown theoretically that the cluster solver can be mapped to a subroutine on a quantum computer whose quantum memory usage scales linearly with the number of orbitals in the simulated cluster and the number of measurements scales quadratically. A quantum computer with a few tens of qubits could therefore simulate the thermodynamic properties of complex fermionic lattices inaccessible to classical supercomputers.

HL 32.3 Tue 14:30 H22

Scattering of photons on Bose-Hubbard lattices — •Kim Georg Lind Pedersen and Mikhail Pletyukhov — Institute for Theory of Statistical Physics, RWTH Aachen, 52056 Aachen

We study the photonic transport of weakly coherent light in various Bose-Hubbard lattice geometries implemented as QED cavity arrays. We use a diagrammatic scattering approach to study the relation between lattice geometry and the second order intensity correlation of the transmitted light. The motivation is twofold: First, a large induced correlation can be used to design circuit elements useful for "photonics applications". Second, the scattering of photons on complex lattices offers a promising way to characterize quantum correlation in a range of different, exotic states of matter theorized to be present in higher-dimensional cavity arrays.

HL 32.4 Tue 14:45 H22

Quantum Simulation of Hawking Radiation With Surface Acoustic Waves — •Raphael Schmit, Bruno G. Taketani, and Frank K. Wilhelm — Saarland University, Theoretical Physics Departement

In 1975, Hawking predicted particles and light to leave the surface of a black hole. This so called Hawking radiation follows the thermal spectrum of a black body with a certain temperature, called Hawking temperature. Its investigation is extremely desired since scientists believe it to provide clues for unanswered questions like the trans-Planckian problem or the information paradox, but a direct observation is challenging since the Hawking temperature is too small or the distance to the black hole is too large. For this purpose, we propose an experimental setup for emulating a black hole and measuring its analogue Hawking radiation. The setup consists of two adjacent piezoelectric semiconducting layers, one of them carrying a flying qubit serving as detector for Hawking radiation, and the other one with an attached MOS diode structure, imposing an effective curved metric on the surface acoustic wave (SAW) propagation. In the moving reference frame of the flying qubit, this metric matches the Painlevé-Gullstrand-metric describing an uncharged, non-rotating black hole with an event horizon for SAWs. We show that for GaAs as used layer material, the system can possess Hawking radiation in the μK regime. The flying qubit interacts with the Hawking phonons via piezoelectrically induced photons, and thus can be used to measure the temperature of the Hawking phonons.

HL 33: Frontiers of Electronic Structure Theory: Focus on Topology and Transport I

Time: Tuesday 14:00–16:00 Location: H24

Topical Talk HL 33.1 Tue 14:00 H24

Topological semimetals and chiral transport in inversion asymmetric systems — •Shuichi Murakami — Department of Physics and TIES, Tokyo Institute of Technology, Tokyo, Japan

Weyl semimetals (WS) are semimetals with nondegenerate 3D Dirac cones in the bulk. We showed that in a transition between different Z2 topological phases, the Weyl semimetal phase necessarily appears when inversion symmetry is broken. In the presentation we show that this scenario holds for materials with any space groups without inversion symmetry. Namely, if the gap of an inversion-asymmetric system is closed by a change of an external parameter, the system runs either into (i) a Weyl semimetal phase or (ii) a nodal-line semimetal, but no insulator-to-insulator transition happens. This transition is realized for example in tellurium (Te). Tellurium has a unique lattice structure, consisting of helical chains, and therefore lacks inversion and mirror symmetries. At high pressure the band gap of Te decreases and finally it runs into a Weyl semimetal phase, as confirmed by our ab initio calculation. We also theoretically propose chiral transport in systems with such helical structures.

HL 33.2 Tue 14:30 H24

Topological orbital magnetic moments — •Manuel dos Santos Dias, Juba Bouaziz, Mohammed Bouhassoune, Stefan Blügel, and Samir Lounis — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

Orbital magnetic moments are usually associated with the spin-orbit interaction (SOI). We explore from first-principles how topological orbital magnetic moments (TOMs) can emerge in non-trivial magnetic spin textures, even without SOI, justifying the 'topological' label. Firstly, the case of magnetic trimers on the Cu(111) surface illustrates the basic symmetry properties of the TOMs, and how to separate their contribution from the usual SOI-driven orbital moments. We then focus on the implications of TOMs for single magnetic skyrmions formed in Pd/Fe/Ir(111) [1], considering their possible use in detecting and distinguishing skyrmions from anti-skyrmions by optical means.

Work funded by the HGF-YIG Programme FunSiLab – Functional Nanoscale Structure Probe and Simulation Laboratory (VH-NG-717).

[1] D.M. Crum et al., Nat. Comms. **6**, 8541 (2015)

HL 33.3 Tue 14:45 H24

The orbital Rashba effect — •Dongwook Go[1,2], Patrick Buhl[1], Gustav Bihlmayer[1], Yuriy Mokrousov[1], Hyun-Woo Lee[2], and Stefan Blügel[1] — [1]Institute for Advanced Simulation and Peter Grünberg Institut, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — [2]Department of Physics, Pohang University of Science and Technology, 37673 Pohang, Korea

We present a new surface phenomenon called the *orbital* Rashba effect, analogous to the spin Rashba effect. The effect is described by the orbital Rashba Hamiltonian, $H_{\text{orb-R}}(\mathbf{k}) = \alpha_{\text{orb-R}}\mathbf{L}\cdot(\hat{\mathbf{z}}\times\mathbf{k})$, where $\mathbf{L}$ is the orbital moment derived from atomic orbitals and $\alpha_{\text{orb-R}}$ is the orbital Rashba constant. This leads to orbital-dependent energy splittings and orbital texture in the $\mathbf{k}$-space. The mechanism behind the emergence of the $H_{\text{orb-R}}(\mathbf{k})$ can be understood as the $\mathbf{k}$-dependent magnetoelectric coupling due to atomic orbital hybridization. In the presence of intra-atomic spin-orbit coupling, the spin moment is aligned parallel or antiparallel to the orbital moment, thus the spin Rashba effect is recovered. As an example, we present a tight-binding and an *ab initio* study of the Bi/Ag(111) surface alloy, where the hybridization between a Ag s-orbital and a Bi p-orbital leads to the orbital Rasbha effect that is dominant over the spin one. The orbital Rashba effect is a key to new physics and to understanding spin-orbit driven physics at surfaces and interfaces, such as Dzyaloshinskii-Moriya interaction, non-collinear magnetism, etc.

HL 33.4 Tue 15:00 H24

Spin and orbital magnetism of Rashba electrons induced by magnetic nanostructures — •Juba Bouaziz, Manuel dos Santos Dias, Phivos Mavropoulos, Stefan Blügel, and Samir Lounis — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

We explore theoretically the spin and orbital magnetism of Rashba

electrons in the presence of noncollinear impurity-induced magnetic states. The Rashba electron gas mediates the Dzyaloshinksii-Moriya interaction between magnetic impurities favoring chiral states [1]. Here we investigate the back-action of such noncollinear magnetic states on the Rashba electron gas. The presence and distribution of ground state spin and orbital currents is analyzed. Surprisingly, when switching off the spin-orbit coupling, chiral magnetic textures generate bound currents, which implies the existence of orbital magnetic moments originating solely from the peculiar topology of the impurities magnetic moments. In the particular case of a single adatom with an out of plane magnetic moment, we found circular currents flowing around the magnetic impurity in agreement with the continuity equation for the electric charge. Similar results were predicted for magnetic adatoms on superconductor surfaces with a finite spin-orbit coupling [2].
[1] J. Bouaziz *et al.* in preparation.
[2] S. S. Pershoguba *et al.* Phys. Rev. Lett. **115**, 116602 (2015).

This work is supported by the HGF-YIG Programme VH-NG-717 (Functional Nanoscale Structure and Probe Simulation Laboratory).

HL 33.5 Tue 15:15 H24

First-principles investigation of the impact of single atomic defects on magnetic skyrmions — •Imara L. Fernandes, Benedikt Schweflinghaus, Juba Bouaziz, Stefan Blügel, and Samir Lounis — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, D-52425 Jülich, Germany

Chiral magnetic skyrmions are topological spin-swirling textures with rich physics and technological potential in the field of information storage. In a device, skyrmions certainly interact with defects and imperfections resulting into pinning phenomena. We explore from first-principles the non-trivial impact of 3d and 4d impurities on the energetics, electronic and magnetic properties of single magnetic skyrmions. Utilizing the newly developed Jülich full-potential relativistic Korringa-Kohn-Rostoker Green function method [1], we focus on topological magnetic objects of sub-5nm diameters stabilized in a single ferromagnetic layer of Fe sandwiched between the Ir(111) surface and one or two Pd layers, where the tunneling spin-mixing magnetoresistance (TXMR) was demonstrated theoretically [2] and experimentally [3]. – Funding provided by the HGF-YIG Program VH-NG-717 and the CNPq (BRAZIL).
[1] D. S. G. Bauer, Schriften des Forschungszentrum, Key Tech. **79** (2014).
[2] D.M. Crum *et al.*, Nat. Comms. **6**, 8541 (2015).
[3] C. Hanneken *et al.*, Nat. Nanotech. Doi:10.1038/nano.2015.218 (2015).

HL 33.6 Tue 15:30 H24

Topological magnons: Any chance to find them? — •Alexander Mook[1], Jürgen Henk[2], and Ingrid Mertig[1,2] — [1]Max-Planck-Institut für Mikrostrukturphysik, D-06120 Halle — [2]Institut für Physik, Martin-Luther-Universität, D-06120 Halle

Topological magnon insulators (TMIs) have a nontrivial topology due to the Dzyaloshinskii-Moriya interaction which results in spatially confined edge states and, thus, energy and spin currents along their edges [1,2]. Several systems have been identified as TMIs, for example, Cu(1,3-benzenedicarboxylate) consisting of kagome planes [3], or the family of ferromagnetic pyrochlore oxides, e. g., $Lu_2V_2O_7$, showing the magnon Hall effect [4]. However, to date, no direct experimental evidence of a topological magnon band has been provided, what comes down to the small total width of the magnon dispersion relation and the energy resolution of surface sensitive measurements.

We propose Fe_3Sn_2 as promising candidate for a TMI. The total width of its magnon dispersion relation is large, and we determine its nontrivial topology by constructing an effective spin Hamiltonian. On this basis, we discuss signatures of topological magnon states that should be looked for in experiments.

[1] L. Zhang et al., PRB **87**, 144101 (2013); [2] A. Mook et al., Phys. Rev. B **89**, 134409 (2014); *eidem*, Phys. Rev. B **90**, 024412 (2014); *eidem*, Phys. Rev. B **91**, 224411 (2015); *eidem*, Phys. Rev. B **91**, 174409 (2015); [3] R. Chisnell et al., Phys. Rev. Lett. **115**, 147201 (2015); [4] Y. Onose et al., Science **329**, 297 (2010).

HL 33.7 Tue 15:45 H24

Acoustic magnons in the long-wavelength limit: resolving the Goldstone violation in many-body perturbation theory — •Mathias C.T.D. Müller, Christoph Friedrich, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Ferromagnetic materials exhibit a spontaneously broken global rotation symmetry in spin space leading to the appearance of massless quasiparticles (zero gap) in the long-wavelength limit. These magnons are formed by the correlated motion of electron-hole pairs with opposite spins, which we describe from first principles employing the T-matrix formalism in the ladder approximation within the FLAPW method [1]. Due to approximations used in the numerical scheme, the acoustic magnon dispersion exhibits a small but finite gap at Γ. We analyze this violation of the Goldstone mode and present an approach that implements the magnetic susceptibility using a renormalized Green function instead of the Kohn-Sham (KS) one. This much more expensive approach shows substantial improvement of the Goldstone-mode condition. In addition, we discuss a possible correction scheme, that involves an adjustment of the KS exchange splitting, which is motivated by the spin-wave solution of the one-band Hubbard model. The new exchange splittings turn out to be closer to experiment. We present corrected magnon spectra for the elementary ferromagnets Fe, Co, and Ni.
[1] E. Şaşıoğlu *et al.*, Phys. Rev. B **81**, 054434 (2010); C. Friedrich *et al.* Top. Curr. Chem. **347**, 259 (2014).

HL 34: Magnetic Semiconductors I (Joint session of HL and MA, organized by MA)

Time: Tuesday 14:00–15:15 Location: H31

HL 34.1 Tue 14:00 H31

Magnetic Semiconductor (Ga,Mn)As Studied by Fluctuation Spectroscopy — •Martin Lonsky[1], Jan Teschabai-Oglu[1], Klaus Pierz[2], Hans Werner Schumacher[2], and Jens Müller[1] — [1]Physikalisches Institut, Goethe-Universität, Frankfurt (M), Germany — [2]Physikalisch-Technische Bundesanstalt, 38116 Braunschweig, Germany

In spintronics, both charge and spin degrees of freedom of the electronic transport properties are utilized. Recent studies on diluted magnetic semiconductors (DMS), as for instance (Ga,Mn)As, raised hopes of applications combining the logic operations of semiconductor devices with the information storage capabilities of magnetic elements. However, ferromagnetism at room temperature has not yet been achieved in DMS, and the underlying mechanism is still subject of investigation. In this context, theoretical studies have discussed the percolation of magnetic polarons as a possible origin of spontaneous magnetization [1]. Motivated by recent results of a diverging $1/f$-noise magnitude in the ferromagnetic semimetal EuB_6, where the existence of percolating nanoscale magnetic clusters has been demonstrated [2], we apply fluctuation spectroscopy to (Ga,Mn)As in order to gain a better understanding of the coupling between charge transport and magnetism. Systematic (magneto-)transport studies are conducted on epitaxial thin films of (Ga,Mn)As [3] with different growth parameters.
[1] A. Kaminski and S. Das Sarma, Phys. Rev. Lett. 88, 247202 (2002)
[2] P. Das et al., Phys. Rev. B 86, 184425 (2012)
[3] A. B. Hamida et al., Phys. Stat. Solidi B 251, 1652 (2014)

HL 34.2 Tue 14:15 H31

Defect induced magnetism in SiC — •Shengqiang Zhou — Helmholtz-Zentrum Dresden Rossendorf, Institute of Ion Beam Physics and Materials Research, Bautzner Landstrasse 400, D-01328 Dresden, Germany

Defect-induced magnetism is attracting intensive research interest. It not only challenges the traditional opinions about magnetism, but also has some potential applications in spin-electronics. SiC is a new candidate for the investigation of defect-induced ferromagnetism after graphitic materials and oxides due to its high material purity and crystalline quality [1, 2]. In this contribution, I will review our comprehensive investigation on the structural and magnetic properties of ion implanted and neutron irradiated SiC sample.

The magnetization in ion irradiated SiC can be decomposed into paramagnetic, superparamagnetic and ferromagnetic contributions [3,4]. The ferromagnetic contribution persists well above room temperature and exhibits a pronounced magnetic anisotropy. By combining X-ray magnetic circular dichroism and first-principles calculations, we clarify that p-electrons of the nearest-neighbor carbon atoms around divacancies are mainly responsible for the long-range ferromagnetic coupling [5]. Thus, we provide a correlation between the collective magnetic phenomena and the specific electrons/orbitals.

[1] APL 98, 222508 (2011); [2] PRB 90, 214435 (2014); [3] PRB 89, 014417 (2014); [4] PRB, 92, 174409 (2015); [5] Sci. Rep., 5, 8999 (2015).

HL 34.3 Tue 14:30 H31

Spin-lattice-relaxation of Bismut doped Silicons slabs in air - a DFT approach. — •Johannes Gugler and Peter Mohn — Center for Computational Materials Science, Vienna, Austria

ESR experiments show that Bismuth doped Silicon exhibits a relaxation-time up to 1 ms at 10 K. These huge values are obtained due to the electron-spin-free surrounding in a Silicon crystal. The absence of electron-spins makes spin-lattice-relaxation a process of interest, when it comes to quantum dots. We present a DFT-investigation of the crystalographic structure, the DOS, the phonon spectra and the configuration of Bismuth doped (100)- and (111)-Silicon surfaces in air. We evaluate the influence of different position of the Bismuth atom inside the silicon slab on the spin-lattice-relaxation mechanisms.

HL 34.4 Tue 14:45 H31

Interface control of electronic transport across the magnetic phase transition in SrRuO3/SrTiO3 heterointerface — •Carmine Autieri[1], Saurabh Roy[2], Biplab Sanyal[1], and Tamalika Banerjee[2] — [1]Department of Physics and Astronomy, Uppsala University, Box-516, 75120 Uppsala, Sweden — [2]Physics of Nanodevices, Zernike Institute for Advanced Materials, University of Groningen, Groningen 9747 AG,The Netherlands

The emerging material class of complex-oxides, where manipulation of physical properties lead to new functionalities at their heterointerfaces, is expected to open new frontiers in Spintronics. For example, SrRuO3 is a promising material where external stimuli like strain, temperature and structural distortions control the stability of electronic and magnetic states, across its magnetic phase transition, useful for Spintronics. Despite this, not much has been studied to understand such correlations in SrRuO3. Here we explore the influence of electron-lattice correlation to electron-transport, at interfaces between SrRuO3 and Nb:SrTiO3 across its ferromagnetic transition, using a nanoscale transport probe and first-principles calculations. We find that the geometrical reconstructions at the interface and hence modifications in electronic structures dominate the transmission across its ferromagnetic transition, eventually flipping the charge-transport length-scale in SrRuO3. This approach can be easily extended to other devices where competing ground states can lead to different functional properties across their heterointerfaces.

HL 34.5 Tue 15:00 H31

Transport effects in $LaCo_5$ and YCo_5 upon electronic topological phase transitions — •Jürgen Weischenberg and Hongbin Zhang — Materialwissenschaft, TU Darmstadt Alarich-Weiss-Straße 2, 64287 Darmstadt, Germany

It is an interesting phenomenon that in $RECo_5$ (RE = La, Y) strong pressure can lead to a Lifshitz transition, which is manifested by an isomorphic lattice collapse. As the lattice collapses and the distance between the atoms decreases, the overlap of their orbitals becomes larger and leads to an alteration of the Fermi surface topology, i.e., an electronic topological phase transition (ETT). Transport properties can be utilized to characterize the ETT, since they are determined by the details of the electronic structure at the Fermi energy level. In this work, to understand recent experiments in $LaCo_5$ [1], we carry out first principle calculations of various transport properties using the full-potential linearized augmented plane-wave method (FLAPW) within density functional theory. In particular, we consider both the intrinsic and the side-jump contribution to the anomalous Hall effect which can be computed directly from the electronic structure of the pristine crystal alone [2]. The impact of the Fermi surface topologies on the electric- as well as on the thermoelectric transport properties in $LaCo_5$ and YCo_5 is discussed. Financial support by German federal state of Hessen through its excellence program LOEWE RESPONSE is gratefully acknowledged.

[1] R. L. Stillwell *et al.*, Phys. Rev. B **92**, 174421 (2015)
[2] J. Weischenberg *et al.*, PRL 107, 106601 (2011)

HL 35: Poster I

Topics: Spintronics, Topological insulators, Group IV (other than C): Si/Ge/SiC, Nitrides: Preparation and Characterization, Nitrides: Devices, III-V semiconductors (other than nitrides))

Time: Tuesday 15:00–19:00 Location: Poster A

HL 35.1 Tue 15:00 Poster A

Properties and definitions of the spin current — •Thorsten Arnold[1], Vidar Gudmundsson[2], and Frank Ortmann[1] — [1]Institute for Materials Science and Dresden Center for Computational Materials Science, TU Dresden, Germany — [2]Science Institute, University of Iceland, Iceland

As opposed to the charge, the spin is not conserved in systems, where spin-orbit interaction or magnetic fields are present. As a consequence, the definition of the spin current is not unique and several suggestions for the definition of the spin current have been proposed [1-3]. The Rashba spin current [3] and the definition $\hat{\mathbf{j}}_\alpha = \frac{1}{2}[\hat{\sigma}_\alpha \hat{\mathbf{v}} + \hat{\mathbf{v}}\hat{\sigma}_\alpha]$ agree for many systems [4]. We use the latter definition to describe a spin current in a tight-binding model to calculate the spin conductivity. We show the spin current in an Aharonov-Casher ring as well as the energy and time resolved spin conductivity in graphene, which we compare to spin relaxation properties of graphene [5].

[1] J. Shi et al., Phys. Rev. Lett. **96**, 076604 (2006).
[2] N. Bray-Ali, and Z. Nussinov, Phys. Rev. B **80**, 012401 (2009).
[3] E.I. Rashba, Phys. Rev. B **68**, 241315 (2003).
[4] T. Arnold et al., Eur. Phys. J. B **87**, 113 (2014).
[5] D. V. Tuan et al., Nature Physics **10**, 857 (2014).

HL 35.2 Tue 15:00 Poster A

Spin Hall conductivity in topological insulators — •Francisco Mireles[1] and John Schliemann[2] — [1]Departamento de Física Teórica, Centro de Nanociencias y Nanotecnología, Universidad Nacional Autónoma de México, Ensenada, BC, 22800, México. — [2]Institut für Theoretische Physik, Universität Regensburg, D-93049 Regensburg, Germany.

Since the discovery of topological insulators in which topological states of matter are protected by time-reversal symmetry, there has been a great deal of interest in the physics of these materials. It is known that they can support helical two-dimensional states at its edges. An important feature is the hexagonal warping of the Hamiltonian of the charge carriers describing these systems. As a result, fundamentally different behavior is expected to appear in the spin and carrier transport in these systems. In particular, the physics of the spin transport and optical spin conductivities in topological insulators is still to be understood. In this work special attention is given to the study of spin-transport properties in such topological insulators. We study the Hall and optical Hall spin-conductivities within the Kubo formalism in linear response. We also present some useful analytical expressions describing the spin-currents in such topological massive Dirac Fermions systems.

* This work was supported by project 'Spin Phenomena in Reduced Dimensions' SFB 689, and DIONICOS project: 612707- FP7-PEOPLE-2013-IRSES.

HL 35.3 Tue 15:00 Poster A

Spin dynamics of Ce^{3+} ions in YAG crystals — •Felix Fobbe[1], Vasilii Belykh[1], Donghai Feng[1], Eiko Evers[1], Dmitry Yakovlev[1,2], and Manfred Bayer[1,2] — [1]Experimentelle Physik 2,

Technische Universitat Dortmund, D-44221 Dortmund, Germany — [2]Ioffe Institute, Russian Academy of Sciences, 194021 St. Petersburg, Russia

Spin dynamics of YAG crystals doped with Ce^{3+} ions were investigated by optical pump-probe Faraday rotation technique in a magnetic field. Resonant spin amplification (RSA) was measured by registering the amplitude of the Faraday rotation as a function of a magnetic field applied either in Voigt or Faraday geometry. Measurements were made at different temperatures and powers of the pump beam.

From the time resolved Faraday rotation it was shown that there are up to five electron spin precession frequencies that correspond to five g-factors ranging from 0.9 to 2.5 which show strong anisotropy. The spin ensemble dephasing time T_2^* is found to be in the range of 10 ns to 50 ns for the different frequencies. The RSA curve shows a strong peak around zero magnetic field in Voigt geometry and a strong dropdown in Faraday geometry. The amplitude of the peak and the dropdown decreases dramatically with increasing temperature. Their origin is presumably related to spin interaction.

HL 35.4 Tue 15:00 Poster A

Fine structure and coherent spin manipulation of the hidden transition of V_{Si} in 4H-SiC — •Matthias Niethammer[1], Sang-Yun Lee[1], Matthias Widmann[1], Ian Booker[2], Torsten Rendler[1], Takeshi Oshima[3], Nguyen Tien-Son[2], Erik Janzón[2], and Joerg Wrachtrup[1] — [1]3.Physikalisches Institut, Universitaet Stuttgart — [2]Department of Physics, Chemistry and Biology, Linkoeping University — [3]Japan Atomic Energy Agency, Takasaki

Silicon carbide has recently been recognized as a promising host material for mainstream room temperature quantum devices based on defects [1]. The silicon vacancy is a point defect with a spin $\frac{3}{2}$ ground state and a zero field splitting of 70MHz which allows for optical control and coherent manipulation even on the single spin level at room temperature [2]. As high impurity density is detrimental for defect based solid state quantum systems, wafer quality is a concern. Here we analyse various fine structures in optically detected spin signal at low magnetic field and present likely models related to wafer quality for their origin. When an axial magnetic field is applied, the spin Hamiltonian predicts three transitions, but usually only two are visible due to equal population. The third transition previously has been revealed by ENDOR measurements [3]. We demonstrate the hidden transition ($m_s = -\frac{1}{2} \leftrightarrow m_s = \frac{1}{2}$) also becomes optically observable by inducing population difference using ELDOR. Additionally we present the coherent manipulation of this hidden transition. 1. Weber et al, PNAS 2010 107 (19) 8513-8518 2. Widmann et al, Nat. Mater 14, 164-168 (2015) 3. Mizuochi et al, Phys. Rev. B 72, 235208 (2005)

HL 35.5 Tue 15:00 Poster A

All optical EPR in magnetically doped quantum structures — •Markus Kuhnert, Ilya Akimov, Dmitri Yakovlev, and Manfred Bayer — Experimentelle Physik 2, TU Dortmund

The field of spintronics, which in contrast to electronics, uses the spin instead of charge as information carrier, presents many interesting possibilities. For proper implementation of spintronic devices, research of adequate materials and methods is required. Here we present the results of our research into Manganese doped GaAs quantum wells, which might offer long lived spin coherence as well as spin manipulation mediated by the magnetic Manganese ions. Following initial studies of electron lifetime in Manganese-doped GaAs quantum wells via time resolved Kerr effect and time resolved Photoluminescence measurements, further investigation into such samples is done by Electron paramagnetic resonance measurements. In this case, a method of all optical Electron paramagnetic resonance was developed. This is achieved by intensity and polarization modulation of the incident laser beam by a frequency of about 9.2 GHz and applying varying external magnetic fields.

HL 35.6 Tue 15:00 Poster A

Spin-flip Raman scattering of the Mn^{2+} ions in (Zn,Mn)Se quantum wells — •Carolin Lüders[1], Henning Moldenhauer[1], Philipp Waldkirch[1], Dennis Kudlacik[1], Victor F. Sapega[1,2], Andreas Waag[3], Jörg Debus[1], and Manfred Bayer[1,2] — [1]Experimentelle Physik 2, Technische Universität, 44227 Dortmund, Germany — [2]Ioffe Institute, Russian Academy of Sciences, 194021 St. Petersburg, Russia — [3]Institute of Semiconductor Technology, University of Braunschweig, 38106 Braunschweig, Germany

A comprehensive and unified picture of the Mn-ion interactions with carriers in diluted magnetic semiconductors is still missing up to now. Therefore, we have studied the resonant spin-flip Raman scattering (SFRS) of the Mn^{2+} ions in $Zn_{1-x}Mn_xSe$/(Zn,Be)Se quantum-well structures with low Mn concentrations ($x \leq 0.04$) and type-I band alignment. Previous studies focused on the multiple Mn^{2+} SFRS in tilted geometries, where the magnetic field direction embraced an angle with the quantum-well growth axis; while, for example, the explanation of the Faraday-geometry mechanism was not yet clarified. We propose a Mn^{2+} spin-flip mechanism for the Faraday geometry, and demonstrate the presence of anti-Stokes Mn^{2+} scattering signals, whose Raman shifts are moreover considerably different to that of the Stokes lines. Additionally, the resonance profile shows that the spin-flips occur preferably under resonant excitation of the heavy-hole exciton.

HL 35.7 Tue 15:00 Poster A

Conductance Correction in semiconductor nanorods with Rashba and Dresselhaus Spin-Orbit Coupling — •Michael Kammermeier[1], Paul Wenk[1], John Schliemann[1], Sebastian Heedt[2], and Thomas Schäpers[2] — [1]Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany — [2]Peter Grünberg Institute and JARA-Fundamentals of Future Information Technology, Forschungszentrum Jülich, 52425 Jülich, Germany

We compute analytically the quantum correction to the Drude conductivity for electrons in zincblende type nanorods following former approaches [1,2]. In the systems of consideration a tubular quantum well is formed below the nanorods surface which can be a result of Fermi surface pinning [3] or band mismatch in core/shell nanowires [4]. The confinement gives rise to both Rashba and Dresselhaus spin-orbit coupling (SOC) which we comprise in our calculations and compare for wires of standard growth directions $\langle 111 \rangle$, $\langle 001 \rangle$ and $\langle 110 \rangle$. The motion on the quasi two-dimensional surface is considered diffusive in both in-plane directions. By fitting the theory to experimental data we extract SOC strength as well as dephasing and relaxation rates.

* * *

[1] S. Kettemann, PRL **98** 176808 (2007)
[2] P. Wenk *et al.*, PRB **83** 115301 (2011)
[3] S. Heedt *et al.*, Nanoscale **7** 18188 (2015)
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HL 35.8 Tue 15:00 Poster A

Identification and magneto-optical properties of the NV center in 4H-SiC — Hans Jürgen von Bardeleben[1], Jean-Louis Cantin[1], Soroush Abbasi-Zargaleh[2], Benoît Eblé[1], Sophie Hameau[1], Eva Rauls[3], and •Uwe Gerstmann[3] — [1]INSP, Université Pierre et Marie Curie, 75005 Paris — [2]Université Paris-Sud, 91405 Orsay — [3]Uni Paderborn, Warburger Strasse 100, 33098 Paderborn

Single spin carrying defects are key elements in quantum information and nanosensing technology with the nitrogen-vacancy (NV) center in diamond being the outstanding example [1], stimulating the search for similar defects in alternative materials with superior material properties. In a combined electron paramagnetic resonance and density functional theory (DFT) study we verify the existence of such NV centers in 4H-SiC in the form of silicon vacancy-nitrogen pairs ($V_{Si}N_C$) and explore their basic magneto-optical properties [2].

Optical polarization of the ground state is indeed very similar to that of the NV center in diamond, whereby in 4H-SiC: (i) the sensitivity with temperature is found to be two times larger, and (ii) the PL spectrum is shifted towards the near infrared. Given the high potential of 4H-SiC as concerns doping and nanostructuring, the NV center in 4H-SiC is expected to be suitable for multiple applications.

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[2] H.J. von Bardeleben, J.L. Cantin, E. Rauls, and U. Gerstmann, Phys. Rev. B **92**, 064104 (2015).

HL 35.9 Tue 15:00 Poster A

Time-resolved photoluminescence and spin dynamics of GaSe crystals — •Maike Halbhuber, Philipp Nagler, Christian Schüller, and Tobias Korn — Institut für Experimentelle und Angewandte Physik, Universität Regensburg, 93040, Regensburg, Germany

Gallium Selenide (GaSe) is a layered semiconductor with a direct band gap of about 2.02 eV at room temperature at the Γ-point. Its peculiar band structure allows optical generation and detection of spin polarization. Here, we investigate the emission spectra of GaSe thin films by means of continuous-wave (cw) and time-resolved μ-photoluminescence (PL). Our samples are prepared by mechanical exfoliation from GaSe

bulk. In temperature-dependent cw PL measurements we could extract a red-shift of the direct free-exciton recombination energy which can be well explained by a Varshni Fit. The degree of spin polarization showed a strong temperature dependence, resulting in a decrease of the time-averaged spin polarization with increasing temperature. Furthermore we studied the lifetime of the PL and the spin polarization by using a streak camera system. Thereby we see dependencies of the spin polarization on both temperature and excitation wavelength. By applying an in-plane magnetic field we observe precession of the spin polarization which enables the determination of the g-factor of GaSe.

HL 35.10 Tue 15:00 Poster A

Low magnetic field wavelength modulation absorption spectroscopy of donor bound excitons in ^{28}Si:P — •Michael Beck[1], Helge Riemann[2], Jens Hübner[1], and Michael Oestreich[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstrasse 2, D-30167 Hannover — [2]Leibniz Institut für Kristallzüchtung, Max-Born-Strasse 2, D-12489 Berlin

Donor atoms in a crystalline silicon host are promising candidates for the implementation of quantum information devices [1]. The decoupling of donor atoms from the nuclear spin bath of the host lattice by means of isotopical enrichment leads to very long coherence times of donor electron spins [2]. We will employ non-perturbative spin noise spectroscopy [3] to unveil the intrinsic spin dynamics of donor bound electrons in weakly doped ^{28}Si:P in the millikelvin temperature regime. As preparatory measurements, we investigate the electronic structure of the donor-bound exciton in a magnetic field by means of modulation absorption spectroscopy, which allows for a determination of the oscillator strength and fine structure. The ultra-narrow linewidth [4] of the bound exciton transition furthermore reveals the magnetic field dependence of the electron and hole Landé g-factor at low magnetic fields.

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[3] J. Hübner *et al.*, Phys. Stat. Solidi (B) **251**, 1824 (2014).
[4] M. L. W. Thewalt *et al.*, J. Appl. Phys. **101**, 081724 (2007).

HL 35.11 Tue 15:00 Poster A

Spin Noise Spectroscopy on single InAs Quantum Dots — •Julia Wiegand[1], Ramin Dahbashi[1], Jens Hübner[1], Klaus Pierz[2], and Michael Oestreich[1] — [1]Leibniz Universität Hannover, Institut für Festkörperphysik, Abteilung Nanostrukturen, Appelstraße 2, D-30167 Hannover, Germany — [2]Physikalisch Technische Bundesanstalt, Bundesallee 100, D-38116 Braunschweig, Germany

The spin dynamics of electrons and holes confined in InAs quantum dots (QDs) are of particular interest for future applications in solid state quantum information processing. We implement spin noise spectroscopy (SNS) to access the intrinsic spin dynamics of confined carriers in individual QDs [1]. Measurements on single heavy hole spins reveal a strong magnetic field dependence of the longitudinal spin relaxation time for low magnetic fields with relaxation times up to 180 μs [2]. The dependence of the relaxation times on the probe laser intensity suggests residual light absorption that shortens the measured times. Improvement of the SNS method for single QDs should be achieved for increased probe laser detunings, that avoid light absorption and allow for higher probe intensities to enhance the signal-to-noise ratio.

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[2] R. Dahbashi, J.Hübner, F. Berski, K. Pierz, and M. Oestreich, Phys. Rev. Lett. **112**, 156601 (2014).

HL 35.12 Tue 15:00 Poster A

Stokes Polarimetry of Magnetic Linear Birefringence in Gallium Arsenide — •Pavel Sterin, Fabian Berski, Agnes Beichert, Jens Hübner, and Michael Oestreich — Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstr. 2, D-30167 Hannover, Germany

Recently, an intriguing excitation mechanism of spin polarized carriers by linearly polarized light was observed in non-centrosymmetric InGaAs. Interestingly, the experimental signatures were interpreted as two dimensional control of the electron spin orientation. [1] However, for an in-depth understanding we employ a highly sensitive, self-built polarimeter and explore the interplay of oblique light propagation and linear birefringence caused by an applied magnetic field. A generalized Mueller-matrix approach allows us to recover unambiguously the complete polarization state of the transmitted laser light. Moreover, the ellipticity and orientation as function of angle of incidence and magnetic field strength are investigated using a 4×4-matrix formalism. [2] Finally, first measurements on well-known gallium arsenide prove the general suitability of our method.

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[2] D. W. Berreman, JOSA **62** 502-510 (1972)

HL 35.13 Tue 15:00 Poster A

Weak Anti-Localization and Bulk-Surface-Correspondence in Topological Insulators — •Sebastian Hutsch and Frank Ortmann — Institute for Materials Science and Dresden Center for Computational Materials Science, TU Dresden, Germany

Topological Insulators have drawn considerable attention in solid state physics in recent years, also leading to investigations of their properties by the means of simulations. Effective models for isolated surface states of 3D TIs have been used to describe experimentally studied phenomena like Weak Anti-Localization of such states. Beyond that, an influence of the bulk states on transport properties as observed in experiment could not be modeled accurately because a full 3D model of the topological insulators (including both, bulk and surface) is needed for realistic simulations.

In this work, the Fu-Kane-Mele model, a 3D generalization of the Quantum-Spin-Hall system graphene, is used for the transport simulations in the Kubo framework, where we study localization behaviour for the strong topological phase and weak disorder.

HL 35.14 Tue 15:00 Poster A

Topological phases in interfacial phase-change materials — •Peter Schmitz[1,3], Wei Zhang[2], Yuriy Mokrousov[3], and Riccardo Mazzarello[1] — [1]Institute for Theoretical Solid State Physics, RWTH Aachen — [2]CAMP Nano, Xi'an Jiaotong university, China — [3]IAS-1 and JARA, Forschungszentrum Jülich

We investigate the topological, spectral and structural properties of $[Sb_2Te_3]_x[GeTe]_y$ compounds, some of which are interfacial phase-change materials (IPCMs), as a function of strain and stacking sequence using density functional theory.
Induced by electric fields and heat, IPCMs can perform fast reversible transitions between crystalline states of different stacking. Since they possess strong SOC and a TI+NI layering, they are a promising platform for nontrivial interface states and switching between topological phases. So far they were shown to exhibit TIs and unstable TI/NI transition points [1], yet no consistent classification exists.
We analyze if the novel **3D topological Dirac semimetal** (TDSM) phase [2] is relevant to these C_3 systems: Under parameter variation, 2 cones move through the bulk spectrum, gapped due to symmetry breaking potentials between the blocks which enables nonzero 3D Z_2 invariants. We show that corresponding states are localized at the interfaces of iPCMs and the effective topological phase is controlled by their van der Waals interaction.

[1] J. Tominaga et al, Adv. Mat. Inter. 1 (2014)
[2] B. Yang and N. Nagaosa, Nature Commun. 5, 4898 (2014)

HL 35.15 Tue 15:00 Poster A

Constructing spintronic devices from topological insulators via combination with ferromagnetic materials — •Matthias Götte, Tomi Paananen, Günther Reiss, Michael Joppe, and Thomas Dahm — Fakultät für Physik, Universität Bielefeld, Germany

Topological insulators with their spin-momentum coupled edge or surface states are promising candidates for future spintronic applications. Combining topological insulators with ferromagnetic materials opens possibilities to control current flow in these states, e.g. via quantum tunneling or proximity induced ferromagnetic exchange fields. Here, we construct tunneling magnetoresistance (TMR) devices from ferromagnet/isolator/topological insulator junctions and calculate their potential TMR ratios using realistic tight-binding models. The theoretical values are of the same order of magnitude as in state of the art TMR devices based on conventional ferromagnets.

By performing numerical transport calculations, we investigate the influence of local ferromagnetic exchange fields on charge transport in edge states of two-dimensional topological insulators. Based thereupon we propose a device that creates pure spin currents along the edge of the topological insulators. All calculations are based on a tight-binding model suitable for the Bi_2Se_3 class of materials.

HL 35.16 Tue 15:00 Poster A

Superconductor-topological insulator junctions based on an Sb_2Te_3/Bi_2Te_3 p-n heterostructure — •Daniel Rosenbach[1], Peter Schüffelgen[1], Martin Lanius[1], Jörn Kampmeier[1], Gregor Mussler[1], Markus Eschbach[1], Ewa Mlynczak[1], Lukasz Plucinski[1], Martina Luysberg[1], Stefan Trellenkamp[1], Martin Stehno[2], Prosper Ngabonziza[2], Alexander Brinkman[2], Detlev Grützmacher[1], and Thomas Schäpers[1] — [1]Peter Grünberg Institut and Jülich Aachen Research Alliance (JARA-FIT), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Faculty of Science and Technology and MESA+ Institute for Nanotechnology, University of Twente, 7500 AE Enschede, The Netherlands

Topological insulators combined with superconducting electrodes are very promising systems for realizing Majorana bound states. However, realizing functional structures including 3D topological insulator (TI) materials suffer from a high unintentional background doping as well as surface state degradation due to oxygen inclusion as soon as the sample is exposed to air. Here, we present the successful integration of niobium superconducting contacts on top of a 3D TI layer system. The TI layers were grown by means of molecular beam epitaxy on Si (111) substrates and are capped *in-situ* by a few nm of aluminumoxide to protect the Dirac-like surface states. Utilizing a layer stack of p-type doped Sb_2Te_3 on top of n-type doped Bi_2Te_3, defining a p-n heterostructure, pushes the Fermilevel at the upper surface to the Dirac-point.

HL 35.17 Tue 15:00 Poster A

Combined structural, electronic and transport investigations on metallic and semiconducting micro flakes from a topological insulator Bi_2Se_3 single crystal — •Dominic Lawrenz[1], Olivio Chiatti[1], Christian Riha[1], Marco Busch[1], Franz Herling[1], Srujana Dusari[1], Jaime Sanchez-Barriga[2], Anna Mogilatenko[3], Lada V. Yashina[4], Sergio Valencia[2], Ahmet A. Ünal[2], Oliver Rader[2], and Saskia F. Fischer[1] — [1]Novel Materials Group, Institut für Physik, Humboldt Universität zu Berlin, D-12489 Berlin — [2]Helmholtz-Zentrum-Berlin für Materialien und Energie, D-12489 Berlin — [3]Ferdinand-Braun-Institut, D-12489 Berlin — [4]Department of Chemistry, Moscow State University, 119992 Moscow, Russia

High-quality Bi_2Se_3 bulk and exfoliated micro flakes are investigated via temperature dependent magneto-transport measurements. To achieve a comprehensive picture, these results are combined with high resolution transmission electron microscopy, energy dispersive x-ray spectroscopy and photoemission electron microscopy to confirm the structure and stoichometry of bulk and flakes. A well-defined bulk band-gap and the presence of a single Dirac cone are proven by angle-resolved photoemission spectroscopy. We investigate Bi_2Se_3 in the regime of high electron density ($> 10^{19}$ cm^{-3}) and find two-dimensional (2D) layered metallic transport in the Shubnikov-de Haas oscillations and quantized Hall resistance. In exfoliated micro flakes the low-field magneto-conductivity shows weak antilocalization that is analyzed in the Hikami-Larkin-Nagaoka (HLN) model for 2D systems.

HL 35.18 Tue 15:00 Poster A

Terahertz radiation induced photocurrents in $(Bi_{1-x}Sb_x)_2Te_3$ based topological insulators — •Helene Plank[1], Leonid E. Golub[2], Stefan Bauer[1], Vasily V. Bel'kov[2], Markus Eschbach[3], Lukasz Plucinski[3], Gregor Mussler[3], Detlev Grützmacher[3], and Sergey. D. Ganichev[1] — [1]Terahertz Center, University of Regensburg, Regensburg, Germany — [2]Ioffe Physical-Technical Institute, St. Petersburg, Russia — [3]Jülich Aachen Research Alliance (JARA-FIT), Jülich, Germany

Here we report on the observation of terahertz (THz) laser radiation induced photocurrents in epitaxially grown $(Bi_{1-x}Sb_x)_2Te_3$ three dimensional topological insulators with antimony concentrations x varying from 0 (n-type) to 1 (p-type conductivity). At normal incidence the photocurrent is dominated by the photogalvanic effect (PGE). It is allowed in the surface states only due to a "symmetry filtration" [1]. However, at oblique incidence the PGE diminishes and a photon drag effect, arising in the trigonal symmetry of the samples due to an in-plane component of the photon momentum, is dominating the photocurrent formation at certain frequencies. We show that this trigonal PDE results in a photocurrent even in the angle of incidence θ and that it is caused by the in-plane gradient of the radiation electric field accompanied by asymmetric elastic scattering. [1] P. Olbrich *et al.*, Phys. Rev. Lett. **113**, 096601(2014)

HL 35.19 Tue 15:00 Poster A

Optical properties of compensated topological insulators — •Alessandro Revelli[1], Nick Borgwardt[1], Jonathan Lux[2], Zhiwei Wang[1,3], Ignacio Vergara[1], Malte Langenbach[1], Achim Rosch[2], Yoichi Ando[1,3], Paul van Loosdrecht[1], and Markus Grüninger[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Institut für theoretische Physik, Universität zu Köln — [3]Institute of Scientific and Industrial Research, Osaka University, Japan

We report on the optical properties of bulk-insulting $BiSbTeSe_2$ for frequencies from 6 meV to 5.5 eV. Combining transmittance data for different sample thicknesses with normal incidence reflectivity data as well as ellipsometric results, we obtain a detailed view on the optical conductivity of the bulk, ranging from $\sigma_1(\omega) = 0.3\,(\Omega\text{cm})^{-1}$ below the gap to $10^4\,(\Omega\text{cm})^{-1}$ at 2eV. At 50 K, we find a nearly fully compensated semiconductor with a carrier density $N \approx 4{\cdot}10^{16}$ cm^{-3}. The intrinsic band gap Δ shows a strong temperature dependence, it shifts from 0.26 eV at 5 K to 0.18 eV at 300 K. Below the gap, the optical conductivity $\sigma_1(\omega)$ reaches values lower than $0.3\,(\Omega\text{cm})^{-1}$ at 50 K. These are the lowest values of $\sigma_1(\omega)$ reported thus far for the entire tetradymite family. Above 50 K, we observe activated behavior of free carriers with an activation energy $E_A \approx 26$ meV, in agreement with transport data. Upon cooling below 50 K, $\sigma_1(\omega)$ rises again due to the formation of puddles of localized carriers which arise from the random potential fluctuations caused by charged defects in a fully compensated semiconductor. Monte Carlo simulations show a screening effect arising from thermally activated carriers, explaining the experimental observations.

HL 35.20 Tue 15:00 Poster A

The structure and electrical properties of Se hyperdoped Si by ion implantation followed by short-time annealing — •Fang Liu[1,2], Slawomir Prucnal[1], Ye Yuan[1,2], Kun Gao[1,2], Yonder Berencén[1], Lars Rebohle[1], Wolfgang Skorupa[1], Manfred Helm[1,2], and Shengqiang Zhou[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Dresden, Germany — [2]Technische Universität Dresden, Dresden, Germany

Si hyperdoped with Se layers was obtained by ion implantation of 60 keV Se at fluence of 5*1E15 cm-2 followed by both pulsed laser annealing (PLA) and flash lamp annealing (FLA). We show that the degree of crystalline lattice recovery of the implanted layers and the Se substitutional fraction depend on the pulse duration and energy density of FLA and PLA. While the annealing at low energy densities leads to an incomplete recrystallization, annealing at higher energy densities results in more defects. The impurities have more chance of redistribution if the sample is maintained at higher temperature for longer time. The electrical properties of the implanted layers can be well correlated to the structural properties resulted from different annealing processing.

HL 35.21 Tue 15:00 Poster A

In situ TEM investigations of the back surface field of aluminum in multi-crystalline silicon — •Hendrik Spende, Patrick Peretzki, and Michael Seibt — IV. Physikalisches Institut der Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

The rear contact of a solar cell requires a uniform low-resistance ohmic contact, minority-carrier reflection, photon reflection and effective gettering of impurities while processing. Standard solar cells use alloyed backside contacts because of their positive effect on the cell efficiency. Screen printing or evaporating Al on the silicon wafer and thermal annealing lead to the formation of an aluminum alloyed back surface field (Al-BSF) at the Al-Si interface. This creates a heavily Al doped p+-region, which forms a pn-junction with the n-type Si, or a p+/p-junction reducing backside recombination.

The formation of the Al-BSF and the effect of grain boundaries in n-type multicrystalline silicon (mc-Si) - used here for preparation issues - were studied by in situ transmission electron microscopy. The grain boundaries were made visible by etching with HNO_3 and HF, then Al was evaporated onto the surface and lamellas were prepared by FIB. During heating the temperature was increased above the eutectic point of Al and Si. The Si dissolved into the Al and then the Al penetrated the Si wafer. During cooling Si doped with Al recrystallized and left a doped BSF region.

HL 35.22 Tue 15:00 Poster A

Si Nanowires Prepared by Glancing Angle Deposition Technique — •Andrii Kulyk[1], Christoph Grüner[1], Andriy Lotnyk[1], Dietmar Hirsch[1], Gal Schkolnik[2], Isom Hilmi[1], and Bernd

Rauschenbach[1] — [1]Leibniz Institute of Surface Modification, Permoserstr. 15, D-04318, Leipzig, Germany — [2]Helmholtz Centre for Environmental Research, Permoserstr. 15, D-04318, Leipzig, Germany

Si nanostructures can be engineered to form a variety of useful shapes by glancing angle deposition there has been recent interest in this new materials class. For example, they can be used as optical sensor, porous electroluminescent material or solar absorber. In this work Si nanostructures are obtained by glancing angle deposition and studied by TEM, XRD, SEM and confocal Raman spectroscopy at various parameters. The nanosphere lithography is used to realize ordered Si nanostructure pattern. Epitaxial and crystalline structures of SiNWs were achieved. Raman spectra have shown high intensity peaks from Si nanostructures in a region from 517 cm-1 to 523 cm-1, which is well agreed with literatures data. XRD investigations identified Si peaks orientated to (111) and (220). The growth of crystalline structure is possible in temperature region 400 - 680 °C.

HL 35.23 Tue 15:00 Poster A

Deep electronic levels in crystalline silicon after irradiation with femtosecond laser pulses in SF_6-atmosphere — •Arne Ahrens[1], Philipp Saring[1], Anna Lena Baumann[2], Stefan Kontermann[2,3], and Michael Seibt[1] — [1]IV. Physikalisches Institut, Georg-August Universität Göttingen, Germany — [2]Fraunhofer Heinrich Hertz Institut, Goslar, Germany — [3]present address: Hochschule RheinMain, Rüsselsheim, Germany

Femtosecond laser pulse irradiation in sulfur hexafluoride (SF_6) atmosphere leads to sulfur incorporation into the silicon beyond the solubility limit (hyperdoping) and structuring of the surface. Enhanced optical absorption in the sub-bandgap range due to introduced deep defect levels is known for such materials. This makes such a material a promising candidate for intermediate band solar cell applications, especially if impurity bands form due to a Mott transition. Considering a p-type silicon substrate, sulfur hyperdoping leads to the formation of a buried pn-junction which has been studied in detail by means of cross-section transmission electron microscopy (TEM) and electron-beam induced current (EBIC) [1] as well as capacitance-voltage (CV) and SIMS measurements [2]. This work presents results of additional cross sectional EBIC and TEM experiments. Furthermore, this work presents the results of an extensive deep-level transient spectroscopy (DLTS) study of deep levels in the vicinity of the buried pn-junction, which points out the existence of two dominant deep levels. [1] P. Saring et al., Appl. Phys. Lett. 103, 061904 (2013). [2] K.-M. Guenther et al., Appl. Phys. Lett. 102, 202104 (2013).

HL 35.24 Tue 15:00 Poster A

Structure and chemistry of crystalline silicon-aluminum oxide interfaces — •Arne Ahrens, Patrick Peretzki, and Michael Seibt — IV. Physikalisches Institut, Georg-August Universität Göttingen, Germany

Aluminum oxide deposited on crystalline silicon by atomic layer deposition (ALD) is known for its high surface passivation capabilities. This surface passivation is attributed to a high negative fixed charge density of about $-4\times10^{12}cm^{-2}$[1] in the aluminum oxide layer close to the silicon-aluminum oxide interface [2]. This makes aluminum oxide an interesting material to increase the efficiency of solar cells by passivation of surface states. Examples of use are passivated emitter and rear cells (PERC) [3] and rear-emitter inversion layer solar cell [4], for which efficiencies of 20% [3] and 18,1% [4] have been reported, respectively.

In this work, we apply transmission electron microscopy (TEM), electron energy loss spectroscopy (EELS) and energy dispersive x-ray spectroscopy (EDX) to study the structure and chemistry of the interface of crystalline silicon and aluminum oxide deposited by ALD for different production parameters, as e.g. post-deposition heat treatments or layer thickness. In addition, we investigate the influence of UV irradiation on the structure and chemistry of the silicon-aluminum oxide interface. [1] F. Werner and J. Schmidt Appl. Phys. Lett. Vol.104, 091604 (2014). [2] B. Hoex et al., J. Appl. Phy. Vol.104, 113703 (2008). [3] J. Schmidt et al., Prog. Photovol: Res. Appl. Vol. 16 461-466 (2008). [4] F. Werner et al., J. Appl. Phy. Vol. 115, 073702 (2014).

HL 35.25 Tue 15:00 Poster A

On deep level transient spectroscopy of extended defects in n-type 4H-SiC — •Jonas Weber, Heiko Weber, and Michael Krieger — Department of Physics, Applied Physics, FAU Erlangen-Nuremberg, Germany

Deep level transient spectroscopy (DLTS) is an electrical measurement technique used for the investigation of point defects having deep levels in the bandgap of semiconductors. In defective materials, negative DLTS signals are frequently observed and ascribed to extended defects, although the origin is not yet understood. We have investigated triangular shaped extended defects in lightly nitrogen doped n-type 4H-SiC epitaxial layers by means of DLTS. For this purpose, triangular defects have been located by photoluminescence mapping and scanning electron microscopy. Schottky contacts for DLTS investigations have been prepared on top of those defects. DLTS measurement parameters, i. e. reverse bias, pulse bias and pulse length have been varied to gain insight into the electrical behavior of the system. It has been found that the appearance of negative DLTS signals depends on the choice of measurement parameters. A model is developed that qualitatively explains the DLTS spectra observed.

HL 35.26 Tue 15:00 Poster A

ion implantation induced damage in nonpolar a-plane GaN films — •Fengfeng Cheng[1,2], Lin Li[2], Slawomir Prucnal[2], M. X. Feng[3], Qian Sun[3], J. Grenzer[2], M. Helm[2], and Shengqiang Zhou[2] — [1]key Lab of Beam Technology and Material Modification of Ministry of Education, College of Nuclear Science and Technology, Beijing Normal University, Beijing Radiation Center, Beijing 100875, China — [2]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, P. O. Box 510119, Dresden 01314, Germany — [3]key Laboratory of Nanodevices and Applications, Suzhou Institute of Nano-Tech and Nano-Bionics (SINANO), Chinese Academy of Sciences (CAS), Suzhou 215123, China

In this study, we investigated ion implantation induced damages in nonpolar alpha-plane GaN films. X-ray diffraction (XRD), Raman scattering, Rutherford backscattering/channeling (RBS/C), are employed to study samples with different implantation fluences. For Si implanted samples, with increasing the implanted fluences, besides the main (102) peak from the XRD $2\theta/\theta$ scan, a bump peak is observed and shifts to a lower angle, which indicates the lattice expansion. It is consistent with newly arising peaks in the Raman spectra, which may associate with the lattice disorder and distortion caused by radiation damage. RBS/C results are also provided as complement to evidence the preview conclusion.

HL 35.27 Tue 15:00 Poster A

Annealing behavior of Er implanted GaN — •Fengfeng Cheng[1,2], Linxiang Chi[2], Ding Li[3], Slawomir Prucnal[2], Fang Liu[2], René Heller[2], M. Helm[2], Xiaodong Hu[3], Guoyi Zhang[3], and Shengqiang Zhou[2] — [1]Key Lab of Beam Technology and Material Modification of Ministry of Education, College of Nuclear Science and Technology, Beijing Normal University, Beijing Radiation Center, Beijing 100875, China — [2]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, P. O. Box 510119, Dresden 01314, Germany — [3]Research Centre for Wide-gap Semiconductor, State Key Laboratory of Artificial Microstructure and Mesosciopic Physics, School of Physics, Peking University, Beijing 100871, China

In this study, we report the annealing behavior of 100 keV Er-implanted GaN with fluence of 1E15/cm2. The microstructural and optical property evolution of samples with different thermal treatment is studied by room temperature photoluminescence (PL), Raman spectra, and Rutherford backscattering. From the results, we try to establish a correlations between microstructural and optical properties. The PL peak around ~1540 nm is clearly observed for all as-implanted and post-annealed samples, with increasing annealing temperature, the PL peak intensity reaches to maximum at annealing temperature of 900 , while the PL intensity reduction with further higher temperature annealing (namely 1050) could be attributed to reduction of optically active Er sites , while RBS/C results shows the out diffusion of Er with increasing annealing temperature.

HL 35.28 Tue 15:00 Poster A

Nanoimprint lithography for selective area growth of GaN-based nanocolumns — •Stefan Behrenz and Philipp Henning — IV. Physikalisches Institut, Georg-August-Universität Göttingen

Ordered arrays of GaN-based nanocolumns provide a promising material basis for novel device applications. Selective area growth by means of a patterned metal mask is a suitable method for the growth of such structures. For the mask preparation a variety of lithography methods is used, most of which are time consuming if applied for a large number of substrates and on large scales. For this scope, nanoimprint

lithography (NIL) has been proven to be an efficient method. Due to the fact that the structure size does not affect the processing time high throughput can be achieved. In this work, we show how NIL can be successfully applied for molecular beam epitaxy of GaN nanostructures. By means of soft imprinting homogeneously patterned arrays of sizes up to (400x400) μm^2 and column diameters ranging from 1200 nm down to 350 nm could be produced. The entire process has been optimized for the selective area growth of GaN. Compared to the growth on masks patterned by electron beam lithography an equally good quality is achieved.

HL 35.29 Tue 15:00 Poster A

Structural and optical properties of a GaN/AlN quantum heterostructure — •Alexander Reuper[1], Gordon Schmidt[1], Silke Petzold[1], Peter Veit[1], Konrad Bellmann[2], Tim Wernicke[2], Frank Bertram[1], Michael Kneissl[2], and Jürgen Christen[1] — [1]Institute of Experimental Physics, Otto-von-Guericke-University Magdeburg, Germany — [2]Institute of Solid State Physics, Technical University Berlin, Germany

III-nitride based quantum dots (QD) are promising candidates for room-temperature quantum emitters due to the large exciton binding energies and strong confinement of this material system. Using transmission electron microscopy combined with cathodoluminescence spectroscopy (STEM-CL) we report on structural and spatially resolved optical properties of a GaN/AlN heterostructure with GaN grown under low V/III ratio to promote QD formation.

The GaN layer has been grown by metal-organic vapor phase epitaxy on a c-plane AlN/sapphire template at 1050°C and immediately capped by AlN.

Structural investigations showed a continuously formed GaN layer with local thickness fluctuations. Nanoscale cathodoluminescence measurements at room temperature as well as 16 K revealed spots of high intensity within GaN-layer. Highly spatially resolved CL investigations show various sharp emission peaks around 300 nm from these spots.

HL 35.30 Tue 15:00 Poster A

Time-resolved photoluminescence spectroscopy of InGaN nanowires — •Vanessa Dahmen[1], Nils W. Rosemann[1], Pascal Hille[2], Jörg Schörmann[2], Felix Walther[2], Martin Eickhoff[2], and Sangam Chatterjee[1] — [1]Faculty of Physics and Materials Science Center, Philipps-Universität Marburg, Renthof 5, D-35032 Marburg, Germany — [2]I. Physical Institute, Justus-Liebig-Universität Gießen, Gießen, Germany

The incorporation of Indium into GaN drastically reduced the band gap of the alloy material. This shift towards the visible regime is exploited in the active material of commercially available blue and green laser diodes. Nanowires (NW) provide a good model system to investigate the intrinsic effects of alloying as they are virtually free of defects due to their self-assembled growth. Here, we study two series of (Ga,In)N NWs by time-resolved photoluminescence. The samples were grown by plasma-enhanced molecular beam epitaxy under different growth conditions. In particular, effects of the plasma power or the nitrogen flux are studied by systematic variations during growth. The time-resolved photoluminescence spectroscopy reveals ensembles of 3 states with similar decay dynamics are found for both series while the spectral position of the peak emissions are shift towards lower energies with increasing nitrogen flux.

HL 35.31 Tue 15:00 Poster A

Time-resolved luminescence studies of rare earth doped high pressure high temperature aluminium nitride — Tristan Koppe, Oliver Beck, Hans Hofsäss, and •Ulrich Vetter — II. Physikalisches Institut der Georg-August-Universität Göttingen, Deutschland

We report on studies of time-resolved defect luminescence processes in undoped and rare earth doped AlN. The material was synthesised by the temperature gradient method in a belt-type HP-HT apparatus. As solvent Li_3AlN_2 is used which was, in the case of doped samples, previously mixed with e. g. EuF_3 to achieve rare earth doped AlN.

The measurements were realised with a tunable femtosecond laser system, which contributes excitation energies from deep UV up to the near infrared region. In combination with a Streak Camera time-resolved spectra with time windows between 1 ns and several hundred milliseconds from 200 - 800 nm with temporal resolutions down to 20 ps are achievable.

To overcome the limitation of the Streak Camera system to measure lifetimes in the millisecond range or above, for e. g. to investigate longer living rare earth decays as well as some types of long living defect related luminescences in AlN, the connected trigger system was extended by an additional trigger unit.

HL 35.32 Tue 15:00 Poster A

Optical Characterization of GaN:Fe — •Sebastian Bauer[1], Matthias Hocker[1], Benjamin Neuschl[1], Maria L. Gödecke[1], Martin Klein[2], Frank Lipski[2], Eberhard Richter[3], Ferdinand Scholz[2], and Klaus Thonke[1] — [1]Institute of Quantum Matter, Semiconductor Physics Group, University Ulm — [2]Institute of Optoelectronics, University Ulm — [3]Ferdinand-Braun Institute, Berlin

Nominally undoped GaN is typically n-type in the range of some $[n] = 10^{16}$-10^{19} cm^{-3} carriers introduced by uncontrolled silicon and oxygen impurities. To remove this background conductivity, incorporation of iron on Ga sites acting as deep acceptors is a viable way to create so-called semi-insulating material, similar to semi-insulating GaAs:Fe. The electrical Fe^{2+}/Fe^{3+} level associated with Fe in GaN is located some 0.6 eV below the conduction band.

In the present study we present electrical and mainly optical data of thick GaN:Fe layers grown by hydride vapour phase epitaxy, using a ferrocen source for Fe. The samples show different concentrations of iron and background donors incorporated, and thus different degrees of compensation. In optical absorption measurements, we established – based on secondary ion mass spectrometry and electrical data – a correlation between the absorption signal and the actually present compensation status of iron.

HL 35.33 Tue 15:00 Poster A

Self-catalyzed and Si-induced growth of vertically aligned InN nanorods by MOVPE — •C. Tessarek[1,2,3], S. Fladischer[4], C. Dieker[4], G. Sarau[1,2], B. Hoffmann[2], M. Bashouti[2], M. Heilmann[2], S. Figge[5], A. Gust[5], E. Spiecker[4], and S. Christiansen[1,2,6] — [1]Institut für Nanoarchitekturen für die Energieumwandlung, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin — [2]Max Planck Institute for the Science of Light, Erlangen — [3]Institute of Optics, Information and Photonics, Friedrich-Alexander-University Erlangen-Nürnberg — [4]Institut für Mikro- und Nanostrukturforschung & Center for Nanoanalysis and Electron Microscopy (CENEM), Friedrich-Alexander-University Erlangen-Nürnberg — [5]Institute of Solid State Physics, University of Bremen — [6]Physics Department, Freie Universität Berlin

InN with its small photonic and large phononic band gap has the potential to be used for hot carrier solar cells. However, InN layers suffer from high defect densities due to the lack of native substrates. A self-catalyzed nanorod approach carried out in metal-organic vapor phase epitaxy is used to reduce the defect density leaving the upper part of the nanorods nearly free of defects. A detailed study of growth parameters influencing the formation and morphology of InN nanorods is carried out. The structural properties are analyzed using transmission electron microscopy, energy dispersive X-ray spectroscopy, X-ray diffraction and Raman spectroscopy. The optical properties are investigated using cathodoluminescence. Finally, the similarities between InN and GaN nanorod growth will be discussed.

HL 35.34 Tue 15:00 Poster A

Carrier-induced refractive index change observed by a whispering gallery mode shift in GaN microrods — •Christian Tessarek[1,2,3], Rüdiger Goldhahn[4], George Sarau[1,2], Martin Heilmann[2], and Silke Christiansen[1,2,5] — [1]Institut für Nanoarchitekturen für die Energieumwandlung, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin — [2]Max Planck Institute for the Science of Light, Erlangen — [3]Institute of Optics, Information and Photonics, Friedrich-Alexander-University Erlangen-Nürnberg — [4]Institut für Experimentelle Physik, Otto-von-Guericke-Universität Magdeburg — [5]Physics Department, Freie Universität Berlin

The influence of the carrier concentration on the refractive index of GaN is investigated. Vertical oriented GaN microrods were grown by metal-organic vapor phase epitaxy. During growth the silane flux was modified to obtain four sections with different n-type carrier concentrations above 10^{19} cm^{-3} along the *c*-axis. Whispering gallery modes can be observed in this type of microrods due to the regular hexagonal shape, the smooth sidewall facets and the sharp edges [1]. The presence of an energy dependent mode shift with respect to the four microrod sections with different doping concentrations is attributed to a carrier-induced refractive index change. The observed mode shift can be calculated by a proper adjustment of the band gap parameter in the analytical expression of the refractive index [2].

[1] C. Tessarek et al., ACS Photonics **1**, 990 (2014).
[2] C. Tessarek et al., New J. Phys. **17**, 083047 (2015).

HL 35.35 Tue 15:00 Poster A

Excitation spectroscopy of higher quantized states in GaInN quantum wells — •Tim Käseberg, Fedor Alexej Ketzer, Heiko Bremers, Uwe Rossow, and Andreas Hangleiter — Institut für Angewandte Physik, Technische Universität Braunschweig

In order to gain better knowledge about their structure and composition, we examine thin GaInN single and multiple quantum well structures with the help of their higher quantized states. Thus we set up a photoluminescence excitation spectroscopy (PLE) experiment. We excite the samples using a 150 W xenon arc lamp in the region of 360 to 520 nm, dispersed by a double-prism monochromator. The photoluminescence is then detected by a second monochromator and a silicon photodiode using a lock-in amplifier. Similar samples with different growth parameters were examined at various excitation wavelengths at room temperature. The composition of the samples influence the overlap of the wave functions and therefore their efficiency. Higher quantized states help to investigate the inner structure of these samples. Since the inhomogeneous broadening is relatively high, higher quantized states are hard to determine. Therefore we computed the absorption spectra of the samples by simulation of the quantum well and compared them to the observed PLE spectra. Similar characteristics are observed.

HL 35.36 Tue 15:00 Poster A

Ohmic Ti/Al/TiN Contacts to n-GaN Fabricated by Sputter Deposition — •Valentin Garbe[1], Juliane Walter[1], Wolfram Münchgesang[1], Alexander Schmid[2], Ronald Otto[2], Thomas Behm[1], Barbara Abendroth[1], and Dirk C. Meyer[1] — [1]Institute of Experimental Physics, TU Bergakademie Freiberg, Leipziger Str. 23, 09599 Freiberg, Germany — [2]Institute of Applied Physics, TU Bergakademie Freiberg, Leipziger Str. 23, 09599 Freiberg, Germany

The annealed Ti/Al/metal/Au contact metallization has emerged as the most used Ohmic contact to n-GaN. While the Ti/Al bilayer is crucial for contact formation, the metal/Au capping layer prevents oxidation and Ga and Al diffusion. However, Au degrades the contact resistance, as itself diffuses to the GaN interface. Here, we present the fabrication and characterization of an Au-free Ti/Al/TiN contact stack to n-GaN with TiN serving as the diffusion barrier. Sputter deposition and lift-off in combination with post deposition annealing at 850 °C for 300 s are used for contact formation. After annealing, contacts show Ohmic behavior to n-GaN and a resistivity of 1.60×10^{-3} Ω cm^2. To understand the contact formation on the microscopic scale, the contacts were characterized by current–voltage measurements, linear transmission line method, X-ray reflectivity, X-ray diffraction, and X-ray photoelectron spectroscopy. Results show diffusion of Ti, Al, N and Ga during annealing, formation of TiN at the GaN/Ti interface, as well as formation of cubic and hexagonal AlN. However, the TiN layer was stable during annealing and proved to be an effective diffusion barrier and prevented oxidation successfully.

HL 35.37 Tue 15:00 Poster A

Influence of the p-AlGaN superlattice on the performance characteristics of deep UV laser diode heterostructures — •E. Ziffer[1], M. Martens[1], C. Kuhn[1], T. Simoneit[1], J. Rass[1], T. Wernicke[1], A. Knauer[2], V. Kueller[2], M. Weyers[2], S. Einfeldt[2], and M. Kneissl[1,2] — [1]Technische Universität Berlin, Institut für Festköperphysik, Berlin, Germany — [2]Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, Berlin, Germany

AlGaN-based deep UV laser diodes (LD) require p-AlGaN cladding layers (CL) with high Al mole fractions. However, with increasing Al content the ionization energy of Mg dopants in AlGaN layers also increases, leading to high series resistance. We have investigated the influence of the p-side CL on AlGaN-based LD structures. The heterostructures consist of AlGaN multiple quantum well (MQW) active regions emitting near 270 nm, embedded in $Al_{0.70}Ga_{0.30}N$ waveguide layers, an $Al_{0.80}Ga_{0.20}N$:Si n-CL and different AlGaN:Mg p-CLs, including a 200 nm thick AlGaN layer, 150 - 200 nm superlattices (SL) with different Al contents and a p-GaN contact layer. The structures were analyzed by transfer length method, I-V characterization and electroluminescence spectroscopy. All diodes exhibit dominant QW emission with peak wavelengths between 258 nm and 276 nm. By increasing the average Al content of the p-SL from 37% to 81%, the diodes' turn-on voltage increases from 17 V to 26 V, whereas the series resistance stays constant on average (60 Ω for a contact size of 100x100 μm^2). This is an improvement in series resistance by one order of magnitude compared to LDs with a bulk $Al_{0.81}Ga_{0.19}N$ p-CL.

HL 35.38 Tue 15:00 Poster A

Influence of acceptor concentration on burn-in effects in AlGaN-based deep UV LEDs — •Jakob Jordan[1], Martin Guttmann[1], Frank Mehnke[1], Johannes Enslin[1], Simon Kapanke[1], Tim Wernicke[1], Mickael Lapeyrade[2], Markus Weyers[2], Sven Einfeldt[2], and Michael Kneissl[1,2] — [1]Technische Universität Berlin, Institut für Festkörperphysik, Berlin, Germany — [2]Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, Berlin, Germany

Light in the deep ultraviolet (UVC) spectral range is used in diverse areas such as sewage water treatment and gas sensing. The toxicity and relative bulkiness of conventional UV mercury lamps necessitates development of light emitting diodes (LEDs) operating in this wavelength region. In this contribution, the optical and electronic properties of AlGaN-based LEDs emitting near 233 nm are analyzed with regards to a variation of the magnesium doping concentration in the electron blocking heterostructure and p-side superlattice. Electroluminescence (EL) measurements are used to determine changes in emission spectrum, light output power, device yield, and temperature response. During measurements, burn-in effects were discovered for LEDs with low Mg-doping. These burn-in effects produce a significant increase in output power that persists after cool down. Annealing in a high temperature environment does not lead to an increase in power, implying that the injected charge carriers are aiding in the activation process. The influence of time, temperature, and current on the observed burn-in effects will be presented and possible explanations will be discussed.

HL 35.39 Tue 15:00 Poster A

Deep UV light emitting diodes with transparent conductive electrodes of multi-layer graphene — •Luca Sulmoni[1], Marc Gluba[2], Norbert Nickel[2], Mickael Lapeyrade[3], Sven Einfeldt[3], Veit Hoffmann[3], Johannes Enslin[1], Christian Kuhn[1], Frank Mehnke[1], Tim Wernicke[1], and Michael Kneissl[1,3] — [1]Technische Universität Berlin, Institut für Festkörperphysik, Berlin, Germany — [2]Institut für Silizium Photovoltaik, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany — [3]Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, Berlin, Germany

Light extraction from bottom-emitting ultraviolet (UV) LEDs is challenging, since all metals typically used as p-contacts strongly absorb the light emitted from the active region. In addition, metal contacts directly on p-AlGaN suffer from high p-contact resistances and Schottky type behavior resulting in large operating voltages. This contribution investigates the current injection in AlGaN-based multi-quantum-well UVC LEDs exploiting UV-transparent multi-layer (ML) graphene-based p-electrodes. The p-(Al)GaN/graphene bi-layer exhibit a sheet resistance of 1200, 700 and 400 Ω/square for 1, 2 and 3 ML, respectively. For deep UV LEDs emitting near 265 nm, the excellent lateral current-spreading of the graphene layers and the vertical current injection into the p-n junction are demonstrated with an output power of 1 mW at 70 mA and 21 V. Finally, highly reflective Al/graphene-based p-electrodes on the same UVC LEDs with and without the absorbing p-GaN cap layer will also be presented.

HL 35.40 Tue 15:00 Poster A

Spectrally pure deep UV LEDs for gas sensing applications — •Frank Mehnke[1], Martin Guttmann[1], Johannes Enslin[1], Simon Kapanke[1], Christian Kuhn[1], Hendrik Krüger[2], Marian Rabe[2], Mickael Lapeyrade[3], Ute Zeimer[3], Sven Einfeldt[3], Tim Wernicke[1], Markus Weyers[3], and Michael Kneissl[1,3] — [1]Technische Universität Berlin, Institut für Festkörperphysik, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Universität Rostock, Institut für Allgemeine Elektrotechnik, Albert-Einstein.Str. 2, 18059 Rostock, Germany — [3]Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, Gustav-Kirchhoff-Str. 4, 12480 Berlin, Germany

Ultraviolet (UV) light emitting diodes (LEDs) emitting at wavelengths near 230 nm could enable compact and highly sensitive NO gas detection systems. Although the required spectral power densities are moderate, spectrally clear single peak emission without parasitic luminescence is of utmost importance. Unfortunately, such very short wavelength LEDs often suffer from various parasitic luminescences which mainly originate from electron leakage into the p-side of the LED and Mg-related deep level transitions. In this contribution, we will present

our recent investigations on the influence of the heterostructure design and p-side doping on the charge carrier injection and the emission characteristics of 233 nm LEDs. By optimizing the electron blocking layer thickness as well as the Mg doping concentration of the p-superlattice we were able to achieve single peak 233 nm LEDs with an emission power of 26 μW at 25 mA. Incorporated into a gas detection system those LEDs are capable to detect nitrogen oxide in the ppm range.

HL 35.41 Tue 15:00 Poster A

Large-scale defect calculations using atomic effective potentials and LATEPP — •Elisabeth Dietze[1], Jerome Jackson[1], and Gabriel Bester[1,2] — [1]Institute for Physical Chemistry, University of Hamburg, Germany — [2]The Hamburg Centre for Ultrafast Imaging, Luruper Chaussee 149, 22761 Hamburg, Germany

We present an electronic structure method which overcomes usual supercell size restrictions for the calculation of point defects in IV-IV and III-V semiconductors. For this we have developed a method to parametrize ab initio the changes in the total Kohn-Sham potential induced by the defect, giving a defect AEP [1, 2] that can be employed in very large supercell calculations.

As an example we present the properties of substitutional Mn defects in Si and GaAs showing that our description reproduces well the results of density functional calculations with the general gradient approximation for system sizes where this is possible, and discuss the energy eigenvalues of the states for very large supercells. The calculations show defect states in the range from shallow to intermediate binding energies, which our method is able to treat in a general way.

[1] J. R. Cardenas and G. Bester, Physical Review B 86, 115332 (2012).

[2] F. Zirkelbach P.-Y. Prodhomme, Peng Han, R. Cherian, and G. Bester, Physical Review B 91, 075119 (2015).

HL 35.42 Tue 15:00 Poster A

Optical Characterization of Ga(N,As,P)/(B,Ga)(As,P)/Ga(N,As,P) Heterostructures — •Julian Veletas[1], Peter Ludewig[2], Nils W. Rosemann[1], Kerstin Volz[1], Wolfgang Stolz[1,2], and Sangam Chatterjee[1] — [1]Faculty of Physics and Materials Science Center, Philipps-Universität Marburg, D-35032 Marburg, Germany — [2]NAsPIII/V GmbH, Am Knechtsacker 19, D-35041 Marburg, Germany

The quarternary semiconductor alloy Ga(N,As,P) is a promising material system for laser devices on silicon substrates to open up new routes towards off-chip optical data transmission. While the active material Ga(N,As,P) is comparatively well characterized many questions remain regarding the optoelectronic properties of the barrier material (BGa)(AsP). In particular, the hetero-offsets at the (B,Ga)(As,P)/Ga(N,As,P) Interface remain under discussion. Several scenarios discussed including a staggered band alignment, which would offer the potential for advanced W-Laser structures at telecom wavelength. Here, a series of Ga(N,As,P) /(B,Ga)(As,P)/Ga(N,As,P) *W-structures* are investigated by modulation and photoluminescence spectroscopy to identify optically allowed transitions and help to clarify the band alignment.

HL 35.43 Tue 15:00 Poster A

Influences of molecular flux gradients on the optical characteristics of GaAs/AlGaAs quantum wells — •Pia Eickelmann, Rüdiger Schott, Andreas D. Wieck, and Arne Ludwig — Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, Universitätsstr. 150, D-44780 Bochum, Germany

Semiconductor heterostructures with quantum wells (QW) find application e.g. in high electron mobility transistors, diode lasers or quantum cascade lasers. A good control of the well thicknesses and alloy compositions during the molecular beam epitaxy (MBE) growth is vital, as these mainly determine the quantization energies.

In this contribution, we present the effect of a spatial molecular flux gradient on an MBE grown GaAs/AlGaAs QW structure. Mounting the substrate in the MBE chamber nonaxially with respect to the Ga and Al effusion cell and stopping the rotation of the wafer cause this present flux gradient. We simulate the QW transition energies due to the change in Al concentration in the barrier and the width of the QW. The trend observed by photoluminescence measurements on the flux gradient grown QW wafer is well reproduced. Furthermore we investigate monolayer steps for the QWs in the same sample.

HL 35.44 Tue 15:00 Poster A

Local etching of a SiO_x layer on Si(111) by Ga droplets and its influence on GaAs nanowire growth — •Tina Tauchnitz[1,2], Harald Schneider[1], Manfred Helm[1,2], and Emmanouil Dimakis[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden — [2]cfaed, TU Dresden, 01062 Dresden, Germany

GaAs nanowires (NWs) can be grown epitaxially on Si(111) substrates in the vapour-liquid-solid mode. Typically, Au is used as catalyst, but affects the NW and substrate properties due to contamination. Thus, the self-catalyzed mode appears to be advantageous. The NW growth is initialized by the formation of Ga droplets on the substrate surface, which is normally covered by a thin SiO_x layer. The yield of vertical NWs depends on the thickness and the nature of the SiO_x [1], pointing out the complex interaction of the liquid Ga with the SiO_x.

This work investigates the local etching of a native SiO_x on Si(111) by liquid Ga droplets, a mechanism, which is thought to precede the NW nucleation. The droplet formation, the etching process, and their effect on the NW growth were studied as a function of the substrate temperature and the etching time using molecular beam epitaxy. In contrast to previous studies, the oxide etching is distinguished from the subsequent NW nucleation by inserting a thermal annealing step, during which the Ga droplets are evaporated completely from the surface. Finally, the yield of vertical NWs and the NW number density can be controlled just by choosing the appropriate conditions for the oxide etching, independent of those used for the subsequent NW growth.

[1] Matteini *et al.*, J. Cryst. Growth **404**, 2014

HL 35.45 Tue 15:00 Poster A

Treatment of concentrated solar radiation PV modules on the basis of AlGaAs-GaAs heterostructures — •Lia Trapaidze[1], Rafiel Chikovani[2], Ia Trapaidze[2], and Gela Goderdzishvii[2] — [1]3 Chavchavadze Ave., 0179 Tbilisi, Georgia — [2]Kostava 77, 0175 Tbilisi, Georgia

Among the alternative and renewable sources of energy the transformation of solar energy directly into electric energy attracts more growing attention. Till present the photoelectric transformers of solar radiation practically have been prepared only on crystalline silicon. The goal of researchers is to increase efficiency of photoelectric transforming systems and to lower the cost. In the present work for fabrication of heterostructures we have used the low-temperature liquid-phase epitaxial method in which we have introduced the changes and identified: a chemical composition of solid solutions of separate layers of multilayer heterostructures; the optimal thicknesses; type and concentration of doping material; the temperature-time modes of the growing processes. As a result in the obtained heterostructures the high value of efficiency coefficient of solar concentrated radiation up to 23,4% (K=100-500) and stability of technological process have been achieved. By using of testing methods of elements and modules we have studied the main parameters both in laboratory and field conditions. We have developed design and fabricated a pilot model of low power tourist mobile photoelectric system.

HL 35.46 Tue 15:00 Poster A

GaAs/air Bragg mirrors to enable strong light-matter interaction — •Meico Heinke-Becker, Sascha René Valentin, Arne Ludwig, and Andreas D. Wieck — Ruhr-Uni Bochum, 44780 Bochum, Deutschland

To obtain strong light matter interaction in cavity QED systems, a small mode volume and high mirror reflectivity is necessary. We present our first attempts to create a distributed Bragg reflector consisting of GaAs/air mirror pairs. This is performed by molecular beam epitaxy (MBE) and partial epitaxial-lift-off techniques.

HL 35.47 Tue 15:00 Poster A

Microfabricated SiN-masks for selective area epitaxy of InAs and GaAs — •Viktoryia Zolatanosha and Dirk Reuter — Optoelectronic Materials and Devices, University of Paderborn, Warburgerstr. 100, 33098, Paderborn, Germany

Selective area epitaxy (SAE) has the potential to open the path to novel semiconductor devices by allowing for laterally patterned material deposition. In SAE various types of masks define local areas, in which materials are deposited. In this contribution, we present a shadow mask approach for SAE in the InAs/GaAs-system.

The mechanical mask is realized from a SiN-membrane by employing nanofabrication technology allowing for hole sizes down to 100 nm. The membrane is made from a Si-wafer covered with 100 nm Si3N4 by anisotropic chemical etching of Si(100) employing KOH. The membrane itself is patterned by electron beam lithography and reactive ion

etching. First test shows that the mask is fully compatible with ultra-high-vacuum and can withstand temperatures up to 800°C. GaAs and InAs deposited on the mask can be re-evaporated without damaging the mask.

HL 35.48 Tue 15:00 Poster A

Growth of Low Density InAs Quantum Dot Molecules — •Nandlal Sharma and Dirk Reuter — Optoelectronic Materials and Devices, University of Paderborn, Warburgerstr. 100, 33098, Paderborn, Germany

In this contribution, we present a modified gradient approach for the fabrication of low density vertically stacked InAs quantum dots (QDs), so called quantum dot molecules (QDM). The samples were grown by solid source molecular beam epitaxy (MBE) on GaAs (100). The density of the QDMs was varied across the wafer by the following approach: the bottom-layer of QDs was grown without substrate rotation, which resulted in an Indium gradient over the substrate surface, generating a QD density gradient. The emission wavelength of the bottom QDs were controlled by partial capping with 2.2 nm GaAs [1]. After growing a GaAs barrier of 6-18 nm, uncapped top-layer QDs were grown with (!) substrate rotation. The influence of the In amount in the top QD layer and of the GaAs inter-dot barrier thickness will be discussed. References [1] S. Fafard et al., Phys. Rev. B 59, 15368 (1999)

HL 35.49 Tue 15:00 Poster A

Emission wavelength tuning of InAs quantum dot molecules by rapid thermal annealing — •Alexander Karlisch, Nandlal Sharma, Stepan Shvarkov, and Dirk Reuter — Optoelektronische Materialien und Bauelemente, Universität Paderborn, Paderborn, Germany

Vertically stacked InAs quantum dots (QDs), so-called quantum dot molecules (QDM), have attracted much interest in the framework of solid state based quantum information processing. The realization of such applications require addressing a single QDM, e. g. by optical methods. To use effective, silicon based detectors and pump lasers that allow single QDM experiments, a ground state emission wavelength of around 950 nm at low temperatures is required. In this contribution, we present a study of emission wavelength tuning by rapid thermal annealing (RTA) for single layer QDs as well as QDM. The samples have been grown by solid-source molecular beam epitaxy on GaAs(100) substrates employing the Stranski-Krastanov growth mode. The as-grown samples show a ground state emission around 1150 nm at low temperatures. The samples have been annealed for 30 s at various temperatures under nitrogen gas atmosphere. To avoid As desorption during annealing, the samples were covered with pieces of a GaAs-wafer as proximity caps. Photoluminescence spectra showed that the emission wavelength at low temperatures could be blue-shifted below 950 nm for the single layer QDs as well as for the QDM while maintaining high luminescence intensities. We attribute the blue-shift to the interdiffusion of Ga and In. The influence of the annealing temperature is discussed in detail.

HL 35.50 Tue 15:00 Poster A

In Plane Gate transistors based on GaAs as sensors for dielectrics — •Benjamin Feldern, Sascha Valentin, Arne Ludwig, and Andreas D. Wieck — Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, Universitätsstraße 150, 44801 Bochum

In-Plane Gate transistors (IPG) [1] based on $Al_xGa_{1-x}As$ / GaAs HEMTs are used for the sensing of gases and liquids in the environment of the IPGs. For this purpose, IPGs are written in GaAs HEMT structures using Focused Ion Beam (FIB) implantation. In this work, the transconductance of IPGs in different gaseous and liquid environments is examined. It is found that the dielectric changes the transconductance of the IPG which in turn is attributed to the change in the electric field in the half space that contains the dielectric. In addition, the effect of surface treatment is examined. It is found that the surface states additionally screen the dielectric and thus reduce the effect of the dielectric. As an outlook, a possible passivation of the devices is envisaged. Hereby, we intend to shorten the time constant of the gate * source/drain transconductance signal path from ms towards the RC-time-constant of the inherent in-plane geometry, being orders of magnitudes shorter. [1] J. Nieder, A D. Wieck, P. Grambow, H. Lage, D. Heitmann, K. v. Klitzing, and K. Ploog, "One-dimensional lateral field-effect transistor with trench gate-channel insulation", Appl. Phys. Lett . 57, 2695 (1990).

HL 35.51 Tue 15:00 Poster A

Growth kinetics of GaP-nanowires employing TBP and TMGa — •Matthias Steidl, Christian Koppka, Peter Kleinschmidt, and Thomas Hannappel — TU Ilmenau, Institute of Physics, Department of Photovoltaics, Gustav-Kirchhoff-Str. 5, D-98693 Ilmenau, Germany

III-V nanowires (NWs) are promising candidates as components of future third generation photovoltaic devices and solar water splitting cells. Here, the moderately high band gap (Eg=2.3eV) and stability in many electrolytes makes GaP a suitable material. Moreover, by adding As or N the band gap can be tuned making the material highly interesting for tandem devices e.g. with silicon sub cells. While the growth kinetics of GaP and GaAs NWs using PH_3 and AsH_3 are already studied in detail, the growth kinetics of GaP NWs applying TBP have not been thoroughly investigated so far. Here, we report on the influence of V/III ratio, temperature and carrier gas on the Au-assisted VLS growth of GaP NWs by MOVPE. We found a great impact of the temperature on the growth behaviour. For low temperatures (450°C) the NW length does not increase linear with time - the longer the NW the smaller its growth rate (GR). In contrast, above 475°C, the GR is constant. The GR reaches its maximum at around 488°C and decreases above. As no Arrhenius dependency can be derived, the growth kinetics in this parameter regime are not governed by only one rate determining step. Moreover, a linear dependency of the GR on the V/III ratio (=5-20) was found for 450°C. Here, changing the carrier gas from pure H_2 to a mixture of H_2/N_2 increases the GR by a factor of two.

HL 36: Poster Ib

Topics: ZnO and II-VI and their relatives, Organic semiconductors, New materials, Surfaces, Heterostructures and interfaces, Optical properties, Ultra-fast phenomena

Time: Tuesday 15:00–19:00 Location: Poster A

HL 36.1 Tue 15:00 Poster A

H_2S-sensing in the ppb regime with ZnO nanowires — •Florian Huber, Sören Riegert, Manfred Madel, and Klaus Thonke — Institute of Quantum Matter / Semiconductor Physics Group, Ulm University

The detection of hydrogen sulfide (H_2S) plays a crucial role in several medical applications. On the one side it indicates different diseases such as asthma, on the other side it is used for therapeutic purposes, e.g. as so called "slow releasing H_2S-donors". However, the detection of small amounts of this gas is still a challenge, and especially for the analysis of the breath of patients a fast sensing method is needed.

In this project we investigate the electrical behaviour of ZnO nanowires towards H_2S detection in order to develop a fast and very sensitive sensor. The goal is the detection of H_2S concentrations in the lower ppb regime. Furthermore, the response of the nanowires to other gases, especially towards oxygen, is investigated in order to realize a breath sensor for medical use.

HL 36.2 Tue 15:00 Poster A

Growth of tilted ZnO nanowires by PLD on pre-structured sapphire substrates — •Alexander Shkurmanov[1], Chris Sturm[1], Guy Feuillet[2], Florian Tendille[3], Philippe De Mierry[3], Holger Hochmuth[1], and Marius Grundmann[1] — [1]Universität Leipzig, Inst. for Exp. Phys. II, Linnéstr. 5, 04103 Leipzig, Germany — [2]CEA/LETI 17, rue des Martyrs, 38054 Grenoble Cedex 9, France — [3]CNRS-CRHEA, rue Bernard Grégory, 06560 Valbonne, France

Nanowires (NWs) are highly interesting since they are building blocks, e.g. in light emitters, sensors and resonators. An advantage of ZnO NWs is that they can be grown self-organized within the bottom up approach. This growth leads typically to randomly organized growth of NWs or to NWs which are well oriented perpendicular to the surface. Here we report the well oriented growth of NW tilted against the surface normal. In doing so, we used a r-plane sapphire substrate where we apply a wet chemical etching process in order to prepare c-plane oriented facets [1]. These c-plane facets are tilted with respect to the r-plane oriented surface by an angle of about 57°. By using a high-pressure pulsed laser deposition process, an oriented growth of ZnO NWs on these c-plane facets along its normal was achieved.

[1] P. de Mierry et al, Appl. Phys. Lett. 96, 231918 (2010)

HL 36.3 Tue 15:00 Poster A

On the E3 deep-level in ZnO crystals — Rainer Pickenhain[1], Matthias Schmidt[2], •Holger von Wenckstern[1], and Marius Grundmann[1] — [1]Universität Leipzig, Institut für Experimentelle Physik II, Abteilung Halbleiterphysik, Linnéstraße 5, 04103 Leipzig — [2]Helmholtz-Zentrum für Umweltforschung GmbH, Abteilung Isotopenbiogeochemie, Permoserstraße 15, 04318 Leipzig

The deep-level E3 is frequently detected in n-doped ZnO crystals. Its thermal activation energy for electron emission into the conduction band amounts to approximately 280meV determined by deep-level transient spectroscopy (DLTS). In this work ZnO crystals from different sources were investigated by various space charge spectroscopic techniques with additional optical excitation. In the experiments the parameters temperature $4\,\mathrm{K} < T < 350\,\mathrm{K}$, photon energy $0.25\,\mathrm{eV} < h\nu < 4\,\mathrm{eV}$ and DLTS rate window $10^{-3}\,\mathrm{Hz} < r < 10^{4}\,\mathrm{Hz}$ were varied. The photo-ionisation cross-sections of two optical emission processes of electrons bound by E3 into the conduction band were measured. The results of these experiments suggest E3 to be a double centre with negative-U properties. Such model also explains the observed optical transitions. Based on the findings in this study a model for the E3 level is suggested. The model is discussed in the context of previously published theoretical work on native defects in ZnO.

HL 36.4 Tue 15:00 Poster A

Electrical properties of ZnO single nanowires — •Markus Stiller, José Barzola-Quiquia, Mahsa Zoraghi, and Pablo Esquinazi — Abteilung für Supraleitung und Magnetismus, Universität Leipzig, Linnestr. 5, D-04103, Germany

We have investigated the electrical resistance $R(T)$ of a ZnO nanowire of $\approx$ 400nm diameter as a function of temperature, between 30K and 300K, and frequency in the range 40Hz to 30MHz. The measurements were done on the as-prepared and after low-energy proton implantation at room temperature. The temperature dependence of the resistance of the wire, before proton implantation, can be well described by two processes in parallel. One process is the fluctuation induced tunneling conductance (FITC) and the other the usual thermally activated process. The existence of a tunneling conductance was also observed in the current-voltage ($I-V$) results, and can be well described by the FITC model. Impedance spectroscopy measurements in the as-prepared state and at room temperature indicate and support the idea of two contributions of these two transport processes in the nanowires. Electron backscatter diffraction confirms the existence of different crystalline regions. After the implantation of H^+ the electrical resistance $R(T)$ as well as the $I-V$ curves can be described by taking into account the contribution of the modified surface of the ZnO nanowire and a third thermally activated process is found. This can be explained by taking into account the impurity band splitting due to proton implantation.

HL 36.5 Tue 15:00 Poster A

B-induced inhomogeneous Broadening of the Electronic Spin Flip Resonance in $Zn_{.94}Mn_{.06}Se$ near the Metal-Insulator Transition — •Alexander Gerhard Knapp[1], Michael Hetterich[2], and Jean Geurts[1] — [1]Universität Würzburg, Experimentelle Physik 3, Würzburg, Germany — [2]Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

The diluted magnetic wide-gap semiconductor $Zn_{1-x}Mn_xSe$ allows the independent tuning of the magnetic and the electronic properties by variation of either the Mn content or the dopant concentration. The strong s-d exchange coupling between the Mn-iond d-levels and the s-type donor electrons gives rise to a giant Zeeman splitting in an external B-field. This short-range exchange interaction with the spatially randomly distributed Mn should result in a B-induced broadening of the donor energy distribution. We have investigated this effect for $Zn_{.94}Mn_{.06}Se$:Cl with various Cl-concentrations up to 4.5 10^{17} cm^{-3} by electron spin flip Raman spectroscopy (ESFRS) at $T = 1.6$ K. In ESFRS, the spin flip transition of the donor-bound electron is mediated by optically induced donor-bound excitons (D^0, X), which results in a sharp resonance of the ESFRS efficiency when the exciting laser photon energy matches the (D^0, X) energy. Therefore, we interpret the spectral dependence of the ESFRS-efficiency (resonance profile) in terms of the energy distribution of the donor states. We actually observe a significant broadening of the ESFRS resonance profiles with increasing B-field, up to 11.5 meV (FWHM) for $B = 5$ T.

HL 36.6 Tue 15:00 Poster A

Analyzing the crystal structure of CdSe nanowires — •Philip Harder, Tobias Redder, Tobias Kipp, and Alf Mews — Institute of Physical Chemistry, University Hamburg, Grindelallee 117, 20146 Hamburg, Germany

Semiconductor nanowires have interesting optical and electronical properties since their diameter scales on the nanometer size whereas their length can reach hundreds of microns. Their electronic properties strongly depend on the crystal structure. CdSe nanowires synthesized in solution via the SLS (solution-liquid-solid) method can exist in Zincblende and Wurtzite crystal structure. We developed a method that can determine the Wurtzite to Zincblende ratio and diameter of nanowires via powder X-ray diffraction measurements. The analalysis of the measured powder diffraction patterns was carried out via differential evolution algorithms and provides results with only few assumptions.

HL 36.7 Tue 15:00 Poster A

Systematic investigation of charge transfer in organic single crystal interfaces — •Yulia Krupskaya[1,2] and Alberto Morpurgo[1] — [1]DQMP, University of Geneva, Geneva, Switzerland — [2]IAPP, Dresden University of Technology, Dresden, Germany

Interfaces formed by two different organic semiconductors often exhibit significantly enhanced electrical conductivity, originating from the charge transfer between the constituent materials. The mechanisms driving the charge transfer and determining its amount are still not well studied and not understood microscopically. We have performed a systematic study of single-crystal charge transfer interfaces based on rubrene and F_x-TCNQ, a family of molecules whose electron affinity can be tuned by increasing the fluorine content. The combined analysis of transport and scanning Kelvin probe measurements reveals that the interfacial charge carrier density, resistivity, and activation energy correlate with the electron affinity of F_x-TCNQ molecules, with a higher affinity resulting in larger charge transfer. Although the transport properties can be described consistently and quantitatively using a mobility-edge model, we find that a quantitative analysis of charge transfer in terms of single-particle band diagrams reveals a discrepancy 100 meV in the interfacial energy level alignment. We attribute the discrepancy to phenomena known to affect the energetics of organic semiconductors, which are neglected by a single-particle description, such as molecular relaxation and band-gap renormalization due to screening.

Financial support: DFG KR 4364/1-1 and KR 4364/2-1

HL 36.8 Tue 15:00 Poster A

Optical properties of aromatic hydrocarbons in vapor phase — •Jonathan Prexl, Andre Rinn, Robin Döring, Nils Rosemann, and Sangam Chatterjee — Faculty of Physics and Materials Sciences Center, Philipps-Universität Marburg, Renthof 5, D-35037 Marburg

Organic single crystals are generally bound by the comparatively weak van-der-Waals interaction between the molecules. Their optical response commonly shows many spectral features which resemble the molecular response in addition to solid-state phenomena such as various exciton resonances. Typically, the molecular properties are investigated in solution. This yields significant influence of the dielectric environment such as the solvent shift or aggregation effects like excimer formation. Measurements in the vapor phase offer potential advantages to solution spectroscopy as they eliminate both. Here, we present a cost-effective, low-pressure heating-chamber-based setup enabling stable high-temperature conditions combined with a low leak rate. This enables reproducible spectroscopic measurements, such as photoluminescence or linear absorption, on pure vapor of the molecules. Exemplary data on various aromatic hydrocarbons are discussed and, e.g., in the case of perylene, compared to the solution and solid state re-

sponses.

HL 36.9 Tue 15:00 Poster A

Optical Spectroscopy on Organic-Inorganic Hybrid Structures - Charge Transfer in Type-II Level Systems — •Ingo Meyenburg[1], Benjamin Heidelmeier[1], Nils Rosemann[1], Christian Prinzisky[2], Jane Falgenhauer[3], Jörg Sundermeyer[2], Derck Schlettwein[3], and Wolfram Heimbrodt[1] — [1]Philipps Universität Marburg Department of Physics and Material Sciences Centre, Renthof 5, 35032 Marburg — [2]Philipps Universität Marburg Department of Chemistry, Hans-Meerwein-Straße, 35032 Marburg — [3]Justus-Liebig-University, Institute of Applied Physics, Heinrich-Buff-Ring 16, 35392 Gießen, Germany

Understanding interface processes is crucial for improvements of existing and new functional materials based on organic-inorganic hybrid semiconductor structures.

The depletion of excited organic states by charge transfer into the inorganic semiconductor helps to determine the level alignment at the interface. Indoline was already successfully used in dye sensitized solar cells (DSSC) which imply a charge transfer from the organic molecules into the inorganic substrate. Indoline dyes on mesoporous ZnO and on other promising substrates have been studied. A variation of the indoline dyes gives acces to different level alignments. The charge transfer time acts as sensor for the interfaces. The influence of the anchoring carboxylate chain on the charge transfer at the interface is clearified. Furthermore, newly sensitized Anthraquinone derivates are discussed regarding their suitability in DSSC.

HL 36.10 Tue 15:00 Poster A

Polarization-resolved reflectance spectroscopy of crystalline perfluoropentacene on various substrates — •Robin Carl Döring, David Leimbach, Tobias Breuer, Gregor Witte, and Sangam Chatterjee — Faculty of Physics and Materials Science Center, Philipps-Universität Marburg, Renthof 5, D-35032 Marburg, Germany

Perfluoropentacene (PFP) is the perfluorinated counterpart and hence n-type organic semiconductor to the prototypical p-type pentacene. It can be grown as highly crystalline thin films on various optically transparent substrates such as NaF, KCl, graphene and also graphene*s opaque multilayer counterpart, highly ordered pyrolytic graphite (HOPG). While PFP forms the typical herringbone motif on both NaF and KCl, it shows a π-stacking polymorph (PSP) on graphene and HOPG. Structural analyses show a π-stacking distance of only 3.07 Å, promising far higher values for electron and hole mobility and therefore greatly improved vertical transport, a desirable feature in potential organic electronic applications. Here, we investigate the influence of the packing motif and hence of the intermolecular coupling on the optoelectronic properties. Making use of polarization-resolved reflection contrast spectroscopy with high spatial resolution, we identify the corresponding exciton transition energies and correlate them with the orientation of crystalline domains and the substrate. Unfortunately, due to the face-on growth of the molecules, the π-stacking axis is inaccessible under normal angle of incidence. Hence, we perform close to grazing incidence photomodulated reflection spectroscopy.

HL 36.11 Tue 15:00 Poster A

The effect of electric field on polaron dynamics in quasi-one-dimensional conjugated polymers — •M.R. Mahani, A. Mirsakiyeva, and Anna Delin — Department of Materials and Nanophysics, School of Information and Communication Technology, Electrum 229, Royal Institute of Technology (KTH), SE-16440, Sweden.

Due to the strong electron-phonon coupling in conjugated polymers, the fundamental electronic excitations in these materials are always accompanied with a lattice distortion. The additional charge carriers dressed with a local structural deformation are called polarons and bipolarons. Among the successful theoretical methods to describe these excitations, density functional theory tends to underestimate the self-localizations, while the Hartree-Fock overestimates them. By use of the adopted Su-Schrieffer-Heeger Hamiltonian which has accurately reproduced the band structure, polaron formation, and other properties of the neutral and doped conjugated polymers, we investigate the effect of electric field on the polaron dynamics. We include an electric field in the Hamiltonian through the time-dependent vector potential via Peierls substitution of the phase factor. We solve the coupled quantum-classical equations for the electrons and the lattice displacements in the polymer chain, using numerical integration scheme. Our calculations elucidate the effect of electric field on the dynamics of polaron in quasi-one-dimensional polymers and contribute to the understanding of the polymer-based light-emitting diodes in which the injected carriers are usually under electric fields with different magnitudes.

HL 36.12 Tue 15:00 Poster A

Determination of trap distributions in organic semiconductors by fractional TSC measurements — •Michael Bretschneider, Alexander Wagenpfahl, and Carsten Deibel — Institut für Physik, Technische Universität Chemnitz, 09126 Chemnitz, Germany

The interplay between traps and charge transport is very important for virtually all organic electronic applications, as the charge carrier mobility has a direct impact on the performance. While hole traps are thoroughly investigated, only indirect information has been available on electron traps until recently. Therefore, we aim at correlating the energetic position and concentration of electron traps in soluble organic semiconductors with their charge transport properties. The properties of these electron trap states will be determined by defect spectroscopy. In particular, we performed thermally stimulated current (TSC) measurements on polymer diodes based on P3HT and PTB7. The resulting density of trap states distribution is compared to the results of time of flight measurements to gain deeper insight in the role of traps on charge transport.

HL 36.13 Tue 15:00 Poster A

Application of metal nanoparticle monolayers as highly tunable room temperature field-effect transistors — •Hauke Lehmann, Svenja Willing, Mirjam Volkmann, and Christian Klinke — Institut für Physikalische Chemie, Universität Hamburg, Grindelallee 117, 20146 Hamburg, Germany

To tackle the need for electrical devices with reduced power-consumption, a limited charge-carrier concentration is advantageous. Single-electron transistors use the Coulomb repulsion that hinders the addition of electrons onto a small island. Due to this Coulomb-blockade effect, the energy levels inside such a small island are quantized. They can be tuned with an electric field which influences the possible transport across the structure. The resulting current oscillations allow for the definition of a conducting and non-conducting state and, thus, the application as transistor with unique periodic transfer characteristics. Colloidally synthesized CoPt nanoparticles are deposited onto substrates with predefined gold electrodes as highly ordered monolayers via the scalable Langmuir-Blodgett method. The nanoparticle array is limited to stripes by means of a resist mask. To influence the transport, a local back-gate electrode is employed underneath the channel for the first time. This enables good electrostatic control over individually addressable devices without interferences from a dielectric capping layer. This new fabrication method yields smoother and more sinusoidally shaped Coulomb oscillations. The predictable and highly reproducible behavior makes systematic investigations, high on/off-ratios and room-temperature operation possible.

HL 36.14 Tue 15:00 Poster A

Synthesis and characterization of free standing Silicene modified with organic groups — •Ravi Kumar Divakar[1], Wladmir Thiessen[1], Ihsan Amin[2], Raul David Rodriguez[3], Manuel Monecke[3], Mahfujur Rahaman[3], and Lukas M. Eng[1] — [1]Institut für Angewandte Physik, TU Dresden, Dresden, Germany — [2]Institut für Makromolekulare Chemie, TU Dresden, Dresden, Germany — [3]Institut für Physik, TU Chemnitz, Chemnitz, Germany

Silicene has attracted remarkable attention in both research and industry due to its potential application for devices such as field effect transistors [1]. Silicene usually is synthesized on Ag substrate using ultra high vacuum system [2]. We present here a novel wet-chemical synthesis route in order to prepare free-standing Silicene monolayers which are modified with organic moieties at the highly reactive Si-atoms at the edges of the sheet. These organic moieties prevent oxidation and provide stability in aqueous surfactant solution. The monolayer with surfactant has a thickness of ~2.5 nm measured by AFM [3]. Furthermore we have performed TEM measurements, showing a honeycomb lattice with the lattice constant a = (2.18 * 0.11) Å, in accordance with DFT calculations [4]. SEM measurements show a stacked morphology of Silicene sheets. The presence of silicon in the synthesized material is confirmed by XPS. In summary, we demonstrate a novel way to synthesize free standing Silicene. [1] Li Tao et al., Nature Nanotechnology

10 (2015) 227. [2] P. Vogt et al., Appl. Phys. Lett. 104 (2014) 021602. [3] M. Ait Ali et al., J. Physics: Conf. Series 491 (2014) 012009. [4] L. Chen et al., Appl. Phys. Lett. 102 (2013) 081602.

HL 36.15 Tue 15:00 Poster A

Investigation of Prussian blue type redox catalysts for artificial photosynthesis — •Franziska Simone Hegner, Núria López, and José-Ramon Galán-Mascarós — Institute of Chemical Research of Catalonia (ICIQ), Av. Països Catalans 16, 43007 Tarragona (Spain)

The development of an efficient, cheap and robust water-splitting catalyst remains the bottleneck step to realizing artificial photosynthesis. Materials based on Prussian blue (iron(III)hexacyanoferrate(II)), which fulfill all those criteria, have shown high catalytic activities with exceeding long-term stabilities. Notwithstanding, the detailed catalytic mechanisms remain unclear. Combining experimental methods with theoretical calculations we shed light on the underlying physics of Prussian blue and its derivatives

Catalytic systems were prepared by coating oxide semiconductors with Co[Fe(CN)6], which has shown to be the highest efficient water-oxidation catalyst. Their electrochemical behaviour and the oxygen evolution were studied under light conditions.

Due to their mixed-valence character, multiple spin configurations and various charge transfer states, Prussian blue and its analogues exhibit a high degree of complexity, which challenges theoretical calculations. We developed a computational approach to investigate these systems. Moreover, we found out new insights about the electronic and magnetic structure.

HL 36.16 Tue 15:00 Poster A

Impact of the nuclear spin bath on the carrier spin noise in InGaAs/GaAs self-assembled quantum dots — •Philipp Glasenapp[1], Dmitri Smirnov[2], Mikhail Glazov[2], Alex Greilich[1], Johannes Hackmann[1], Frithjof Anders[1], and Manfred Bayer[1] — [1]Technische Universität Dortmund, 44227 Dortmund, Germany — [2]Ioffe Physical-Technical Institute, 194021 St. Petersburg, Russia

Spin noise of self-assembled InGaAs/GaAs quantum dots doped with single electron or hole spins, and grown under identical conditions, is measured optically in the limit of low probe laser intensity. This allows to reveal fundamental properties of carrier spin dynamics due to interaction with surrounding nuclei on a level close to thermal equilibrium. These dynamics include for example Overhauser precession of electron spins due to isotropic hyperfine interaction. The most remarkable result is the decoupling of the carrier spins from the nuclei under longitudinal magnetic fields, leading to a crossover to 1/log (t) spin dynamics. This happens regardless of the type of carrier spin, and we find that under these conditions both electrons and holes obey comparable timescales of dephasing - an observation that can be seen as an evidence of nuclear quadrupolar effects in the quantum dots that do not depend on carrier spin doping, and which provide additional channels of spin dephasing beyond hyperfine interaction. We compare our results to existing theoretical models and find good agreement.

HL 36.17 Tue 15:00 Poster A

Electronic and magnetic properties of the ideal Fe/GaAs(110) interface — •Tim Iffländer[1], Steffen Rolf-Pissarczyk[1], Lars Winking[1], Rainer G. Ulbrich[1], Ali Al-Zubi[2], Stefan Blügel[2], and Martin Wenderoth[1] — [1]IV. Physikalisches Institut - Solids and Nanostructures, Georg-August-Universität Göttingen — [2]Peter Grünberg Institut (PGI-1) & Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

By means of scanning tunneling microscopy (STM) and spectroscopy (STS) in cross-sectional geometry we investigate the electronic properties of the ideal Fe/GaAs(110) interface. Highly-resolved STS measurements at the metal-semiconductor contact exhibit a continuum of metal-induced gap states (MIGS) in the first few atomic layers at the interface. Three-dimensional finite element calculations yield a precise value for the Schottky barrier height and additional information on the local density of states inside the valence and conduction band at the interface. Our density functional theory (DFT) calculations are in excellent agreement with the STS data showing that our experimental approach serves as an excellent probe to study the process of Schottky barrier formation on the atomic scale [1]. Furthermore, we investigate the magnetic properties of the ideal Fe/GaAs(110) interface by means of in situ magneto-optical Kerr effect measurements. We find a unidirectional magnetic anisotropy for 2-3 ML thin Fe films. Our results indicate that this anisotropy is the manifestation of a more complex spin structure. This work was supported by the DFG SPP 1285.

[1] T. Iffländer et al., Phys. Rev. Lett. 114, 146804 (2015).

HL 36.18 Tue 15:00 Poster A

Terahertz spectroscopy and ultrafast electron dynamics of a broad single GaAs/AlGaAs quantum well — •Johannes Schmidt[1,2], Stephan Winnerl[1], Martin Teich[1], Aaron M. Andrews[3], Gottfired Strasser[3], Harald Schneider[1], and Manfred Helm[1,2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany — [2]Technische Universität Dresden, 01062 Dresden, Germany — [3]Technische Universität Wien, A-1040 Vienna, Austria

Ultrafast electron dynamics in quantum well (QW) structures is investigated by applying a strong terahertz (THz) field with a photon energy resonant to an intersubband transition. In particular, if the THz field is in resonance with the transition between the second and third subband, so-called Autler-Townes (or AC Stark) splitting could be observed when probing the 1-2 transition. This effect has been observed previously at mid-infrared wavelengths in an n-type multiple QW [1]. Our efforts aim at investigating the AC-Stark effect in the THz regime using a broad, 36 nm wide single QW where the carrier density can be tuned electrically. We will present our first results indicating absorption by an intersubband transition in the QW, where the electron population can be controlled by an electrical modulation technique. Furthermore, ultrafast electron dynamics in the ps-regime is investigated by narrowband single-color pump-probe measurements performed using a THz free-electron laser.

[1] J. F. Dynes, M. D. Frogley, M. Beck, J. Faist, and C. C. Phillips, Phys. Rev. Lett. 94, 157403 (2005)

HL 36.19 Tue 15:00 Poster A

Atomic Layer Deposition of high-k dielectrics on III-V substrates — •Soraya Karimzadah[1,2,3], Torsten Rieger[1,2], Ullrich Pietsch[3], Detlev Grützmacher[1,2], and Mihail Ion Lepsa[1,2] — [1]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich GmbH, 52425 Jülich — [2]JARA-FIT — [3]Festkörperphysik, Universität Siegen, 57072 Siegen

Deposition of high-k dielectrics on III-V substrates by atomic layer deposition (ALD) is considered as a novel generation of gate oxide for nanodevices and surface passivation of nanowires (NWs). The thin film layers deposited by ALD are extremely uniform and conformal which is highly important for high aspect ratio structures such as NWs. We have investigated the in-situ ALD deposition of Al2O3 on MBE grown GaAs layers using TMA and H2O as ALD precursors. Experiments were carried out in a state of the art multi-material nanocluster tool composed of UHV growth and deposition systems. The window for the thermal ALD deposition of Al2O3 on Si substrate is determined. Later on, the in situ process of deposition of Al2O3 on GaAs substrate has been performed. The GaAs layers were grown by MBE and transferred to the ALD chamber without exposing the sample to air. In this way, the formation of the native oxide and any other contamination on the GaAs surface is avoided improving the quality of the oxide-semiconductor interface. The samples were characterized by ellipsometry, XRR, AFM, TEM, XPS and CV measurements. High-k dielectrics on III-V substrates with high quality as well as in-situ formed interfaces open the way to nanoscale devices with improved characteristics.

HL 36.20 Tue 15:00 Poster A

Electrical and topological analysis of silicon after laser pulse irradiation in a sulfur-containing atmosphere — Julian Sickel and •Michael Seibt — Georg August Universität IV. Physikalisches Institut, Göttingen, Deutschland

Enhanced infrared absorption of sulfur hyperdoped crystalline silicon has drawn attention to fs laser irradiation in SF6 atmosphere [1]. Such treatments lead to highly S doped surface-near regions and buried pn-junctions if p-type substrates are used. Furthermore, depending on the number of pulses per spot different surface topologies have been observed as well as the formation of extended defects such as twins and dislocations [2]. Here we focus on so called gray silicon which is named after its appearance due to a five double fs pulse laser treatment per spot with a wavelength of 800 nm. Using atomic force microscopy (AFM) the topology of the samples was characterized. Electrically sensitive techniques such as Kelvin-Probe atomic force microscopy (KFM) and electron beam induced current (EBIC) have been used on the same areas in order to study correlations between electrical properties like

work-function or excess carrier recombination and the surface micro structure. The results of this work show special structural formation of hillocks and valleys at the surface as well as lower excess carrier recombination rates and higher work-functions within the hillocks. In addition, experimental results indicate a special distribution of work-functions inside the hillocks. [1] A.L. Baumann, et al., Energy Procedia 27 (2012) 480-484 [2] P. Saring, et al., Appl. Phys. 103, 061904 (2013)

HL 36.21 Tue 15:00 Poster A

Microscopic Theory of the Refractive Index — •Ronald Starke[1] and Giulio Schober[2] — [1]TU Bergakademie Freiberg, Inst. f. theo. Phys — [2]Uni. Heidelberg, Inst. f. theo. Phys

We re-examine the refractive index from the viewpoint of modern first-principles materials physics and find that the standard formula, $n^2 = \epsilon_r \mu_r$, is downright wrong. Even worse, the allegedly approximate Maxwell relation, $n^2 = \epsilon_r$, which is being used for most practical purposes, can only be justified in the long-wavelength limit. In order to obtain the true wave-equation in materials, one instead has to start from the fundamental, Lorentz covariant electromagnetic wave-equation in terms of the proper response tensor. From this we prove a general theorem by which the electric field in materials is restricted to the kernel of the microscopic dielectric tensor thus elucidating the analogy to the theory of plasmons.

HL 36.22 Tue 15:00 Poster A

Very slow decay of a defect related PL emission band in AlN: signatures of the Si related DX state — •Matthias Lamprecht[1], Christiane Grund[1], Benjamin Neuschl[1], Zachary Bryan[2], Ramón Collazo[2], Zlatko Sitar[2], and Klaus Thonke[1] — [1]Institute of Quantum Matter / Semiconductor Physics Group, Ulm University, 89081 Ulm, Germany — [2]Department of Materials Science and Engineering, North Carolina State University, Raleigh, North Carolina 27606, USA

We investigated the defect related PL emission band at 2.4 eV in aluminum nitride bulk crystals using different methods including time-resolved photoluminescence (TRPL) investigations. Two slow processes with decay times of 13 ms and 153 ms were found for this band in the low-temperature limit. Based on temperature dependent TRPL and PL experiments, the faster process is assigned to a donor-acceptor pair transition (involving a shallow, effective-mass like silicon donor), and the slower process is attributed to a transition between a more localized electron at a silicon DX center and the same deep acceptor.

HL 36.23 Tue 15:00 Poster A

Density functional study of structural, electronic and optical properties of point defects in 2D transition metal dichalcogenides — •Soumyajyoti Haldar[1], Hakkim Vovusha[1], Manoj Yadav[2], Olle Eriksson[1], and Biplab Sanyal[1] — [1]Div. of Materials Theory, Dept. of Physics & Astronomy, Uppsala University, Sweden — [2]Nepal Academy of Science and Technology, Nepal

Using density functional theory, we have studied structural, electronic and magnetic properties of various point defects in 2D transition metal dichalcogenides MX_2, (M = Mo, W; X = S, Se, Te). Our results shows that the X interstitial defect has the lowest formation energy ($\sim$ 1 eV) for all the systems under the X rich condition whereas for M rich condition, X vacancy has the lowest formation energy except for MTe_2 systems. At experimental growth temperatures (1000 - 1200 K), these defects have high equilibrium defect concentrations. In general, the defect states appears in the band gap, which can affect electronic and optical properties of the pure system. Calculation of optical properties show that the optical transitions occurs at $\sim$ 1.0 eV due to defect states. Our results are expected to guide the experimental nanoengineering of defects to achieve suitable properties related to band gap modifications and characterization of defect fingerprints via optical absorption measurements.

HL 36.24 Tue 15:00 Poster A

Power-dependent resonant Rayleigh scattering of exciton-polaritons — •Bernd Berger[1], Johannes Schmutzler[1], Daniel Schmidt[1], Marc Assmann[1], Martin Kamp[2], Christian Schneider[2], Sven Höfling[2], and Manfred Bayer[1] — [1]Experimentelle Physik 2, Technische Universität Dortmund, D-44221 Dortmund, Germany — [2]Technische Physik, Physikalisches Institut, Wilhelm Conrad Röntgen Research Center for Complex Material Systems, Universität Würzburg, D-97074 Würzburg, Germany

In a two dimensional DBR-microcavity a condensate of exciton-polaritons is formed by resonant excitation. Due to the non-zero in-plane momentum resulting from resonant excitation the condensate propagates inside the microcavity and undergoes Rayleigh scattering at structural defects of the sample. Characteristic scattering rings in the Fourier space image of transmitted light are identified and examined. Especially the influence of different excitation parameters on the scattering patterns is examined systematically and will be presented.

HL 36.25 Tue 15:00 Poster A

Overview of band-edge and defect related luminescence in aluminium nitride — Tristan Koppe, Hans Hofsäss, and •Ulrich Vetter — II. Physikalisches Institut der Georg-August-Universität Göttingen, Deutschland

We present a compact overview of results published in the last decades describing near band-edge as well as defect related luminescence in aluminium nitride. Especially in the case of defect related luminescences associated with oxygen or oxygen vacancy complexes, the different points of view in literature are outlined and compared to each other.

In many cases luminescence signals in the band-gap region are assigned to specific band to impurity or donor acceptor pair transitions without regarding other possible origins. One problem are the various theories describing the same transitions based on experimental observed emission or absorption signals in combination with simulations which show sometimes contradicting results too. Due to the large number of different possible sources for defect related luminescences a detailed investigation of the stoichiometric composition of samples is necessary.

Therefore, in order to provide a point of reference, more than 200 publications investigating aluminium nitride in experiments as well as in simulations were analysed and are presented in a neatly arranged manner to provide an overview of the existing assignments.

HL 36.26 Tue 15:00 Poster A

Influence of growth temperature on the optical and structural properties of Ga(N,As,P) quantum wells on silicon for laser application — •Sarah Karrenberg, Sebastian Gies, Martin Zimprich, Tatjana Wegele, Andreas Beyer, Wolfgang Stolz, Kerstin Volz, and Wolfram Heimbrodt — Faculty of Physics and Material Science Center, Philipps University Marburg, D-35032 Marburg, Germany

Realizing suitable light sources for optical data transmission on silicon is one of the major goals of optoelectronic integration nowadays. The quaternary Ga(NAsP) is a promising candidate for this. Previously, we had optimized the annealing procedure of the necessary rapid-thermal-annealing. Here, we present an analysis of the influence of growth parameters on Ga(NAsP) quantum wells (QWs) on silicon. The optical and electronic properties are revealed using photoluminescence (PL), PL excitation and Raman spectroscopy. The structural properties are analyzed by transmission electron microscopy and high resolution X-ray diffraction. The conjunction of these methods reveals the striking influence of the growth temperature on the Ga(NAsP) QW composition, interfaces and luminescence properties. An in-depth analysis of the Ga(NAsP) disorder is presented. Furthermore, the changes in disorder upon increasing the growth temperature are connected to the accompanying structural changes in the QWs morphology. This allows us to reveal the optimal growth parameters in terms of structural and electronic properties of the Ga(NAsP)/Si material system.

HL 36.27 Tue 15:00 Poster A

Optical properties of InGaN/GaN core-shell nanowires — •Florian Krause[1], Johannes Dühn[1], Jürgen Gutowski[1], Christian Tessarek[2,3], Martin Heilmann[2], Silke Christiansen[2,3], and Kathrin Sebald[1] — [1]University Bremen, Institute of solid state physics, Bremen, Germany — [2]Max-Planck-Institute for the Science of Light, Erlangen, Germany — [3]Helmholtz-Zentrum Berlin for Materials and Energy, Berlin, Germany

Nanowires (NWs) based on GaN and InGaN can be utilized to increase the efficiency of optoelectronic applications like white light sources due to the improvement of their structural quality in comparison to planar structures. Therefore we are interested in InGaN/GaN core-shell NWs which were grown on sapphire substrates by using metalorganic vapour phase epitaxy. The NWs consist of a N-polar Si-doped GaN core with mixed polarity surrounded by an InGaN/GaN multiple quantum well shell covered by non-doped GaN. The NW size varies in diameter and height within a range of a few micrometers and their aspect ratio is between 1:2 and 1:10. The GaN core has a Ga-polar column embedded in a N-polar tube. The column favours the formation of a small pyra-

midal tip on the top facet of the NW and it is also covered by InGaN. To investigate the optical properties of single and ensemble NWs, their micro-photoluminescence spectra are analyzed in dependence on temperature and excitation density. In particular, the optical properties of the top facets of single NWs are most interesting with respect to carrier confinement in the InGaN accumulation zones in these facets which could be employed as single photon sources.

HL 36.28 Tue 15:00 Poster A

Investigation of the impact of gold nanodots deposited in porous GaP template by Raman Spectroscopy — •Andrei Tiron[1,2], Cameliu Himcinschi[2], Jens Kortus[2], Eduard Monaico[1], and Ion Tiginyanu[1,3] — [1]Technical University of Moldova, Stefan cel Mare Avenue 168, MD-2004 Chisinau, Republic of Moldova — [2]TU Bergakademie Freiberg, Institute of Theoretical Physics, Leipziger Str. 23, D-09599 Freiberg, Germany — [3]Institute of Electronic Engineering and Nanotechnologies, Academy of Sciences of Moldova, Academy str. 3/3, Chisinau MD-2028, Republic of Moldova

Porous gallium phosphide (GaP) without and with gold deposited inside the pores were investigated by micro-Raman spectroscopy. The anodization causes a breakdown of the polarization selection rules, inherent to a (100) surface, accompanied by a downward shift of the LO-phonon frequency [1]. The appearance of two surface-related phonon modes in porous GaP templates without and covered with gold nanodots was detected. The influence of the temperature and laser annealing on the Raman spectra also were investigated. Au deposition in porous GaP templates induced an enhancement of the Raman signal.

[1] Micro-Raman-scattering study of surface-related phonon modes in porous GaP. (I. M. Tiginyanu, G. Irmer, J. Monecke, H. L. Hartnagel) Phys. Rev. B, volume 55, 6739-6742 (1997).

HL 36.29 Tue 15:00 Poster A

Nonlinear optical excitation of a two-level system with a superoscillating field — •Daniel Berghoff, Matthias Reichelt und Torsten Meier — Department of Physics and CeOPP, University of Paderborn, Warburger Str. 100, D-33098 Paderborn, Germany

Although superoscillations are a well known phenomena [1], the impact on a nonlinearly photoexcited two-level system (TLS) was only recently investigated by Baranov et al. [2]. Here, the excitation with different electric fields is studied. Among other things we show that the TLS can be excited by off-resonant superoscillations. Furthermore, parameters are numerically obtained, for which a maximum population inversion is observed.

[1] Y. Aharonov, F. Colombo, I. Sabadini, D. C. Struppa, and J. Tollaksen, Some mathematical properties of superoscillations, J. Phys. A **44**, 365304 (2011).
[2] D. G. Baranov, A. P. Vinogradov, and A. A. Lisyansky, Abrupt Rabi oscillations in a superoscillating electric field, Optics Letters **39**, 6316 (2014).

HL 36.30 Tue 15:00 Poster A

Temporal coherence properties of a polariton condensate in a disordered environment — Martin Thunert, •Stefan Lange, Helena Franke, Chris Sturm, Tom Michalsky, Marius Grundmann, and Rüdiger Schmidt-Grund — Universität Leipzig, Inst. für Exp. Physik II, Linnestr. 5, 04103 Leipzig

We report on the temporal coherence properties of an exciton-polariton Bose-Einstein condensate (BEC) in a disordered ZnO-based bulk planar microcavity (MC). The momentum space intensity distribution of the BEC emission is strongly influenced by disorder even at high excitation powers. We found theoretically that this lack of BEC stabilization relies on the driven dissipative nature of the condensate, leading to disorder induced, density independent phase fluctuations [1]. To prove whether the observed emission arises from a temporally coherent condensate, we applied interferometry measurements with variable path length difference or rather temporal delay between both interferometer arms. With this procedure, we found a coherence time of about 24 ps for the BEC emission, which is by a factor of 150 larger than the lifetime of the uncondensed polaritons [1]. Using time-resolved, energy-momentum-space imaging, BEC emission was observed up to 100 ps after the decay of the exciting laser pulse. Consequently, the coherence of the investigated quantum system is conserved during the multiple reabsorption and reemission processes that can thus be identified as a polariton condensate.

[1] M. Thunert, A. Janot *et al.*, ArXiv (2014), arXiv:1412.8667

HL 36.31 Tue 15:00 Poster A

Photoconductivity of a new material: $K_2Hg_2Se_3$ — •Sina Lippert[1], Günther Thiele[2], Felix Fahrnbauer[3], Philipp Bron[2], Oliver Oeckler[3], Arash Rahimi-Iman[1], Bernhard Roling[2], Stefanie Dehnen[2], and Martin Koch[1] — [1]Faculty of Physics and Materials Sciences Center, Philipps-Universität Marburg, D-35037 Marburg — [2]Department of Chemistry and Materials Sciences Center, Philipps-Universität Marburg, D-35043 Marburg — [3]Faculty of Chemistry and Mineralogy, Institut of Mineralogy, Crystallography and Materials Science, D-04275 Leipzig

$K_2Hg_2Se_3$ is a new photoconducting material with a direct band gap of around 1.4 eV, identified by both absorption and photocurrent experiments, and verified by comparison with impedance spectroscopy measurements and band structure calculation [1]. The compound shows a semiconductor-type behavior with current-voltage characteristics comparable to GaAs.

The presented material is a chalcogenido-mercurate, which was obtained by means of solvothermal treatment of the corresponding solid precursors on large scales and compromises unprecedented, covalently linked selenidomercurate columns.

In our recent study, we found that presence of heavy element atoms in $K_2Hg_2Se_3$ leads to unique material properties regarding optoelectronic, photophysical and thermoelectric properties. Their functionality can be further adjusted by a variation of the elements within a family of structurally related compounds.

[1] G. Thiele et al., Chem. Mater. 27, 2015, 4114-4118.

HL 36.32 Tue 15:00 Poster A

Nonlinear Optical Response of Functionalized Chalcogenide Cluster Molecules — •Nils W. Rosemann[1], Jens Eussner[2], Ulrich Huttner[1], Andreas Beyer[1], Kerstin Volz[1], Stephan W. Koch[1], Mackillo Kira[1], Stefanie Dehnen[2], and Sangam Chatterjee[1] — [1]Faculty of Physics and Materials Science Center, Philipps-Universität Marburg, Renthof 5, D-35032 Marburg, Germany — [2]Faculty of Chemistry and Materials Sciences Center, Philipps-Universität Marburg, Hans-Meerweinstraße, D-35043 Marburg, Germany

Chalcogenide clusters in combination with various different ligands offer a large variety of structural and physical properties. In particular, their nonlinear optical response can be tuned, e.g., enabling second harmonic generation by varying the compositions and constituents of cluster cores and ligands. Modifying the core primarily influences the band gap energy, whereas changing the ligand influences the anharmonicity of the electronic potential and thus the efficiency of nonlinear processes.

HL 36.33 Tue 15:00 Poster A

Exciton polaritons in CdMgTe / CdZnTe waveguides — •Felix Spitzer[1], Ilya Akimov[1], Manfred Bayer[1], Nils Weber[2], Cedrik Meier[2], Torsten Meier[2], Régis Andre[3], and Henri Mariette[3] — [1]Experimentelle Physik II, TU Dortmund, D-44221 Dortmund, Germany — [2]Department Physik, Universität Paderborn, D-33098 Paderborn, Germany — [3]Institut Néel (Centre National de la Recherche Scientifique), 25 Avenue des Martyrs, 38042 Grenoble, Frankreich

The steady-state reflectivity of a CdMgTe / CdZnTe waveguide structure was measured using Fourier imaging spectroscopy. One dimensional metallic gratings are used to couple far field radiation with waveguiding modes. The angular and wavelength resolved reflectivity exhibits the underlying waveguide dispersion and its interaction with the excitonic resonance. The polarization resolved data shows TE- and TM-waveguiding modes. These results are consistent with angle resolved photoluminescence, where the emission is coupled out under a given angle, depending on the grating period.

The dispersion of waveguiding modes flattens strongly in the vicinity of exciton resonance. Here we demonstrate, that the group velocity can be increased by more than one order of magnitude.

HL 36.34 Tue 15:00 Poster A

Phonon dispersion by fitting effective potentials to ab initio data — •Philipp Risius, Marcel Giar, Andreas Rühl, and Christian Heiliger — Institut für theoretische Physik, Justus-Liebig-Universität, 35392 Gießen

Direct *ab initio* calculation of the forces on atoms is not feasible for materials with small defect concentrations, which have to be represented by large supercells. Effective potentials as used in molecular dynam-

ics simulations could allow this and subsequently enable calculation of phonon dispersion curves.

Defect-free silicon is used as a model system. Effective potentials are generated by matching predicted forces to those calculated with *ab initio* methods. The resulting potentials are tested for reproduction of small and long-range forces and phonon dispersion curves are calculated from them.

It is found that a modified Embedded Atom Method [1] is best suited for reproducing the reference forces. Here, the phonon dispersion can be reproduced accurately, whereas other potential models perform worse.

[1] Lenosky et al. *Model. Simul. Mater. Sci. Eng.* **8**, 825 (2000).

HL 36.35 Tue 15:00 Poster A

Anisotropy measurement using ultrafast photocurrents — •Christian Schmidt, Shekhar Priyadarshi, and Mark Bieler — Physikalisch-Technische Bundesanstalt, Braunschweig, Germany

The linear surface magneto-photocurrent (LSMC) is based on an optically induced anisotropic carrier distribution which is scattered asymmetrically at the surface of semiconductors [1]. Here, we investigate the LSMC induced in bulk GaAs by optical femtosecond excitation on a sub-picosecond time scale. For this we detect its THz radiation via electro-optical sampling [2]. Comparing the LSMC measurements with a time-dependent model of the LSMC we are able to extract the anisotropy relaxation time from our measurements.

We found a double exponential decay of the anisotropy with the fast time constant being on the order of 10 fs and the slow time constant ranging from 100 fs to 190 fs. We attribute the fast and slow relaxation times to anisotropy relaxation of heavy holes and electrons, respectively. Variations of the photocarrier density in the range of $10^{15}\mathrm{cm}^{-3}$ to $5 \times 10^{17}\mathrm{cm}^{-3}$ indicate that phonon-carrier scattering is the major anisotropy relaxation mechanism for electrons. Our data compares well to previously reported anisotropy relaxation times ranging from 30 fs to 190 fs [3], [4] and shows that the LSMC is a novel intrinsic probe for anisotropy relaxation in semiconductors.

[1] V.L. Alperovich et al., JETP Lett. 49, 702 (1989).
[2] C.B. Schmidt et al., Appl. Phys. Lett. 106, 142108 (2015).
[3] J.L. Oudar et al., Phys. Rev. Lett. 53, 384 (1984).
[4] M.T. Portella et al., Appl. Phys. Lett. 60, 2123 (1992).

HL 36.36 Tue 15:00 Poster A

Exciton-Polariton Propagation in CdZnTe — Jan Lohrenz[1], Stephan Melzer[1], Claudia Ruppert[1], Ilya Akimov[1], Matthias Reichelt[2], •Alexander Trautmann[2], Torsten Meier[2], and Markus Betz[1] — [1]Experimentelle Physik 2, TU Dortmund, Otto-Hahn-Str. 4, 44221 Dortmund, Germany — [2]Department of Physics and CeOPP, University of Paderborn, Warburger Str. 100, D-33098 Paderborn, Germany

In bulk CdZnTe light is significantly slowed down in a spectral range close to the lower exciton-polariton (LP) branch. [1] We present different methods for modelling light pulses centered near the LP resonance, i.e., numerical and analytical approaches allowing for slow light propagation and the diffusion of the wave packet. [2] These light fields are used to interpret nonlinear optical signatures in a recently performed ultrafast pump-probe experiment. [3]

[1] T. Godde, I. A. Akimov, D. R. Yakovlev, H. Mariette, and M. Bayer, Phys. Rev. B **82**, 115332 (2010).
[2] A. Trautmann, Bachelor Thesis, University of Paderborn, submitted.
[3] J. Lohrenz, S. Melzer, C. Ruppert, I.A. Akimov, M. Reichelt, A. Trautmann, T. Meier, M. Betz, to be published.

HL 36.37 Tue 15:00 Poster A

Nonlinear Phononics and the interaction of Light and Phonons — •André Bojahr[1], Matthias Rössle[1], Wolfram Leitenberger[1,2], Peter Gaal[2], Mathias Sander[1], Matthias Reinhardt[2], Alexander von Reppert[1], Jan-Etienne Pudell[1], and Matias Bargheer[1,2] — [1]Institut für Physik und Astronomie, Universität Potsdam, Karl-Liebknecht-Str. 24-25, 14476 Potsdam, Germany — [2]Helmholtz-Zentrum Berlin, Wilhelm-Conrad-Röntgen Campus, BESSY II, Albert-Einstein-Str. 15, 12489 Berlin, Germany

Phonons are often regarded as delocalized quasiparticles with certain energy and momentum. The anharmonic interaction of phonons determines macroscopic properties of the solid, such as thermal expansion or thermal conductivity, and a detailed understanding becomes increasingly important for functional nanostructures. By the use of ultrashort laser pulses we are able to excite monochromatic phonon wave packets with a wavelength in the nanometer range. To observe the anharmonic interaction of these phonons we use time-resolved Brillouin scattering with a white light probe pulse and ultrafast X-ray diffraction. [1] With these methods we were able to observe the nonlinear mixing of a narrowband coherent phonon wave packet in strontium titanate (SrTiO3) to its second harmonic. [2] Furthermore, we present concepts to amplify monochromatic phonons by stimulated Raman scattering to overcome the limits of the maximum phonon amplitude in the excitation process mainly given by the damage threshold due to ultrafast heating above the melting temperature. [1] Opt. Express, 21, 18, 21188-21197 [2] Phys. Rev. Lett., 115, 195502

HL 36.38 Tue 15:00 Poster A

Influence of the growth temperature on LT- GaAs photoconductive antennas for THz generation — •Oday Mazin Abdulmunem[1], Norman Born[1], Martin Mikulics[2], Jan C. Balzer[1], and Martin Koch[1] — [1]Faculty of Physics and Materials Sciences Center, Philipps-Universität Marburg, D-35037, Marburg — [2]Peter Grünberg Institut (PGI-9), Forschungszentrum Jülich GmbH, D-52425, Jülich

THz technology is becoming a fully developed technology which is used for fundamental research as well as for industrial applications. There are several approaches to optically generate THz radiation. Most of them are based on femtosecond lasers whose spectrum is transformed into the low THz frequency range (0.1 THz to 10 THz). This can for example be achieved by optical rectification in a nonlinear crystal or by using a photoconductive antenna (Auston switch).

In this work we concentrate on the characterization of photoconductive antennas. They are based on a semiconductor material with a low carrier lifetime (< 1 ps). A well suited candidate for an excitation wavelength of 800 nm is low temperature grown GaAs (LT-GaAs). We characterize samples which were grown with various temperatures (between 200°C and 300°C). They are analyzed in a specially designed setup which allows for easy switching of the antennas. We found a clear correlation between the growth temperature of the antennas and their performance in a THz time domain spectrometer.

HL 37: Ultrafast Phenomena II

Time: Tuesday 14:45–16:00 Location: H10

HL 37.1 Tue 14:45 H10

Optical phonon relaxation and dynamic Fano effects of silicon (100) investigated by time-resolved spontaneous Raman scattering — •Jingyi Zhu, Rolf Baldwin Versteeg, Prashant Padmanabhan, Thomas Koethe, and Paul Herbertus Maria van Loosdrecht — II. Physikalisches Institut - Universität zu Köln, Zülpicher Straße 77, 50937 Cologne, Germany

The interaction of photo-induced charge carriers with photons initiates a complex dynamics including carrier cooling, carrier phonon scattering, and phonon relaxation. Here we revisit the incoherent optical phonons dynamics, electronic scattering, and hole-phonon interaction dynamics in silicon using time-resolved spontaneous Stokes and anti-Stokes Raman spectroscopy. Surprisingly, we observe a dynamic spectral asymmetry between the Stokes and anti-Stokes Raman scattering processes. The unusual asymmetry is thought to be mainly caused by the effects of the optically induced changes in the Fano interference between phonon and hole scattering.

HL 37.2 Tue 15:00 H10

Dynamics of exciton-polariton condensates in semiconductor microcavities with periodic potentials — •Xuekai Ma[1], Stefan Schumacher[1], and Oleg Egorov[2] — [1]Physics Department, Universität Paderborn, Warburger Strasse 100, 33098 Paderborn, Germany — [2]Institute of Condensed Matter Theory and Solid State Optics, Abbe Center of Photonics, Friedrich-Schiller-Universität Jena, Max-

Wien-Platz 1, 07743 Jena, Germany

Exciton-polaritons are quasi-particles made of quantum well (QW) excitons coupled to cavity photons. They have very small effective mass (10-4me) and lifetimes on the tens of picoseconds scale. Due to their photonic properties, they can be excited by light and probed, respectively. Due to their excitonic properties, nonlinearity is introduced into this system at elevated densities. Polaritons, which are composite bosons, can undergo a condensation process (with similarities to Bose-Einstein condensation) under incoherent excitation. Many features in the dynamics of polariton condensates can be described by a modified Gross-Piteavskii equation (GPE). Here, we study the nonlinear dynamics of polariton condensates in periodic potentials. In the presence of a periodic potential, a band structure including a band-gap can be obtained. We show that polariton condensates can occupy and switch between different energy states by changing the pump excitation intensity and shape. Our simulation results agree very well with recent experimental results.

HL 37.3 Tue 15:15 H10

Controlling the optical spin Hall effect — •Przemyslaw Lewandowski[1], Ombline Lafont[2], Samuel Luk[3], Nai Kwong[3], Jerome Tignon[2], Stefan Schumacher[1], Emmanuel Baudin[2], and Rolf Binder[3] — [1]Universität Paderborn, Warburger Strasse 100, 33098 Paderborn, Germany — [2]Ecole Normale Supérieure, 75231 Paris Cedex 05, France — [3]University of Arizona, Tucson, AZ 85721, USA

As an optical counterpart of the spin Hall effect, the optical spin Hall effect (OSHE) describes a spatial spin-separation of ballistically propagating polaritons in planar semiconductor microcavities [1]. This remarkable feature is driven by a transverse-longitudinal cavity-mode splitting, which acts as an effective magnetic field and therefore gives rise to a pseudo-spin orbit coupling. Here, we present an approach to control the OSHE using only all-optical means [2]: For a sufficiently strong cw-excitation the effective magnetic field vector can be tilted out of the cavity plane to which it is otherwise confined. We show that this nonlinear effect, based on the polariton-polariton interaction, allows the modification of the spin-current, making the OSHE a promising candidate for potential spin-optotronic applications. Our experimental and numerical results confirm well our analytical predictions, based on a microscopic semiconductor theory.

[1] A. Kavokin, G. Malpuech and M. Glazov, Phys. Rev. Lett. 95, 136601 (2005). [2] O. Lafont, M.H. Luk, P. Lewandowski, N.H. Kwong, K.P. Chan, M. Babilon, P.T. Leung, E. Galopin, A. Lemaitre, J. Tignon, S. Schumacher, E. Baudin, R. Binder (submitted).

Invited Talk HL 37.4 Tue 15:30 H10

Blasting semiconductor electrons with terahertz fields — •Mackillo Kira — Univ. Marburg, Germany

Present-day experiments can generate terahertz (THz) pulses having peak-field strengths around 100MV/cm. By limiting the THz pulse to few-cycles, one can both avoid structural damage and dominance of electron scattering during an excitation creating roughly a 1eV gradient over a 1Å distance. I will overview a cluster-expansion-based theory[1,2] to systematically explain how electrons as well as Coulomb-bound electronhole clusters[3] are excited and transported by extremely strong THz pulses. I will explain how a strong THz field induces an interplay of interband polarization and intraband currents during high-harmonic generation[4] (HHG) and an electronic quantum interference yielding a massive reshaping of the time-resolved harmonic emission[5]. Coulombic effects are demonstrated with THz wave mixing among Landau electrons[6] and with harmonic sideband generation (HSG) around an excitonic resonance. The identified HHG, HSG, quantum interference, and many-body effects can be combined to steer ultrafast processes in solids and to develop new light sources.

[1] M. Kira and S.W. Koch, *Semiconductor Quantum Optics*, (Cambridge Univ. Press, 2011). [2] M. Kira, Nat. Comm. **6**, 6624 (2015). [3] O. Vänskä *et al.*, Phys. Rev. Lett. **114**, 116802 (2015). [4] O. Schubert *et al.*, Nat. Photon. **8**, 119 (2014). [5] M. Hohenleutner *et al.*, Nature **523**, 572 (2015). [6] T. Maag *et al.*, Nat. Phys., doi:10.1038/nphys3559 (2015).

HL 38: Oxide Semiconductors II

Oxide Semiconductors except for ZnO

Time: Tuesday 14:45–15:45 Location: H13

HL 38.1 Tue 14:45 H13

Signatures of quantum coherence in Rydberg excitons in Cu_2O — •Peter Grünwald[1], Marc Assmann[2], Dietmar Fröhlich[2], Manfred Bayer[2], Heinrich Stolz[1], and Stefan Scheel[1] — [1]Institut für Physik, Universität Rostock, D-18059 Rostock, Germany — [2]Experimentelle Physik 2, Technische Universität Dortmund, D-44221 Dortmund, Germany

In a recent breakthrough experiment, excitons in Cu_2O have been optically excited to Rydberg states with principal quantum numbers upto $n = 25$ [1]. These fragile objects show very similar behaviour compared to their atomic counterpart, including the concept of a quantum defect [2].

We present first results on the study of the quantum optical properties of Rydberg excitons. The details of the absorption spectrum of excitons with large n can only be understood by including coherent excitation dynamics [3]. The measured absorption spectrum includes both the probability for absorbing a laser photon as well as a contribution relating to the coherent and incoherent parts of the intensity spectrum of the excitons. For increasing n, the incoherent spectrum becomes relevant. In particular, additional resonances appear between the exciton peaks, which vanish if the laser pumping is substituted for white-light excitation. These resonances indicate the onset of quantum-coherent light-exciton interaction.

[1] T. Kazimierczuk *et al.*, Nature **514**, 343 (2014).
[2] F. Schöne *et al.*, arXiv:1511.05458 [cond-mat.mes-hall].
[3] P. Grünwald *et al.*, arXiv:1511.07742 [cond-mat.mes-hall].

HL 38.2 Tue 15:00 H13

Hybrid density functional calculations of small polarons and bi-polarons in oxides — •Sebastian Kokott, Sergey V. Levchenko, and Matthias Scheffler — Fritz Haber Institute of the MPS, Berlin, Germany

Formation of polarons, i.e. phonon-"dressed" holes or electrons, plays an important role in optical spectra and electrical conductivity of materials. For the formation of small (localized) polarons microscopic properties of the systems are crucial, and the use of an *ab initio* theory is necessary for its description. For this reason we calculate small polarons in a supercell approach using density functional approximations (DFA).

We find that the results can be strongly affected by self-interaction and finite supercell size errors. However, using constraints from exact DFT, such as the IP-theorem[1], the binding energy of polarons can be reformulated in terms of energies obtained from the neutral system[2]. With this we show, that the dependence on the underlying XC functional of the reformulated polaron binding energy can be drastically reduced. The effect will be demonstrated for small polarons and bipolarons in MgO for the entire range of the the exact-exchange fraction in the HSE hybrid functional. We also demonstrate the dependence of the results on the supercell size and give results on the binding energies of polarons in the extrapolated dilute limit.

[1] J. Perdew et al., Phys. Rev. Lett. **49**, 1691 (1982) [2] B. Sadigh Phys. Rev. B **92**, 075202 (2015)

HL 38.3 Tue 15:15 H13

Stark-Effect Measurements on Rydberg Excitons in Cu_2O — •Marcel Freitag, Julian Heckötter, Marc Assmann, Dietmar Fröhlich, and Manfred Bayer — Technische Universität Dortmund, Fakultät Physik, Experimentelle Physik II, 44221 Dortmund, Germany

We report on Stark-Effect measurements of Rydberg excitons[1] in Cu_2O with quantum numbers up to $n = 25$. These excitons have extensions up to $2\,\mu$m. As known from hydrogen, the dipole matrix elements for $\Delta n = 0$ and $\Delta l = \pm 1$ grow quadratically with n. Due to the electric field induced coupling, we observe S- and D-excitons of the yellow series and from $n = 5$ we are even able to identify G-excitons in

fields as low as 50 V/cm. Measurements are done on a 30 μm sample with a single frequency dye laser ($\Delta E = 5$ neV) and a broadband white-light source at temperatures down to 1.2 K. Contrary to hydrogen, the Stark-Effect measurements can be done in a longitudinal configuration ($K_{laser} \parallel E$).

[1] T. Kazimierzuk et al. Nature 514, 343 (2014)

HL 38.4 Tue 15:30 H13

Optical properties of β -Ga_2O_3 — •Nadja Jankowski[1], Christian Nenstiel[1], Gordon Callsen[1], Zbigniew Galazka[2], and Axel Hoffmann[1] — [1]Technische Universität Berlin, Berlin, Deutschland — [2]Leibniz Institut für Kristallzüchtung, Berlin, Deutschland

β-Ga_2O_3 is a wide band gap semiconductor, which is suitable for many possible applications, such as transparent conducting oxides, UV-devices, high-temperature-stable gas sensors and dielectric coating for solar cells.

Structural and optical properties of the investigated β-Ga_2O_3 single crystal were examined by the means of Raman and photoluminescence spectroscopy.

As the exact band gap value of β-Ga_2O_3 is still under discussion, this work focuses on the determination of the band gap by performing photoluminescence excitation spectroscopy. The measurements exhibit excitation channels in the region of 4.6 to 5.0 eV, below the theoretically calculated band gap within recent publications. To clarify the origin of the excitation channel at 4.91 eV, temperature dependent photoluminescence excitation spectroscopy and absorption spectroscopy were performed.

HL 39: Silicon-based Semiconductors II

Time: Tuesday 14:45–15:45 Location: H14

HL 39.1 Tue 14:45 H14

Doping of 4H-SiC with group IV elements — •Maximilian Rühl[1], Tomasz Sledziewski[1], Günter Ellrott[1], Theresa Palm[1], Heiko Weber[1], Michael Krieger[1], and Michel Bockstedte[2,3] — [1]Department of Physics, Applied Physics, FAU Erlangen-Nürnberg, Germany — [2]Department of Physics, Solid State Theory, FAU Erlangen-Nürnberg, Germany — [3]Department of Chemistry and Physics of Materials, Universität Salzburg, Austria

An enhancement of the electrical conductivity of 4H-SiC was achieved recently by in-situ germanium doping [1]. Since Ge behaves isoelectrically in SiC, a Ge-related modification of the defect equilibrium was suggested. Here we combine experiment and theory to reveal the underlying physics. Our analysis of n-type 4H-SiC samples implanted with Ge or tin (Sn) by deep level transient spectroscopy (DLTS) shows that the mobility-limiting $Z_{1/2}$ center can be strongly reduced with increasing implantation dose. Simultaneously new defects are formed which are assumed to be Ge-/Sn-related. Using hybrid density functional theory we investigate the electronic properties and abundance of Ge-related defects. We find that the most abundant ones are the electrically inactive substitutional center at the Si-site (Ge_{Si}), the deep substitutional center at the C-site (Ge_C), and a complex with a carbon vacancy (Ge_{Si}-V_C). The Ge_{Si}-V_C complex can be associated with new defect centers observed in DLTS. Our combined approach suggests that kinetic effects drive the observed reduction of $Z_{1/2}$ (=V_C , [2]).

[1] Sledziewski *et al.* Mater. Sci. Forum **778-780** (2014) 216.

[2] Kawahara *et al.* J. Appl. Phys. **115** (2014) 143705.

HL 39.2 Tue 15:00 H14

LDOS matching in nanophotonic cavities using position-defined quantum dots — Magdalena Schatzl, •Florian Hackl, Martin Glaser, Moritz Brehm, Reyhaneh Jannesari, Friedrich Schäffler, and Thomas Fromherz — Institute of Semiconductor and Solid State Physics, Johannes Kepler University, A-4040 Linz, Austria

Si integrated optics is an absolutely required next step for the implementation of data rates currently required in data storage centers and in near future also for inter- and intra-chip communication. As a technologically less demanding alternative to hybrid integration of III-V material based emitters into a SOI based integrated optical platform, the monolithic integration of group IV based emitters for the telecom wavelength region is highly attractive. While for coherent radiation strained Ge, SnGe and glassy QD based lasers have been demonstrated recently, as emitter on the single photon level SiGe quantum dots combined with ultra-high Q nano-optical cavities are promising candidates. In our work, we combine site controlled growth of SiGe QDs with L3 type photonic crystal resonators defined by e-beam lithography for a systematic study of the influence of the QD position within the cavity on the photoluminescence efficiency. Using a series of identical cavities, each containing a single QD at accurately and systematically varied positions, by these experiments we map out the photonic local density of states (LDOS) of several optical cavity modes and demonstrate that by placing the QD at the correct position, we are able to control the emission mode of QDs.

HL 39.3 Tue 15:15 H14

Tellurium hyperdoped Si: Flash lamp annealing vs. pulsed laser melting — •Mao Wang[1,2], Fang Liu[1,2], Ye Yuan[1,2], Slawomir Prucnal[1], Yonder Berencén[1], Lars Rebohle[1], Wolfgang Skorupa[1], Manfred Helm[1,2], and Shengqiang Zhou[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Bautzner Landstr. 400, 01328 Dresden, Germany — [2]Technische Universität Dresden, 01062 Dresden, Germany

Chalcogen-hyperdoped silicon has been a topic of great interest due to its potential optoelectronic applications owing to the sub-band gap absorption [1-3]. In our work, tellurium hyperdoped Si was fabricated by ion-implantation with different fluences ranging from 1.09*1015 to 1.25*1016 cm-2 followed by two kinds of ultra-short annealing processing: flash lamp annealing (FLA) and pulsed laser melting (PLM). The Raman spectroscopy results reveal the high-quality recrystallization of tellurium implanted Si by both FLA and PLM. From the transport measurements, the conductivity increases with increasing tellurium concentration. High tellurium concentration samples show a finite conductivity as temperature trend 0. This indicates that the high concentration doping of tellurium induces an insulator-to-metal transition in Si although Te introduces a deep donor in Si.

[1] Kim, T. G., et al., Appl. Phys. Lett. 88, 241902 (2006) [2] Tabbal, M., et al., Appl. Phys. A 98, 589*594 (2010) [3] Umezu, I., et al., J. Appl. Phys. 113, 213501 (2013)

HL 39.4 Tue 15:30 H14

Disentangling Surface from Bulk Conductivity by Distance-dependent Four-Probe Transport Measurements Combined with an Analytical Conductance Model — •Sven Just[1], Helmut Soltner[2], Stefan Korte[1], Vasily Cherepanov[1], and Bert Voigtländer[1] — [1]Peter Grünberg Institut (PGI-3) and JARA-FIT, Forschungszentrum Jülich — [2]Central Institute for Engineering, Electronics and Analytics (ZEA-1), Forschungszentrum Jülich

Distance-dependent four-probe measurements performed with a multi-tip scanning tunneling microscope (STM) allow to distinguish between 2D and 3D charge transport channels. In combination with a conductance model for mixed 2D-3D geometries, a disentanglement of surface transport from bulk contributions and a determination of the surface conductivity is possible. Often a very simple parallel circuit model of surface and bulk is used, but it has a very limited applicability due to the rough approximation of only two layers. So, an analytical model for charge transport in N layers is derived from the solution of Poisson's equation, which e.g. can be used for semiconductors in combination with a calculation of the near-surface band-bending to model very precisely the measured four-point resistance on the surface. By applying this model to published data on Ge(001), Si(100) and Si(111) with different doping concentrations, the surface conductivity of these materials can be determined without any further needs of special sample preparation. Furthermore, this generic approach for determining surface conductivity can be easily applied to other material systems, e.g. to topological insulators.

HL 40: On-Chip Quantum Photonics II

Organizers: Simone Portalupi and Peter Michler (Universität Stuttgart)

Time: Tuesday 14:45–16:00 Location: H16

Invited Talk HL 40.1 Tue 14:45 H16

On-chip generation, routing and detection of nonclassical light — •Kai Müller[1,2], Kevin A. Fischer[1], Constantin Dory[1], Günther Reithmaier[2], Fabian Flassig[2], Konstantin G. Lagoudakis[1], Tomas Sarmiento[1], Michael Kaniber[2], Jonathan J. Finley[2], and Jelena Vuckovic[1] — [1]E. L. Ginzton Laboratory, Stanford University, Stanford, California 94305, USA — [2]Walter Schottky Institut, Am Coulombwall 4, 85386 Garching, Germany

Nonclassical light can be generated on chip using self-assembled quantum dots strongly coupled to photonic crystal cavities. However, the highly dissipative nature of such systems typically limits the achievable fidelities. Here we show that detuning emitter and cavity mode [1] and understanding the coupling to phonons [2] facilitates high-fidelity generation of single photons. Moreover, by exploiting a novel self-homodyne suppression technique [3] we demonstrate generation of highly-indistinguishable photons [4].

On-chip detection can be realized by integration of superconducting single photon detectors. To this ends, we fabricate patterned NbN films directly onto GaAs waveguides. The absorption of a single photon produces a measurable electric signal which allows us to demonstrate on-chip detection of emission from single quantum dots [5-6].

[1] K. Müller et al. Phys. Rev. Lett. 114, 233601 (2015) [2] K. Müller et al. Phys. Rev. X. 5, 031006 (2015) [3] K. A. Fischer et al. arXiv:1512.04102 (2015) [4] K. Müller et al. arXiv:1512.05626 (2015) [5] G. Reithmaier et al. Scientific Reports 3, 1901 (2013) [6] G. Reithmaier et al. Nano Letters, 15 (8), 5208 (2015)

Invited Talk HL 40.2 Tue 15:15 H16

On-chip quantum optics using quantum dot microcavities and waveguide structures — Pierce Munnelly[1], Matthias Karow[1], Arsenty Kaganskiy[1], Jan-Hindrik Schulze[1], Andre Strittmatter[1], Martin Kamp[2], Sven Rodt[1], Sven Höfling[2], Tobias Heindel[1], Christian Schneider[2], and •Stephan Reizenstein[1] — [1]Institute of Solid State Physics, Technische Universität Berlin, 10623 Berlin, Germany — [2]Technische Physik, Universität Würzburg, 97074 Würzburg, Germany

The generation, manipulation, and detection of single photons on an integrated semiconductor platform containing passive and active elements is a central goal of on-chip quantum optics. Progress in this field will strongly benefit from monolithically integrated and electrically contacted building blocks.

In this talk I will present an on-chip device concept which is based on monolithically integrated and electrically driven whispering gallery mode quantum dot (QD) microlasers which can resonantly excite single-QD microcavity structures operating in the regime of cavity quantum electrodynamics (cQED). This concept is used to observe cQED effects in a fully integrated platform, to generate non-classical light, and to detect light in an on-chip configuration. Moreover, I will present work on planar waveguide structures with deterministically integrated quantum dots.

HL 40.3 Tue 15:45 H16

On-chip Photodetectors using Electrically Contacted Quantum Dot Micropillars — •Pierce Munnelly[1], Matthias Karow[1], Tobias Heindel[1], Martin Kamp[2], Sven Höfling[2], Christian Schneider[2], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, Berlin, Germany — [2]Technische Physik, Universität Würzburg, Würzburg, Germany

An important goal of nanophotonics is to unite the generation of coherent or single-photon states of light with efficient manipulation and detection techniques for advanced schemes in quantum information science. As the optical parts of the circuits are more heavily integrated and components are shrunk to smaller and smaller scales, it will also become harder to assess and control the quality of light sources within optoelectronic devices via conventional out-of-plane detection methods such as micro-photoluminescence spectroscopy.

In this contribution, a novel, micrometer-scaled, on-chip photon detector will be presented. The detector is based on an electrically contacted quantum dot micropillar and operates in the regime of cavity quantum electrodynamics. The potential of our concept is exemplarily demonstrated by determining the input-output characteristics and the threshold current of a monolithically integrated whispering gallery mode laser.

HL 41: Graphene: Optics (Joint session of HL and TT, organized by HL)

Time: Tuesday 14:45–15:45 Location: H17

Invited Talk HL 41.1 Tue 14:45 H17

Ultrafast carrier dynamics in monolayer graphene — •Daniele Brida — Department of Physics and Center for Applied Photonics, University of Konstanz, Universitätsstr. 10, D-78464 Konstanz, Germany

The impulsive optical excitation of carriers in graphene creates an nonequilibrium distribution, which thermalizes on an ultrafast timescale. The hot Fermi-Dirac distribution subsequently cools via phonon emission within few hundreds of femtoseconds. We investigated the initial stages of the thermalization process that are dominated by electron-electron scattering events. By comparing the two-color pump-probe experimental data with different models, that solve the quantum Boltzmann equation by implementing three different screening methods, we can visualize the importance of Auger recombination processes, such as carrier multiplication, in the ultrafast relaxation of the electronic distribution along the Dirac cone in graphene. Recent theoretical and experimental work also emphasizes the role of the polarization state of the light pulses used for the excitation. When carriers are excited with linearly polarized light, the resulting occupation in momentum space is not isotropic due to the pseudospin selection rules. To observe this anisotropy we compare the transient absorption signal arising for probe pulses with polarizations parallel and perpendicular to the pump pulse. We identify electron-phonon scattering as main driving mechanism of isotropization of the electronic distribution across the Dirac cone since it occurs in approximately 100 fs.

HL 41.2 Tue 15:15 H17

Noncollinear Coulomb scattering in graphene — •Jacob C. König-Otto[1,2], Martin Mittendorff[3], Torben Winzer[4], Ermin Malic[5], Andreas Knorr[4], Alexej Pashkin[1], Harald Schneider[1], Manfred Helm[1,2], and Stephan Winnerl[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]Technische Universität Dresden, Germany — [3]University of Maryland, USA — [4]Technische Universität Berlin, Germany — [5]Chalmers University of Technology, Sweden

Utilizing the anisotropy of the optical excitation in graphene, we reveal the twofold nature of Coulomb scattering in graphene. The initial non-equilibrium charge carrier distribution in graphene created by linearly polarized light possesses a pronounced anisotropy, which has been observed in our recent experiment [1]. In the present study we perform polarization-dependent pump-probe measurements using a photon energy of 88 meV to suppress efficiently the optical phonon scattering. In this case the relaxation dynamics leading to an isotropic distribution is dominated by noncollinear Coulomb scattering. By varying the pump fluence over a range of several orders of magnitudes we are able to successfully control the efficiency of this process. This reveals a surprising twofold nature of Coulomb scattering in graphene: Whereas collinear Coulomb scattering is known to be a very fast process on the fs timescale, noncollinear scattering is remarkably slow, resulting in a thermalization time of several ps in our experiment. Our experimental findings are complemented by the results of microscopic modelling.

[1] M. Mittendorff et al., Nano Lett. **14**, 1504 (2014).

HL 41.3 Tue 15:30 H17

Gate-Voltage Dependency of Förster Transfer in Graphene - Quantum Dot Photo Detection — •Lorenz Maximilian Schneider[1], Ruifeng Li[2], Huizhen Wu[2], Martin Koch[1], and Arash Rahimi-Iman[1] — [1]Faculty of Physics and Materials Sciences Center, Philipps-Universität Marburg, 35032 Marburg, Germany — [2]Department of Physics and the State Key Laboratory of Silicon Materials, Zhejiang University, Hangzhou, 310058, P.R. China

Graphene photodetectors functionalized by colloidal Quantum dots (cQDs) have been recently demonstrated for effective photo detection. Nevertheless, the transfer of the energy or charge carriers from cQDs to graphene is not sufficiently understood. Here, we present a respective study of a graphene field-effect transistor, which is functionalized with CdSe/ZnS Core-Shell QDs covering it's conductive channel. In order to investigate energy transfer dynamics in this system, we have investigated the time-resolved photo-luminescence from the cQDs as function of the applied gate voltage. A clear change in the photo-luminescence lifetime has been observed, indicating a change of the decay channels. In support of our findings, we provide data for a Förster-like energy transfer model as a function of the gate voltage. The model shows that by applying a backgate voltage to the photo detector, absorbance can be tuned with respect to the photo-luminescence of the cQDs, changing the energy transfer rate of the photo-detector.

HL 42: Organic Electronics and Photovoltaics I (Joint session of CPP, DS, HL and O, organized by CPP)

Time: Tuesday 14:00–15:30 Location: H37

HL 42.1 Tue 14:00 H37

Elucidating the Morphology of Organic Bulk Heterojunction Solar Cells Using Nanoanalytical Transmission Electron Microscopy — •Stefanie Fladischer[1], Tayebeh Ameri[2], Christoph Brabec[2], and Erdmann Spiecker[1] — [1]FAU, CENEM, Erlangen, Deutschland — [2]FAU, i-MEET, Erlangen, Deutschland

Organic photovoltaics is one of the most promising technologies for low cost energy production with the advantages of semi-transparency, flexibility and solution processing. Significant improvement of the power conversion efficiency could be achieved in the last years using novel materials and adapted device engineering. To further improve the efficiency of solar cells the knowledge of the morphology is essential, as it decisively influences the device performance. The morphology of organic bulk heterojunction (BHJ) active layers depends not only on the involved materials but also on their molecular weight and their treatment like thermal annealing and solvent vapor annealing. Analytical Transmission Electron Microscopy (TEM) is a versatile tool to characterize the morphology of organic solar cells concerning on the one hand the interfaces of the various layers and on the other hand the material distribution in BHJ active layers. Combining high-resolution imaging with analytical techniques like electron energy-loss spectroscopy (EELS) and energy filtered TEM (EFTEM) as well as energy-dispersive X-ray spectroscopy (EDXS) the morphology can be determined and thus the device performance can be understood and further improved.

HL 42.2 Tue 14:15 H37

Links between organic solar cell performance and morphological properties — •Daniel Moseguí González[1], Christoph J. Schaffer[1], Stephan Pröller[2], Johannes Schlipf[1], Lin Song[1], Sigrid Bernstorff[3], Eva M. Herzig[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748, Garching, Germany — [2]TU München, Munich School of Engineering, Herzig Group, 85748 Garching, Germany — [3]Elettra Sincrotrone Trieste S.C.p.A., Basovizza, 34149 Trieste, Italy

Many attempts have been made to establish solid links between morphology and performance of organic solar cells (OSCs) as well as the potential suitability of some materials for solar devices. Eventually, many of these attempts have yielded deeper insight into the physics governing excitonic solar cells. In this regard, one of the most innovative approaches consists in the in-operando observation of solar devices under working conditions in time-resolved grazing incidence X-ray scattering experiments. This configuration allows for simultaneous tracking of morphological and electronic properties as a function of time, making the appearing co-dependences among studied parameters more remarkable. The presented work focuses on the first in-operando observations that showed strong correlations between the crystalline state of P3HT:PCBM OSCs' active layers and the open-circuit voltage delivered by the devices. Up to now, this link was only addressed in a multi-step fashion with works featuring interdependences between properties like crystallinity, recombination, energy disorder, open-circuit voltage, or exciton/charge carrier transport.

HL 42.3 Tue 14:30 H37

Strong influence of morphology on charge transport and recombination in solution processed small molecule based solar cells — •Alexey Gavrik[1], Andreas Baumann[2], Yuriy Luponosov[3], Sergey Ponomarenko[3,4], and Vladimir Dyakonov[1,2] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Bayerisches Zentrum für Angewandte Energieforschung (ZAE Bayern), 97074 Würzburg — [3]Enikolopov Inst Synthet Polymer Mat, 117393 Moscow, Russia — [4]Lomonosov Moscow State University, 119991 Moscow, Russia

Solution processed small molecules (SSM) are promising materials for solar cell (SC) applications due to their well defined structure and high chemical reproducibility. Donor-acceptor-donor layout of SSM provides enhanced exciton splitting, as well as good possibility for effective charge transfer. The blend morphology in a bulk-heterojunction (BHJ) SC is assumed to play a crucial role in the cell performance. Therefore, we set to find optimal BHJ fabrication method keeping track of corresponding transport properties. In this work we studied DTS(EtHex)$_2$-(2T-DCV-Me)$_2$:PC$_{60}$BM BHJ SC using the photogenerated charge carrier extraction technique OTRACE in order to analyze non-geminate recombination and determine charge carrier mobility in context of varying blend morphology. We show that different preparation conditions have a strong impact on the blend morphology and thus on the charge carrier transport (i.e. mobility and recombination rate). Furthermore, introduced modifications allowed to achieve a 4-fold enhancement of SC efficiency up to 4.3%.

HL 42.4 Tue 14:45 H37

Direct visualization of charge-extraction in metal-mesh based OPV cells by light-biased LBIC — •Mathias Gruber[1,2], Arne Hendel[1], Vladislav Jovanov[1], Manfred J. Walter[2], and Veit Wagner[1] — [1]Department of Physics and Earth Sciences, Jacobs University Bremen, 28759 Bremen, Germany — [2]PolyIC GmbH & Co. KG, 90763 Fürth, Germany

Metal-mesh based electrode systems are a highly conductive, versatile and unexpensive alternative to ITO-electrodes for organic photovoltaic (OPV) cells. However, as a metal-mesh does not offer full surface conductivity it is usually combined with a less conductive PEDOT:PSS layer, which enables lateral charge-transport in the area in between the metal tracks. The sheet conductivity of this additional lateral conductive layer (LCL) needs to be carefully tuned with respect to the distance of the metal tracks to reduce short circuit current (J_{sc}) losses and additional series resistance due to resistive losses in the LCL material. Usually this is done via electrical simulation or via analysis of IV-measurements of a large number of devices with different LCL sheet conductivities. Here we present a direct way to measure the current collection losses due to PEDOT:PSS sheet resistance by integrating a white light-bias into a LBIC measurement (Light-bias LBIC). We show that we are not only able to directly measure and visualize charge extraction under real device operation conditions but are also able to determine the intrinsic PEDOT:PSS sheet resistance in the operating OPV device.

HL 42.5 Tue 15:00 H37

Morphological Degradation of Polymer-Fullerene Bulk-Heterojunction Solar Cells — •Christoph J. Schaffer[1], Claudia M. Palumbiny[1], Martin A. Niedermeier[1], Christian Burger[1], Gonzalo Santoro[2], Stephan V. Roth[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS

Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — [2]DESY, Notkestr. 85, 22607 Hamburg

Organic solar cells offer a wide range of advantages based on their mechanical flexibility, their optical tunability and their ease of production in comparison to conventional photovoltaics. However, elongating their lifetime remains the main challenge after efficiencies exceeding the 10% marker have been recently reported [1]. We focus on the stability of the active bulk-heterojunction layer of polymer-fullerene solar cells. Using in-situ GISAXS and simultaneous current-voltage tracking we have previously shown that the active layer is morphologically unstable during operation of a P3HT:PCBM based solar cell, causing device degradation [2]. In our recent work we observe different degradation mechanisms occurring in other polymer-fullerene blends. This knowledge shows that tailored stabilization methods must be found for each specific material system.

[1] S.-H. Liao et al., Scientific Reports 2014, 4, 6813.
[2] C. J. Schaffer et al., Adv. Mater. 2013, 25, 6760.

HL 42.6 Tue 15:15 H37

Illumination dependent parasitic resistances in organic bulk hetero junction solar cells. — •Arne Hendel and Veit Wagner — Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany

During outdoor operation, the solar cell is exposed to AM1.5G during noon only. For other daytimes and for indoor applications the performance of the solar cell at lower light intensities is important. In this study, bulk hetero junction solar cells were exposed to light irradiation from 10^{-5} to several suns intensity. We find a strong illumination dependence of the parasitic resistances. For the different light intensities I-V characteristics were performed. In addition the Jsc-Voc analysis was done to obtain series resistance free I-V measurement. It was found that the series and shunt resistance, which are critical for the solar cell performance, strongly depend on illumination intensity. The light intensity induced conductivity change of the solar cell shows different dependencies for forward and reverse operation. For low light intensities, the shunt resistance can be directly measured via the open circuit voltage assuming the Shockley model for the diode. From these measurements a strong light dependence is obtained. Based on the experimental data a model for the light dependent shunt resistance and series resistance is presented.

HL 43: Symposium SYTI: Topological Insulators: Status Quo and Future Directions (Joint session of DS, HL, MA, O and TT, organized by TT)

Time: Wednesday 9:30–13:00 Location: H1

Invited Talk HL 43.1 Wed 9:30 H1

Topological insulators and topological superconductors — •Shoucheng Zhang — Dept of Physics, Stanford University

In this talk, I will first give a brief overview on topological insulators and superconductors. I will then discuss the recent theoretical prediction and the experimental observation of the quantum anomalous Hall effect in magnetic topological insulators. I shall present a newly predicted material called stanene, and discuss its potential applications.

Invited Talk HL 43.2 Wed 10:10 H1

Three-dimensional topological insulators and superconductors — •Yoichi Ando — II. Physikalisches Institut, Universität zu Köln

A topological quantum state of matter is characterized by a nontrivial topological structure of its Hilbert space. 3D topological insulators are characterized by non-trivial Z_2 topology, which is due to band inversion caused by strong spin-orbit coupling [1]. Intriguingly, when superconductivity shows up upon doping charge carriers into 3D topological insulators, the resulting superconducting state can also be topological [2], because the strong spin-orbit coupling could lead to an unconventional gap function characterized by a new Z_2 topological invariant [3]. In this talk, I will present experimental realizations of these materials and report recent efforts to address their exotic properties.

[1] Y. Ando, J. Phys. Soc. Jpn. **81**, 102001 (2013)
[2] Y. Ando and L. Fu, Ann. Rev. Cond. Mat Phys. **6**, 361 (2015)
[3] S. Sasaki, M. Kriener, K. Segawa, K. Yada, Y. Tanaka, M. Sato, and Y. Ando, PRL **107**, 217001 (2011)

Invited Talk HL 43.3 Wed 10:50 H1

Interplay of magnetic and electronic states in pyrochlore iridates — •Leon Balents — University of California, Santa Barbara, CA, USA

The pyrochlore iridates are a series of compounds undergoing antiferromagnetic ordering and metal-insulator transitions. They are of interest because they combine electron correlation effects and the potential for non-trivial band topology. We will discuss the theoretical picture of these materials, from electronic structure to magnetism and phase transitions, and how they may be controlled through applied fields and temperature. Comparison will be made between theory and recent experiments.

10 min. break

Invited Talk HL 43.4 Wed 11:40 H1

Magnetic imaging of edge states — •Kathryn Moler — Stanford University

Beautiful theoretical proposals launched the field of topological materials, followed rapidly by great initial successes in synthesizing and demonstrating several topological insulators. The challenges now are to understand and control edge and surface scattering, to find materials with no bulk states and large gaps for high-temperature operation, and most importantly, to fabricate integrated devices that include gates, superconductors, and ferromagnets. Scanning SQUID microscopy can aid this effort by imaging magnetism, superconductivity, and current flow. Images of current flow in two quantum spin hall insulators verify that currents really do flow on the edges, provide images of the developing edge states with voltage and temperature, and also help reveal the conditions for achieving topological vs. trivial edge states. Sensitive magnetic measurements characterize superconductor * topological insulator structures, and help to determine the conditions for achieving exotic Josephson junctions.

Invited Talk HL 43.5 Wed 12:20 H1

Sub-nm wide edge states at the dark side of a weak topological insulator — •Markus Morgenstern — II. Institute of Physics B and JARA-FIT, RWTH Aachen, 52074 Aachen

Three-dimensional insulating crystals, which respect time reversal symmetry, can be classified as trivial insulators, strong topological insulators and weak topological insulators (WTIs). Many examples of trivial or strong topological insulators are known, but WTIs have barely been probed. They offer pairs of topologically protected surface states on most surfaces, but exhibit one dark surface without such surface states. The step edges of this dark surface naturally belong to the bright surfaces such that they contain spin helical edge states with perfect e^2/h conductivity. The first WTI $Bi_{14}Rh_3I_9$ was synthesized recently [1]. Here, we show by scanning tunneling spectroscopy that the edge states indeed exist and are below 1 nm wide. They can be scratched into the surface using an atomic force microscope providing a simple tool to guide them [2]. Moreover, it is shown that the edge state can be removed by chemically dimerizing adjacent layers of the WTI. Strategies to bring the edge state to the Fermi level are discussed.

[1] B. Rasche, A. Isaeva, M. Ruck, S. Borisenko, V. Zabolotnyy, B. Büchner, K. Koepernik, C. Ortix, M. Richter, and J. van den Brink, Nature Mater. **12**, 422 (2012)
[2] C. Pauly, B. Rasche, K. Koepernik, M. Liebmann, M. Pratzer, M. Richter, J. Kellner, M. Eschbach, B. Kaufmann, L. Plucinski, C. M. Schneider, M. Ruck, J. van den Brink, and M. Morgenstern, Nature Phys. **11**, 338 (2015)

HL 44: Optical Properties I

Time: Wednesday 9:30–13:15 Location: H10

Invited Talk HL 44.1 Wed 9:30 H10

Rydberg excitons in cuprous oxide — •Manfred Bayer — Experimentelle Physik 2, TU Dortmund, Germany

Excitons, bound electron-hole complexes, are decisive for the optical properties of semiconductors. Thereby their description as hydrogen atom-like complexes has turned out to be extremely useful. In Rydberg atoms an electron is promoted into a state with high principal quantum number. The atom becomes a mesoscopic object then with dimensions in the micrometer-range, with which, for example, the transition from quantum to classical dynamics can be studied. Recently it has been shown that also excitons can be highly excited by observing states with principal quantum number up to n=25 in high-quality natural cuprous oxide crystals [1]. This corresponds to an average radius of more than a micrometer so that the exciton wave function is extended over more than 10 billion crystal unit cells. In this contribution similarities and differences of these Rydberg-excitons with their atomic counterparts will be addressed.

[1] T. Kazimierczuk, D. Fröhlich, S. Scheel, H. Stolz, and M. Bayer, Nature 514, 343 (2014).

HL 44.2 Wed 10:00 H10

Quantum Chaos of Rydberg Excitons in Cu_2O — •Johannes Thewes, Marc Assmann, Dietmar Fröhlich, and Manfred Bayer — Experimentelle Physik 2, Technische Universität Dortmund, D-44221 Dortmund, Germany

The yellow exciton series of Cu_2O exhibits a complex transition towards quantum chaos under the influence of an external magnetic field. The observed quadratic level repulsion in the chaotic regime indicates a non-trivial breaking of the time reversal symmetry in the system. We argue that an asymmetric scattering process with crystal phonons is the reason for the non-trivial breaking of time reversal symmetry in Cu_2O.
In a hydrogen-like system like this, the breaking of time reversal symmetry by the magnetic field itself is not sufficient to observe quadratic level repulsion. For such systems, there is still a combined symmetry operation available that leaves the system invariant. Hence, the Hamiltonian of these systems can be represented by a real and symmetric matrix which is only the prerequisite for linear level repulsion in the chaotic regime.

HL 44.3 Wed 10:15 H10

Strong coupling in a resonant inorganic/organic microcavity — •Michael Höfner[1], Sergey Sadofev[1], Björn Kobin[2], Stefan Hecht[2], and Oliver Benson[1] — [1]Humboldt-Universität zu Berlin, Institut für Physik, Newtonstr. 15, 12489 Berlin — [2]Humboldt-Universität zu Berlin, Institut für Chemie, Brook-Taylor-Str. 2, 12489 Berlin

We present strong exciton photon coupling in a hybrid microcavity containing ZnO/ZnMgO quantum wells and specially synthesized ladder-type oligo-(*p*-phenylene) molecules. An epitaxially grown ZnMgO based Bragg reflector followed by six ZnO quantum wells and the active molecule embedded in a polymer matrix. The cavity is completed by evaporating a SiO_2/ZrO_2 based dielectric mirror. The system is investigated by low temperature angular resolved reflectivity revealing a clear anticrossing related to the Frenkel and Wannier-Mott exciton creating three polariton branches. At an angle of incidence of 35° an equal mixing of all resonances is reached [1]. Through careful adjustment of the oscillator strength of both active materials and the cavity design, we reach an equal mixing in the middle polariton branch. A hybrid exciton-polariton with equal contribution of the photon, Frenkel and Wannier-Mott resonance is created. This makes this new material combination an excellent candidate for tailoring the phonon assisted polariton relaxation and creating a polariton laser.

[1] M. Höfner, S. Sadofev, B. Kobin, S. Hecht and F. Henneberger, Hybrid polaritons in a Resonant Inorganic/Organic Semiconductor microcavity, Appl. Phys. Lett. 107, 181109, 2015.

HL 44.4 Wed 10:30 H10

Quantum Defects of Excitons in Cu_2O — Florian Schöne, •Sjard Ole Krüger, Peter Grünwald, Heinrich Stolz, and Stefan Scheel — Institut für Physik, Universität Rostock, D-18059 Rostock, Germany

Recent experiments have shown a clear deviation of the yellow exciton series in Cu_2O from an ideal (hydrogen) Rydberg series [1]. We present numerical calculations for the exciton binding energies based on the nonparabolicity of the Γ_7^+ valence band using a group theoretical band hamiltonian [2]. The momentum space Schrödinger equation has been reduced to a set of Fredholm integral equations for the radial part of the wavefunction, which could be solved numerically. Describing the deviation from a Rydberg series through quantum defects, we analyzed the influence of the valence band nonparabolicity on the exciton binding energies for angular momenta $l = 0, \ldots, 3$.

[1] T. Kazimierczuk, D. Fröhlich, S. Scheel, H. Stolz, M. Bayer, doi:10.1038/nature13832

[2] F. Schöne, S.-O. Krüger, P. Grünwald, J. Thewes, M. Aßmann, J. Heckötter, D. Fröhlich, M. Bayer, H. Stolz, and S. Scheel, arXiv:1511.05458 [cond-mat.mes-hall].

HL 44.5 Wed 10:45 H10

DIP: Organic Small Molecules for Strong Coupling — •Felix Lemke, Hartmut Fröb, and Karl Leo — Institut für Angewandte Photophysik, TU Dresden, Germany

Due to recent reports on polariton lasing with reduced threshold compared to conventional lasing, the investigation of strong coupling is of large interest. Organic molecules are promising candidates for studying light matter interaction due to their high exciton binding energy, creating a large polaritonic splitting. Since organic molecules are often unstable, there is ongoing research on small, thermally evaporable organic molecules for strong coupling.

In this work, we discuss Bu4-Ph4-DIP evaporated in between two mirrors to form a microcavity. Reflection measurements of different sample structures (one DBR/one metal mirror or two metal mirrors) are presented, showing a splitting between both polariton branches of several tens of meV. In the structure made of two metal mirrors, even a third branch arising from higher vibronic states of the molecule can be identified. The measurements are compared to calculations based on the transfer matrix algorithm.

30 min. Coffee Break

HL 44.6 Wed 11:30 H10

Exciton-Polaritons in doped semiconductor microcavities with finite hole mass — •Dimitri Pimenov[1], Oleg Yevtushenko[1], Jan von Delft[1], and Moshe Goldstein[2] — [1]Arnold Sommerfeld Center for Theoretical Physics, Ludwig-Maximilians-Universität München, D-80333 München, Germany — [2]School of Physics and Astronomy, Tel Aviv University, Tel Aviv 69978, Israel

As shown in recent experiments, spectral properties of exciton-polaritons in optical microcavities with an embedded semiconductor quantum well are strongly affected by doping of the semiconductor. Previous theoretical studies concerned with nonzero Fermi-energy mostly relied on the approximation of infinite valence band hole mass, which is appropriate for low-mobility samples only. For high-mobility samples, one needs to consider large but finite hole mass. We present an analytical diagrammatic approach to tackle this problem for a model of short-ranged (screened) electron-hole interaction, studying its two different regimes. In the first regime, where the Fermi-energy dominates over the exciton binding energy, one can make use of the summation of parquet diagrams introduced by Mahan and Nozières. As a trend, finite mass effects cut off the excitonic features in the polariton spectra, in qualitative agreement with the experimental findings. In the second regime of dominant binding energy, we perform a low-density summation of ladder diagrams. As opposed to the previous case, the excitonic features are enhanced by the finite mass, which can be understood based on phase-space arguments.

HL 44.7 Wed 11:45 H10

Coherent manipulation of photonic crystal microcavities with metallic electric contacts — •Wadim Quiring[1], Björn Jonas[1], Ashish Rai[2], Dirk Reuter[1], Andreas Dirk Wieck[2], and Artur Zrenner[1] — [1]Center for Optoelectronics and Photonics Paderborn (CeOPP), Universität Paderborn, Paderborn, Germany — [2]Ruhr-Universität Bochum, Bochum, Germany

We present our results of a two pulse experiment on a photonic crystal cavity (PhCC). We use MBE-grown GaAs membranes, which are designed as n-i-Schottky structures with an InGaAs wetting layer as active layer in the intrinsic region. From this we have fabricated PhCCs with narrow electrodes, which provide an electric connection to the defect and allow for photocurrent (PC) readout. The samples were first characterized by PC spectroscopy under resonant cw excitation [1]. The measured Q factors are around 5000. Double pulse excitation was realized by a 3.5 ps Ti:Sa laser followed by a Michelson interferometer. The pulse separation and relative phase could be precisely controlled over a long range. Changing the time delay we simultaneously monitored the interferogram (i) of the laser fields and (ii) of the cavity response using photocurrent detection. The excitation wavelength was chosen to be either on the cavity resonance or in defined detuning conditions. Our experiments clearly show the coherent control of the PhCC and its phase evolution with respect to the driving laser field. [1] W. Quiring et. al, Appl. Phys. Lett. 107, 041113 (2015)

HL 44.8 Wed 12:00 H10

Tailored Scattering Layers to Homogenize Light Emission from Large-Area Organic Light-Emitting Diodes — •Frederik Mayer[1], Robert Schittny[1], Amos Egel[2], Andreas Niemeyer[1], Jan Preinfalk[2], Ulrich Lemmer[2], and Martin Wegener[1,3] — [1]Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76128 Karlsruhe, Germany — [2]Light Technology Institute and Institute of Microstructure Technology, Karlsruhe Institute of Technology (KIT), 76128 Karlsruhe, Germany — [3]Institute of Nanotechnology, Karlsruhe Institute of Technology (KIT), 76128 Karlsruhe, Germany

For large-area organic light-emitting diodes, the relatively high sheet resistance of the transparent electrode layer is often compensated for by adding a metallic electrode grid on top. However, these electrodes cast a shadow, leading to a spatially inhomogeneous light emission of the OLED. In this talk, based on recent findings on diffusive-light cloaking, we present a method to homogenize this light emission and thereby hide the contact grid by adding an additional light-scattering layer on top, consisting of regions with different concentrations of scattering particles. We design this light-scattering layer using Monte-Carlo simulations of light transport through multiply-scattering media and show corresponding experiments on a scaled-up model structure.

HL 44.9 Wed 12:15 H10

Circular Bragg grating cavity design for efficient sources of single photons fabricated within a deterministic technology platform — •Anna Musiał[1,2], Benjamin Wohlfeil[3], Sven Burger[3], Tobias Heuser[1], Arsenty Kaganskiy[1], Esra Yarar Tausher[1], Ronny Schmidt[1], Sven Rodt[1], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, Germany — [2]Faculty of Fundamental Problems of Technology, Wrocław University of Technology, Poland — [3]Computational Nano Optics, Zuse Institut Berlin, Germany

Growing interest in quantum information processing and secure communication requires realization of efficient single-photon sources (SPS). Reliable implementation of advanced quantum protocols makes deterministic fabrication technologies desirable. A further key requirement is maximizing the extraction efficiency of emission from QDs acting as single-photon emitters. To tackle these issues we propose to deterministically integrate single QDs into circular Bragg grating cavities (CBGC). We present results based on the modelling of GaAs/air CBGCs using a finite element method which allows us to optimize the cavity design parameters for maximum extraction efficiency. For this purpose, a detailed knowledge of the influence of cavity geometry on the electro-magnetic field distribution, mode energy, cavity quality factor and optimal position of the QD in the cavity is indispensable. Optimized design parameters are used to realize CBGCs that include single In(Ga)As QDs by combining cathodoluminescence spectroscopy and in-situ electron-beam lithography.

HL 44.10 Wed 12:30 H10

Nonlinear optical coefficients of III-V semiconductors measured by Raman spectroscopy — •Christian Röder, Gert Irmer, Cameliu Himcinschi, and Jens Kortus — TU Bergakademie Freiberg, Institute of Theoretical Physics, Leipziger Str. 23, D-09599 Freiberg, Germany

Applications based on nonlinear waveguides, frequency doubling, frequency mixing or phase conjugation require for design and optimization of devices an accurate knowledge of the linear and nonlinear optical response. Johnston and Kaminow [1] demonstrated for GaAs that Raman scattering can be used to determine the nonlinear optical coefficients below the bandgap. In case of wz-GaN there have been several experimental and theoretical studies with significant divergences concerning the coefficients of the second-harmonic generation (SHG) and the linear-optical effect (LEO). Due to the wurtzite structure of GaN symmetry requires three SHG and LEO coefficients to be considered independently. In the present study Raman scattering experiments were performed in order to determine all six coefficients of wz-GaN for the first time.
This work is financially supported by the European Union (European Social Fund) and by the Saxonian Government (grant no. 100231954).

[1] W.D. Johnston, Jr. and I.P. Kaminow: Phys. Rev. **188**, 1209 (1969)

Invited Talk HL 44.11 Wed 12:45 H10

From a loophole-free Bell test to a secure quantum Internet — •Ronald Hanson — QuTech and Kavli Institute of Nanoscience, Delft University of Technology, The Netherlands

For more than 80 years, the counterintuitive predictions of quantum theory have stimulated debate about the nature of reality. In his seminal works, John Bell showed that in any theory in which events only have local causes, the correlations between distant measurements satisfy an inequality and, moreover, that this inequality can be violated according to quantum theory. In the past decades, numerous ingenious Bell inequality tests have been reported. However, because of experimental limitations, all experiments to date required additional assumptions to obtain a contradiction with local realism, resulting in "loopholes".

In this talk I will explain our recent Bell experiment that is free of any such additional assumption [1], in which we entangle two electron spins in diamond separated by more than 1 km. I will discuss the implications of its result for possible models of nature. Furthermore, I will speculate how this result, combined with recently achieved control over individual nuclear spins in diamond [2] and teleportation between separated diamond chips [3], may lead to a quantum Internet secured through device-independent protocols - reaching the ultimate physical limits of privacy [4].

[1] B. Hensen et al., Nature 526, 682 (2015). [2] J. Cramer et al., arXiv:1508.01388 (2015). [3] W. Pfaff et al., Science 345, 532 (2014). [4] A. Ekert and R. Renner, Nature 507, 443 (2014).

HL 45: Hybrid and Perovskite Photovoltaics III (Joint session of CPP, DS and HL, organized by CPP)

Time: Wednesday 9:30–11:45 Location: H11

HL 45.1 Wed 9:30 H11

Impact of Preparation Conditions on the Ionization Energy and Electronic Structure of CH3NH3PbI3 Perovskites — •Jennifer Emara[1], Tobias Schnier[1], Neda Pourdavoud[2], Thomas Riedl[2], Klaus Meerholz[1], and Selina Olthof[1] — [1]University of Cologne, Institute for Physical Chemistry, Luxemburger Straße 116, 50939 Köln, Germany — [2]Institute of Electronic Devices, University of Wuppertal, Rainer-Grunter-Straße 21, 42119 Wuppertal, Germany

Hybrid organic/inorganic halide perovskites have lately been a topic of great interest in the field of solar cell applications, with the potential to achieve device efficiencies exceeding other thin film device technologies. Yet, large variations in device efficiency and basic physical properties are reported. This is due to unintentional variations during film processing, which have not been systematically investigated so far. We therefore conducted an extensive study of the electronic structure of a large number of CH3NH3PbI3 perovskite films produced by different preparation methods and by varying precursor ratios. We

show that variations in film stoichiometry lead to vast changes in the density of states (DOS), and changes in ionization energy, which can be intentionally tuned by almost 1 eV. Using x-ray diffraction measurements, we find the variations in film stoichiometry are not due to the formation of separate phases, but that interstitials and vacancies are homogeneously distributed within the material. Implementing the prepared perovskite layer materials in solar cells, we find a clear correlation between the changes in DOS with the overall power conversion efficiency.

HL 45.2 Wed 9:45 H11

Two dimensional organometal halid perovskite nanosheets in light emitting application — •Rui Wang[1], Zhendong Fu[1], Vitaliy Pipich[1], Alexandros Koutsioumpas[1], Stefan Mattauch[1], Peter Müller-Buschbaum[2], and Henrich Frielinghaus[1] — [1]Jülich Center for Neutron Science, outstation at FRM II, Lichtenbergstr. 1, 85747 Garching — [2]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching

Two dimensional functional materials have created intensive research interest for high efficiency solar cells. Recently low dimensional pervoskite nanocrystals, such as 2D perovskite nanosheets have been reported to possess reduced fluorescence decay times, an increased exciton binding energy and low conductivity in certain crystallographic directions. Consequently, these lower dimensional perovskites can be utilized for light emitting applications. In the present work, 2D nanosheet perovskites are formed by using octylamine bromide as capping ligands. GISANS combined with neutron reflectivity (NR) are applied to investigate the structure buried inside the thin films. GISANS had proven to be a powerful technique for thin film morphology investigations. NR guarantees that information about nanometer sized layers can be accessed. We present the determined structures in terms of optical properties, grain size information and stacked layered characteristic.

HL 45.3 Wed 10:00 H11

Morphology and crystal orientation of hybrid perovskite thin films for application in high efficiency solar cells — •Johannes Schlipf[1], Lukas Oesinghaus[1], Nadja Giesbrecht[2], Yinghong Hu[2], Sigrid Bernstorff[3], Thomas Bein[2], Pablo Docampo[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — [2]Department of Chemistry and CENS, LMU München, 80539 München, Germany — [3]Elettra-Sincrotrone Trieste S.C.p.A., Basovizza, 34149 Trieste, Italy

Organo-metal halide perovskites mark a paradigm shift in photovoltaic research, as they combine high efficiencies challenging conventional inorganic solar cells with easy processing and cheap abundant precursor materials. Recent reports of power conversion efficiencies around 20% are possible due to remarkable material properties and their highly crystalline nature even when processed from solution. However, photovoltaic performance is directly linked to film morphology which in turn depends on the fabrication method. We investigate hybrid perovskite thin films of high efficiency solar cells prepared by various synthesis protocols with X-ray diffraction, GIWAXS and GISAXS. Thereby, we evidence different crystallization mechanisms that lead to certain morphologies and crystal orientations reflecting the chosen synthesis method [1]. We link these findings to the photovoltaic performance and aim at a rational development of new synthesis methods for high efficiency perovskite solar cells.

[1] Schlipf et al: J. Phys. Chem. Lett, 6, 1265-1269, 2015.

HL 45.4 Wed 10:15 H11

Influence of annealing time on crystal structure and composition of CH3NH3PbI3-xClx mixed halide perovskite film — •Maryline Ralaiarisoa[1], Yan Busby[2], Johannes Frisch[1], Ingo Salzmann[1], Jean-Jacques Pireaux[2], and Norbert Koch[1] — [1]Humboldt-Universität zu Berlin, Institut für Physik, Brook-Taylor-Str. 6, 12489 Berlin, Germany — [2]Research Center in the Physics of Matter and Radiation , Laboratoire Interdisciplinaire de Spectroscopie Electronique (LISE), University of Namur, 5000 Namur, Belgium

Thermal annealing is a crucial step for the formation of crystalline perovskite films from precursor solution. However, the structural evolution during perovskite film formation and particularly its composition during annealing have not been thoroughly characterized yet. Such characterization is essential to understand the mechanisms leading to the complete conversion to perovskite. Using ToF-SIMS, we monitored the changes in composition and structure of CH3NH3PbI3-x Clx perovskite films after two different annealing stages, that is, before and after complete perovskite crystallization. At the early stage of annealing, our results show phase separation throughout the entire film depth into one where perovskite was formed and another where mostly the inorganic precursor PbCl2 was detected. After sufficiently long annealing, we found a single perovskite phase of homogeneous composition on the micrometer scale. By means of UPS, we further observed that perovskite films become more n-type for longer annealing time, which correlates the morphological evolution and the surface electronic structure.

15 min. break.

HL 45.5 Wed 10:45 H11

Ferroelasticity in methylammonium lead halide perovskite? — Ilka Hermes[1], Simon Bretschneider[1], Victor Bergmann[1], Dan Li[1], Alexander Klasen[1,2], Julian Mars[1], Wolfgang Tremel[2], Frédéric Laquai[1], Hans-Jürgen Butt[1], Markus Mezger[1,2], Rüdiger Berger[1], Brian Rodriguez[3], and •Stefan Weber[1,2] — [1]MPI for Polymer Research, Mainz — [2]Johannes Gutenberg University, Mainz — [3]University College Dublin, Ireland

Methylammonium lead halide ($MAPbX_3$) perovskite materials show an outstanding performance in photovoltaic devices. However, some material properties, especially the possible ferroic behavior, remain unclear. We observed distinct nanoscale periodic domains in the piezoresponse of $MAPbI_3$(Cl) grains. The structure and the orientation of these striped domains is indicating ferroelasticity as their origin. By correlating vertical and lateral piezoresponse force microscopy experiments performed at different sample orientations with x-ray diffraction, the preferred domain orientation was assigned to the $a_1 - a_2$-phase. The observation of the twin domains appears to strongly depend on the preparation route and the film texture and is thought be induced by internal strain during the cubic-tetragonal phase transition.

HL 45.6 Wed 11:00 H11

XPS study of the ALD growth of Al_2O_3 on the $CH_3NH_3PbI_3$ — •Małgorzata Sowińska[1], Chittaranjan Das[1], Konrad Wojciechowski[2], Henry Snaith[2], and Dieter Schmeisser[1] — [1]Brandenburgische Technische Universität Cottbus-Senftenberg, Angewandte Physik-Sensorik, Konrad-Wachsmann-Allee 17, 03046 Cottbus, Germany — [2]Clarendon Laboratory, University of Oxford, Parks Road, Oxford, OX13PU, UK

Organic-inorganic lead halide perovskites have emerged as very attractive absorber materials for the fabrication of low cost and high efficiency solar cells, but a delicate nature of these films is one of the main challenges for a successful commercialization. Typically, when exposed to air or moisture, perovskite films degrade within a couple of hours or days. Moreover, the methylammonium lead triiodide ($CH_3NH_3PbI_3$) perovskite cannot sustain a prolonged annealing at temperatures around 85°C. In this work, we are investigating stability (upon air and thermal exposure) of a $CH_3NH_3PbI_3$ perovskite film coated with a thin layer of Al_2O_3 deposited by atomic layer deposition (ALD). In particular, the chemical and electronic changes occurred at the $Al_2O_3/CH_3NH_3PbI_3$ interface during the first 50 ALD cycles were monitored ex-situ by high-resolution and surface-sensitive synchrotron-based X-ray photoelectron spectroscopy (SR-XPS). The advantage of the ALD as a deposition method is that it can produce extremely dense layers with a very precise thickness control at room temperature. Detailed SR-XPS data analysis and a stability test of the perovskite film with alumina will be presented.

HL 45.7 Wed 11:15 H11

Water based hybrid solar cells: spray deposition of the active layer monitored with x-ray scattering methods — •Volker Körstgens[1], Christoph Mayr[1], Stephan V. Roth[2], Hristo Iglev[3], Reinhard Kienberger[3], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, James-Franck-Str. 1, 85748 Garching — [2]DESY Photon Science, Notkestr. 85, 22607 Hamburg — [3]TU München, Physik-Department, LS Laser- und Röntgenphysik, James-Franck-Str. 1, 85748 Garching

Spray-coating is a technique suitable for the large-scale and cost-effective preparation of hybrid photovoltaics. Unique environmentally friendly processing of hybrid solar cells can be realized with systems based on the solvent water. Using an active layer consisting of laser-ablated titania nanoparticles and water-soluble poly[3-(potassium-6-hexanoate)thiophene-2,5-diyl] (P3P6T) hybrid solar cells were realized.

[1] For the performance of these devices the morphology of the active layer is of major importance. We followed the development of the morphology in situ with high spatial and temporal resolution. The mesoscale was probed with GISAXS and the crystallinity of the polymer and the inorganic component was probed with GIWAXS. The changes of the morphology of the active layer with increasing thickness and the dependence on the blocking layer chosen as the initial substrate are discussed and implications for an improved spray protocol will be given.

[1] Körstgens et al., Nanoscale 7, 2900 (2015).

HL 45.8 Wed 11:30 H11

A low temperature route towards hierarchically structured titania films for thin hybrid solar cells — •Lin Song[1], Amr Abdelsamie[1], Christoph J. Schaffer[1], Volker Körstgens[1], Weijia Wang[1], Nicola Hüsing[2], Paolo Lugli[3], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — [2]Materialchemie, FB Chemie und Physik der Materialien, Universität Salzburg, Hellbrunnerstr. 34, 5020 Salzburg, Austria — [3]TU München, Department of Electrical Engineering and Information Technology, Institute for Nanoelectronics, 80333 München, Germany

Fabricating titania based solar cells at low temperature has a high significance regarding energy efficacy , since most of photovoltaic devices with titania require high-temperature calcination. Moreover, a low-temperature process offers the potential for flexible solar cells. However, this kind of solar cells has a low efficiency. In order to improve the device performance, we make superimposed structural order on titania films from nanometer to submicrometer length scales. Hierarchical structural order enhances light harvesting in solar cells, thereby enhancing the photovoltaic performance. Titania nanostructures are obtained via PS-b-PEO template assisted sol-gel processing. Nanoimprint lithography (NIL) provides ordered submicrometer patterns as a superstructure over nanostructured titania films. SEM and AFM measurements map the film surface morphology, and GISAXS measurements yield information about the bulk film morphology. The optoelectronic properties are examined by UV/Vis spectroscopy.

HL 46: Organic Semiconductors

Time: Wednesday 9:30–11:30 Location: H13

HL 46.1 Wed 9:30 H13

Exciton-Polaritons in Open Organic Microcavities — •Simon Betzold, Christof P. Dietrich, and Sven Höfling — Technische Physik, Julius-Maximilians-Universität Würzburg, Am Hubland, 97074 Würzburg

Frenkel excitons, characteristic of organic semiconductors, possess large binding energies and are stable at room temperature, making polariton experiments at ambient air conditions feasible. Organic materials further exhibit very large oscillator strengths and thus strongly interact with a cavity field. Circumventing the issue that organic materials are very sensitive to the depositing of semiconductor layers on top of them, we use an open cavity system, which makes non-invasive investigation of the active material possible.

Open cavities are tunable systems and comprise a bottom semiconductor distributed Bragg reflector (DBR) with the active material (the organic semiconductor) on top and a concave top DBR separated by a micrometer sized air gap. This configuration allows a 3D photonic confinement and brings unprecedently high quality factors into reach.

Here, we show the versatility of open cavities by performing reflectivity and photoluminescence measurements in Fourier imaging configuration and exemplarily investigate the strong exciton-photon coupling between a red-emitting polymer and the dielectric cavity. We emphasize that the open cavity approach can easily be extended to more complex active regions including two-dimensional monolayer materials or hybrid organic-inorganic bilayers.

HL 46.2 Wed 9:45 H13

Multi-scale modeling of spin transport in organic semiconductors — •Amaury Souza[1], Shayan Hemmatiyan[1], Erik Mcnellis[1], Denis Andrienko[2], and Jairo Sinova[1] — [1]Johannez Gutenberg Universy - Mainz — [2]Max Planck Institute for Polymers - Mainz

In this work, we present our theoretical framework to simulate simultaneously spin and charge transport in amorphous organic semiconductors. By combining several techniques e.g. molecular dynamics, density functional theory and kinetic Monte Carlo, we are be able to study spin transport in the presence of anisotropy, thermal effects, magnetic and electric field effects in a realistic morphologies of amorphous organic systems. We apply our multi-scale approach to investigate the spin transport in amorphous Alq3 (Tris(8-hydroxyquinolinato)aluminum) and address the underlying spin relaxation mechanism in this system as a function of temperature, bias voltage, magnetic field and sample thickness.

HL 46.3 Wed 10:00 H13

Conformal growth of ultra-thin p-conductive polymer layers on n-type semiconductor nanostructures by oxidative chemical vapour deposition — •Linus Krieg[1], Stephanie Bley[2], Max Rückmann[2], Jürgen Gutowski[2], Florian Meierhofer[3], Lutz Mädler[3], and Tobias Voss[1] — [1]Institute of Semiconductor Technology and LENA, Braunschweig University of Technology — [2]Institute of Solid State Physics, Semiconductor Optics, University of Bremen — [3]Foundation Institute of Material Science, Department of Production Engineering, University of Bremen

Inorganic-organic hybrid systems consisting of conjugated polymers and inorganic semiconductors are promising for the development of cheap, versatile and tailored electronic and optoelectronic devices. A gentle approach for polymer layer deposition is offered by the oxidative chemical vapour deposition (oCVD), a solventless and dry method where the oxidising agent and the monomer are provided in the gaseous phase. In our experiments, we use $FeCl_3$ as an oxidising agent and monomers of the p-conductive polymers polypyrrole (PPy) and poly(3,4-ethylenedioxythiophene) (PEDOT) to conformally coat n-type ZnO and GaN wafers and nanowires. SEM and TEM measurements confirm that we can achieve conformal coating of the entire nanowire with the conductive polymer while the optical properties of the inorganic semiconductors show no substantial deterioration. The layer thickness is in the order of a few tens of nanometres and can be controlled by the total amount of the oxidising agent provided during the coating process.

30 min. Coffee Break

HL 46.4 Wed 10:45 H13

α,ω-Dihexyl-sexithiophene thin films for solution-gated organic field-effect transistors — •Hannah Schamoni[1], Simon Noever[2], Bert Nickel[2], Max Kraut[1], Martin Stutzmann[1], and Jose A. Garrido[3] — [1]Walter Schottky Institut und Physik-Department, Technische Universität München, Deutschland — [2]Fakultät für Physik und CeNS, Ludwig-Maximilians-Universität München, Deutschland — [3]Catalan Institute of Nanoscience and Nanotechnology, CSIC and The Barcelona Institute of Science and Technology, Barcelona, Spain

While organic semiconductors are being widely investigated for chemical and biochemical sensing applications, major drawbacks such as the poor device stability and low charge carrier mobility in aqueous electrolytes have not yet been solved to complete satisfaction. In this work, solution-gated organic field-effect transistors (SGOFETs) based on the molecule α,ω-dihexyl-sexithiophene are presented as a promising platform for in-electrolyte sensing. It is shown that the performance of the SGOFETs can be improved by choosing suitable growth parameters which lead to a two-dimensional film morphology and a high degree of structural order. Furthermore, the capability of the SGOFETs to detect changes in the pH or ionic strength of the gate electrolyte is demonstrated and successfully simulated. Excellent transistor stability is confirmed by continuously operating the device over a period of several days. Altogether, our results demonstrate the feasibility of high performance and highly stable organic semiconductor devices for chemical or biochemical applications.

HL 46.5 Wed 11:00 H13

Correlation of Crystalline Structure and Optical Properties

of Perylene: a Comprehensive Experiment-Theory Comparison — •Andre Rinn[1], Tonatiuh Rangel[2], Andrè Pick[1], Gregor Witte[1], Leeor Kronik[3], Jeffrey Neaton[2], and Sangam Chatterjee[1] — [1]Faculty of Physics, Philipps Universität Marburg, Renthof 5, D-35032 Marburg, Germany — [2]Molecular Foundry, Lawrence Berkeley National Laboratory, University of California, Berkeley, 1 Cyclotron Road, MS 67R3207 Berkeley, CA 94720, U.S.A. — [3]Faculty of Chemistry, Weizmann Institute of Science, Rehovot 76100, Israel

Aromatic molecules such as perylene and its derivatives find wide spread usage in electronic devices and as dyes as this class of material shows strong light-matter coupling. Here, we show a comprehensive study of the optical properties of the model semiconductor perylene. It adopts two distinctive crystalline polymorphisms, both of which show vastly different excitonic structure and carrier dynamics. The comparison of a detailed theoretical analysis based on first-principles calculations with the polarization-resolved experimental linear absorption spectra yields excellent agreement. In particular, we discuss the importance of electron-hole interaction effects beyond a standard two-particle picture and implications of different approximations commonly made in calculations using density functional theory and many-body perturbation theory formalisms.

HL 46.6 Wed 11:15 H13

Strain and Pressure Dependent Electronic Properties of Polyacetylene — •Franz Knuth[1], Christian Carbogno[1], Volker Blum[2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin, Germany — [2]MEMS Department, Duke University, Durham, NC 27708, USA

Strain, stress, and pressure can influence the electronic properties of organic semiconductors [1]. In this contribution, we present the changes of electronic and transport properties for crystalline *trans*-polyacetylene under strain and hydrostatic pressure in the framework of density-functional theory. We critically discuss the role of approximations in the exchange-correlation functional and show that the fraction of exact exchange included in the calculations with hybrid functionals is non-trivial to choose and essential for the correct description of polyacetylene. The pressure studies are performed with the help of the analytical strain derivatives (stress tensor) including the contributions coming from van-der-Waals corrections and exact exchange [2]. Our calculations also reveal that the electronic band structure and gap of polyacetylene are not only determined by the dimerization of the carbon chain but are at least as much influenced by interchain interactions.

[1] J. H. Kim, S. Seo, and H. H. Lee, Appl. Phys. Lett. **90**, 143521 (2007); G. Giri *et al.*, Nature. **480**, 504 (2011)
[2] F. Knuth *et al.*, Comp. Phys. Comm. **190**, 33 (2015)

HL 47: Quantum Hall Effect

Time: Wednesday 9:30–11:45 Location: H14

HL 47.1 Wed 9:30 H14

Impact of the dynamically tuned 2DEG density on the photoluminescence of modulation-doped CdTe and CdMnTe quantum wells — •Janina Rautert[1], Dion Braukmann[1], Jörg Debus[1], Vitalii Yu. Ivanov[2], Dmitri R. Yakovlev[1,3], Grzegorz Karczewski[2], Tomasz Wojtowicz[2], and Manfred Bayer[1,3] — [1]Experimentelle Physik 2, Technische Universität Dortmund, 44227 Dortmund, Germany — [2]Institute of Physics, Polish Academy of Sciences, 02668 Warsaw, Poland — [3]Ioffe Institute, Russian Academy of Sciences, 194021 St. Petersburg, Russia

A highly concentrated two-dimensional electron gas (2DEG) in a modulation-doped semiconductor quantum well (MDQW) shows many interesting features in both transport measurements and optical spectroscopy, like the integer and fractional quantum Hall effect (QHE). It is known that the formation of trion and exciton complexes in a MDQW strongly depends on the 2DEG density, which can be controlled by the laser power and its energy as well as by an external magnetic field. We study the competition between the 2DEG and negative trion photoluminescence (PL) in the stationary and time-resolved regime (showing up for several hundreds of μs) for a CdTe MDQW at different magnetic fields. By comparison, in a CdMnTe MDQW the exciton magneto-PL shows variations in the energy for transitions between different QHE regimes at elevated temperatures above 1.5 K. Moreover, the 2DEG and exciton PL lines may anticross at different points of time with increasing magnetic field.

HL 47.2 Wed 9:45 H14

Terahertz induced oscillations of magnetoresistivity in AlGaAs/GaAs quantumwells (QW) — •Tobias Herrmann[1], Ze Dong Kvon[2], Dmitriy A. Kozlov[2], Vasily V. Bel'kov[3], Bruno Jentzsch[1], Martin Schneider[1], Peter Olbrich[1], Dominique Bougeard[1], Dieter Weiss[1], and Sergey D. Ganichev[1] — [1]University of Regensburg, Regensburg, Germany — [2]Institute of Semiconductor Physics, Novosibirsk, Russia — [3]Ioffe Institute, St. Petersburg, Russia

We report on the observation of MIRO-like oscillations (Microwave Induced Resistivity Oscillations) in GaAs-based two dimensional electron systems (2DES). The 1/B periodic oscillations are detected in corbino disk very low and high mobility QW samples excited by radiation with $f = 0.69$ THz. Strikingly we observe that the oscillations* amplitudes, in contrast to cyclotron resonance (CR), only slightly depend on the radiation helicity, even in the vicinity of CR. This result is insofar important that existing theories predict the amplitude of MIRO to depend on the helicity of the circular polarization via the factor $1/[(\omega \pm \omega_c)^2 + 1/\tau^2]$, where the minus (plus) sign corresponds to active (inactive) polarization[1]. Furthermore, scanning the beam across the sample with the beam size smaller than the corbino disc diameter we observed that the oscillations are excited in the 2DES and not at the structure edges. This observation demonstrates that edge effects caused by pondermotive forces[2] are not responsible for the observed MIRO-like oscillations. [1] Dmitriev et al., Rev. Mod. Phys., 84. 1709 (2012) [2] Mikhailov, Phys. Rev. B, 89, 045410 (2014)

HL 47.3 Wed 10:00 H14

GaSb/InAs double quantum wells for Topological Insulator application — •Maximilian Schwarz[1], Georg Knebl[1], Pierre Pfeffer[1], Monika Emmerling[1], Lukas Worschech[1], Sven Höfling[1,2], and Martin Kamp[1] — [1]Technische Physik and Wilhelm Conrad Röntgen Research Center for Complex Material Systems, University of Würzburg — [2]SUPA, School of Physics and Astronomy, University of St. Andrews, St. Andrews KY16 9SS, United Kingdom

The topological insulator phase is theoretical predicted for InAs/GaSb double quantum wells (DQW) embedded in AlSb barrier layers. In HgTe/CdTe-QW structures the transition between the normal and the topological insulator state can only be achieved by variation of the QW-thickness. For InAs/GaSb-DQW structures it is shown that one can tune between trivial and topological phase by front and back gates. Dry and wet etching as well as optical and electron beam lithography were used and compared processing structures. Transport data for differently processed samples will be compared and reversible switching majority carriers from electrons to holes by optical doping will be shown.

Financial support by the DFG SPP166, Elitenetzwerk Bayern IDK TOIS and the State of Bavaria is gratefully acknowledged.

HL 47.4 Wed 10:15 H14

Probing magnetic nanostructures with non-diffusive Hall crosses — •Stefan Fasbender[1], Jakob Schluck[1], Mihai Cerchez[1], Thomas Heinzel[1], Klaus Pierz[2], Sibylle Sievers[2], and Hans Werner Schumacher[2] — [1]Heinrich Heine Universität Düsseldorf — [2]PTB Braunschweig

Hall sensing is performed on a localized magnetic field pattern using a Hall cross device that can be tuned from diffusive to ballistic by decreasing the temperature. As the ballistic regime is entered, the Hall resistance develops a pronounced peak as a function of the magnetic field amplitude. This non-monotonic response exemplifies qualitatively the failure of conventional Hall sensing with ballistic Hall crosses. It is shown that the magnetization can still be determined from such measurements by a numerical correction based on the Landauer-Buettiker model as long as the functional form of the magnetic field profile is

known.

30 min. Coffee Break

HL 47.5 Wed 11:00 H14

Narrow-gap semiconductor nanostructures in the quantum Hall regime — •Olivio Chiatti[1], Christian Riha[1], Johannes Boy[1], Sergio Pezzini[2], Steffen Wiedmann[2], Christian Heyn[3], Wolfgang Hansen[3], and Saskia F. Fischer[1] — [1]Novel Materials Group, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — [2]High Field Magnet Laboratory, Radboud University Nijmegen, 6525ED Nijmegen, The Netherlands — [3]Institut für Angewandte Physik, Universität Hamburg, 20355 Hamburg, Germany

The quantum Hall edge channels (QHECs) are crucial for our understanding of the underlying physics of the quantum Hall effect (QHE). Our experimental work has been directed at studying the role of spin-orbit interaction (SOI). We have combined quantum point contacts (QPCs) with in-plane gates and Hall-bars in a narrow-gap semiconductor heterostructure with strong SOI. The constriction was fabricated by micro-laser photolithography and wet-chemical etching from an InGaAs/InAlAs quantum well with an InAs-inserted channel [1]. We have performed transport measurements at temperatures down to 300 mK in the combined QPC and Hall-bar structures in magnetic fields perpendicular to the 2DEG up to 33 T. We observe conductance quantization through the QPC when QHECs are formed. We investigate the effect of symmetric and asymmetric in-plane gate voltages on the transport by QHECs through the QPC.
[1] Chiatti *et al.*, Appl. Phys. Lett. **106**, 052102 (2015).

HL 47.6 Wed 11:15 H14

Coupling non-equilibrium transport and the stationary many particle Fermi Sea for numerical modelling of the integer quantum Hall effect regime — •Josef Oswald[1] and Rudolf Römer[2] — [1]Institute of Physics, Leoben University, Franz Josef Str. 18, A-8700, Leoben, Austria — [2]Department of Physics, University of Warwick, Coventry CV4 7AL, UK

Even 35 years after discovery, the quantum Hall effect (QHE) remains an interesting and still challenging topic of research. The challenge of modelling experiments in the QHE regime is the need of a link between the Fermi Sea as a stationary many particle quantum state and the experimentally injected non-equilibrium.

This is handled by two modules : One addresses the stationary many particle Fermi sea on the basis of a self-consistent numerical Hartree-Fock (HF) approach and the other addresses the non-equilibrium electron transport by a network approach. It allows us to simulate directly the distributions of the experimentally injected non-equilibrium potentials at arbitrary contact configurations in arbitrarily shaped sample geometries, including native and artificial in-homogeneity. The associated resistances need to be calculated only in a post processing step like it is also the case in real experiments. The screening behaviour of the electron system is addressed by the HF module that allows seeing effects like filling factor dependent screening, Landau-level broadening and enhanced g-factor. These effects enter the properties of the transport module and allow a modelling that is much more close to real systems and real experiments then most of other models.

HL 47.7 Wed 11:30 H14

The Physics of the Integer and Fractional Quantum Hall Effects — •Horst Jürgen Andrä — Former member of Institut für Kernphysik, Universität Münster, Wilhelm-Klemm-Str. 9, 48149 Münster

A framework is presented for the understanding of both the Integer(I)- and the Fractional(F)-Quantum Hall Effect (QHE), including the widths of their plateaus. It is based on the condition of neutrality which enforces any change in the population of the 2-Dimensional Electron System (2DES) to also occur in an adjacent positive 2-Dimensional Hole Layer (HL). The near perfect exchange between the 2DES and the HL allows the description of the IQHE independent of any potential distribution across the 2DES. When on the contrary the HL is nearly constant for all magnetic fields then also the number of electrons in the 2DES has to be nearly constant for all magnetic fields. This is the condition for the description of all ever observed FQHE-signals as the result of a spatial electron and magnetic flux quantization. Experiments are proposed to proof these descriptions. The particular ν=5/2-, 7/2-, 9/2-, etc. FQHE states are interpreted as due to inter-Landau electron-electron interactions with specific selections rules. Tilted field experiments can be interpreted in terms of symmetry breaking. Hints on the origin of the reentrant integer quantum Hall states are given. For more details see DOI: 10.13140/RG.2.1.3864.7766

HL 48: Quantum Dots and Wires: Microcavities

Time: Wednesday 9:30–12:00 Location: H15

HL 48.1 Wed 9:30 H15

Temperature-stable strong light-matter coupling in the solid state with quantum dot-micropillars — •Anna Musiał[1,2], Caspar Hopfmann[1], Maximillian Strauss[1], Andreas M. Barth[3], Martin Gläßl[3], Alexei Vagov[3], Micha Strauss[4], Christian Schneider[4], Sven Höfling[4,5], Martin Kamp[4], Vollrath M. Axt[3], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, Germany — [2]Faculty of Fundamental Problems of Technology, Wrocław University of Technology, Poland — [3]Institut für Theoretische Physik III, Universität Bayreuth, Germany — [4]Technische Physik, Universität Würzburg, Germany — [5]School of Physics and Astronomy, University of St. Andrews, UK

Strong coupling (SC) regime of cQED is important for implementation of quantum networks. We address experimentally and theoretically the crucial issue of its temperature stability. Experiments and statistical analysis of temperature influence on the vacuum Rabi splitting (VRS) performed for 89 cases of SC in a broad temperature range (10*50) K revealed behavior beyond the strong confinement approximation. The unprecedented temperature stability is attributed to compensation of phonon-induced renormalization of VRS in laterally-extended In0.4Ga0.6As QDs and their unique optical properties resulting from complex electronic structure. The calculations within path integral formalism reproduces observed behavior. Observed persistence of SC demonstrates appealing possibility to counteract detrimental phonon effects.

HL 48.2 Wed 9:45 H15

Experimental and theoretical investigation of a strong optical Stark effect in a semiconductor micropillar cavity — •Fabian Hargart[1], Kaushik Roy-Choudhury[2], Tilmann John[1], Simone Luca Portalupi[1], Christian Schneider[3], Sven Höfling[3], Martin Kamp[3], Stephen Hughes[2], and Peter Michler[1] — [1]Institut für Halbleiteroptik und Funktionelle Grenzflächen, Universität Stuttgart, Allmandring 3, 70569 Stuttgart — [2]Department of Physics, Engineering Physics and Astronomy, Queen's University, Kingston, Ontario, Canada K7L 3N6 — [3]Technische Physik and Wilhelm Conrad Röntgen Research Center for Complex Material Systems, Physikalisches Institut, Universität Würzburg, Am Hubland, 97074 Würzburg

The energy shift of a two-level system by intense, oscillating electric fields—commonly known as AC Stark shift—is studied experimentally and theoretically for a cavity-driven, detuned quantum dot-cavity system. The electric field enhancement inside the cavity facilitates exceptionally strong line shifts of up to $4\,\mu eV/\mu W$. The effect is systematically investigated in dependence of the driving Rabi frequency Ω and the QD-cavity detuning δ. The fine structure splitting of exciton states $|X\rangle$ and $|Y\rangle$ can be increased by magnitudes of orders due to their unequal QD-cavity coupling strengths g_X and g_Y. By extending the system to four levels, including also the biexciton state, we explain the observation of an unexpected opposite Stark shift within a dressed-state picture. The experimental results are reproduced using a simple Hamiltonian for the QD-cavity system and the driving laser field.

HL 48.3 Wed 10:00 H15

Far-field and quality factor optimized GaAs-based photonic crystal cavities for high collection efficiencies in quantum optical applications — •Stefan Hepp, Ulrich Rengstl, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen, Research Center SCoPE and Center for

Integrated Quantum Science and Technology IQ^{ST}, University of Stuttgart, Allmandring 3, 70569 Stuttgart, Germany

Photonic crystal cavities in combination with integrated semiconductor quantum dots have become a fundamental element in present photonic research. High quality factors in combination with ultra-low mode volumes, below one cubic wavelength, make these photonic crystal structures interesting for a wide range of applications, such as the generation of non-classical light states or the investigation of cavity quantum electrodynamic (cQED) effects. However, a major issue is the off-plane radiation profile that features maxima at emission angles around 70° leading to very low collection efficiencies even with high numerical aperture (NA) objectives.
Here, we present a GaAs-based L3-photonic crystal cavity optimized for high quality factors with integrated InAs quantum dots. Additionally, we have modified the far-field emission properties for high collection efficiencies with low numerical aperture objectives that could be useful for quantum optical applications. Theoretical studies show, that the collection efficiency with a standard objective with NA=0.5 can be increased by a factor of 10 from around 7% up to almost 70%.

HL 48.4 Wed 10:15 H15

Deterministic generation of bright single resonance fluorescence photons from a Purcell-enhanced quantum dot-micropillar system — •Stefan Gerhardt[1], Sebastian Unsleber[1], Sebastian Maier[1], Yu-Ming He[1,3], Chao-Yang Lu[3], Jian-Wei Pan[3], Martin Kamp[1], Christian Schneider[1], and Sven Hoefling[1,2] — [1]Technische Physik, Physikalisches Institut and Wilhelm Conrad Roentgen-Research Center for Complex Material Systems, Universitaet Wuerzburg, Am Hubland, 97074 Wuerzburg — [2]SUPA, School of Physics and Astronomy, University of St Andrews, St Andrews, KY16 9SS, United Kingdom — [3]Hefei National Laboratory for Physical Sciences at the Microscale and Department of Modern Physics & CAS Center for Excellence and Synergetic Innovation Center in Quantum Information and Quantum Physics, University of Science and Technology of China, Hefei, Anhui 230026, China

We report on the observation of bright emission of single photons under pulsed resonance fluorescence conditions from a single quantum dot (QD) in a micropillar cavity. The brightness of the QD fluorescence is greatly enhanced via the coupling to the fundamental mode of a micropillar with an extraction efficiency of (20.8 ± 0.8) % per linear polarization basis with a $g^{(2)}(0)$ of 0.072 ± 0.011 at a QD-cavity detuning of 75 μeV. We observe the first Rabi-oscillation in a weakly coupled quantum dot-micropillar system under coherent pulsed optical excitation, which enables us to deterministically populate the excited QD state.

30 min. Coffee Break

Invited Talk HL 48.5 Wed 11:00 H15

Exciton-polariton thermodynamics in ZnSe-based microcavities — •Sebastian Klembt[1,5], Emilien Durupt[1], Sanjoy Datta[2], Thorsten Klein[3], Yoan Léger[4], Augustin Baas[1], Charsten Kruse[3], Detlef Hommel[3], Anna Minguzzi[2], and Maxime Richard[1] — [1]Institut Néel, CNRS-CEA-Université Grenoble Alpes, France — [2]LPMMC, CNRS-Université Grenoble Alpes, France — [3]IFP, Universität Bremen, Germany — [4]CNRS, FOTON, Insa de Rennes, France — [5]Technische Physik, Universität Würzburg, Germany

Exciton-polaritons have attracted considerable interest since they allowed for fundamental understandings of light-matter interactions such as polariton Bose-Einstein condensation and superfluidity. At high density, polaritons constitute indeed a driven dissipative quantum fluid of half-light, half-matter integer spin quasi-particles, which is embedded in a solid-state crystalline environment. The thermodynamic properties of polariton fluids have been mostly overlooked so far. An intriguing specificity of polariton condensates is their contact with three different reservoirs: the thermal phonon bath, the exciton bath and the electromagnetic vacuum. We show experimentally and theoretically that phonons can be efficiently absorbed by inelastic scattering with polaritons. A Raman spectroscopy based technique is presented using anti-Stokes fluorescence (ASF) and we show that under suitable conditions a net cooling rate can be generated by polariton ASF. By using high-Q ZnSe-microcavities the interaction between polariton condensates at up to T=270 K with the respective phonon baths is also investigated.

HL 48.6 Wed 11:30 H15

cQED effects in resonantly excited quantum dot-micropillar cavities — •Caspar Hopfmann[1], Alexander Carmele[2], Anna Musiał[1,3], Micha Strauss[4], Christian Schneider[4], Sven Höfling[4,5], Martin Kamp[4], Andreas Knorr[2], and Stephan Reitzenstein[1] — [1]Institute of Solid State Physics, Technische Universität Berlin, Germany — [2]Institute of Theoretical Physics, Technische Universität Berlin, Germany — [3]Faculty of Fundamental Problems of Technology, Wrocław University of Technology, Poland — [4]Technische Physik, Universität Würzburg, Germany — [5]School of Physics and Astronomy, University of St. Andrews, UK

Resonant excitation of quantum systems offers the unprecedented possibility of coherent control important for both fundamental study and applications due to minimized dephasing and direct addressing of a chosen state, enabling observation of phenomena not accessible otherwise. We employed resonance fluorescence (RF) to study cavity quantum electrodynamics effects in strongly coupled quantum dot (QD) - micropillar system. An advanced 90 degree excitation/detection scheme as well as spatial filtering is employed to extract the signal. For large detunings between the exciton (X) and the cavity mode (CM) both direct RF and a cavity-mediated signal is monitored and provides direct insight into the X-CM coupling. Varying the excitation power on resonance enabled observation of co-existence of a strongly coupled X-CM system and a laser-driven uncoupled QD transition, this is supported by theory based on Fourier-transformed first-order autocorrelation functions including multi-photon scattering.

HL 48.7 Wed 11:45 H15

Auger-recombination in a single self-assembled quantum dot: Quenching and broadening of the charged exciton — •Annika Kurzmann[1], Arne Ludwig[2], Andreas D. Wieck[2], Axel Lorke[1], and Martin Geller[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, Lotharstraße 1, 47057 Duisburg, — [2]Chair for Applied Solid State Physics, Ruhr-Universität Bochum, Universitätsstraße 150, 44780 Bochum, Germany

The Auger-recombination is a non-radiative process, where the electron-hole recombination energy is transferred to a third charge carrier. While this process was extensively studied in colloidal quantum dots [1], it was considered, unimportant for self-assembled quantum dots (QDs). Here, we show that in a single self-assembled QD the Auger recombination rate can directly be determined using time-resolved resonance fluorescence (RF) measurements. Furthermore, the Auger recombination quenches and broadens the charged exciton transition (two electrons and one hole).

The QD is embedded in a field-effect transistor, and the tunneling rate from the charge reservoir into the dot is about $1/\mu$s. The measured Auger-recombination rate is of the same order of magnitude as this tunneling rate. This leads to an uncharged QD and a quenched RF signal. Our measurements show the relevance of the ratio between the Auger-recombination rate and the tunneling rate for the properties of the charged exciton transition. A model, based on rate equations, is in good agreement with our measurements.

[1] V. I. Klimov et al., Science **287**, 1011 (2000)

HL 49: Focus Session: Many-body effects in two-dimensional materials (Joint session of HL and O, organized by HL)

Organizers: Christopher Gies and Tim Wehling (Universität Bremen)

Time: Wednesday 9:30–13:00 Location: H16

Invited Talk HL 49.1 Wed 9:30 H16

Probing bandgap renormalization, excitonic effects, and in-

terlayer coupling in 2D transition metal dichalcogenide semiconductors — •Miguel M. Ugeda[1], Aaron Bradley[1], Sufei Shi[1], Felipe H. Jornada[1], Yi Zhang[2,3], Diana Qiu[1], Wei Ruan[1], Sebastian Wickenburg[1], Alexander Riss[1], Jiong Lu[1], Sung-Kwan Mo[2], Zahid Hussain[2], Zhi-Xun Shen[3], Feng Wang[1], Steven G. Louie[1], and Michael F. Crommie[1] — [1]Department of Physics, University of California, Berkeley, CA 94720, USA. — [2]Advanced Light Source, Lawrence Berkeley National Lab., Berkeley, CA 94720, USA. — [3]Stanford Institute for Materials and Energy Sciences, Menlo Park, CA 94025, USA.

Reduced screening in 2D metal dichalcogenides (TMDs) has been predicted to result in dramatically enhanced Coulomb interactions that should cause giant bandgap renormalization and excitonic effects. Here we present direct experimental observation of extraordinarily high exciton binding energy and band structure renormalization in a single-layer of semiconducting TMD[1]. We have determined the binding energy of correlated electron-hole excitations in monolayer MoSe2 grown via molecular beam epitaxy on bilayer graphene by using a combination of scanning tunneling spectroscopy and photoluminescence spectroscopy. We have also studied the role of interlayer coupling and layer-dependent carrier screening on the electronic structure[2] of few layer MoSe2. We find that the electronic quasiparticle bandgap decreases by nearly 1 eV when going from one layer to three. [1]Nature Materials 13, 1091 (2014). [2]Nano Letters 15, 2594 (2015).

HL 49.2 Wed 10:00 H16

A Tight Binding Approach to Strain and Curvature in Monolayer Transition-Metal Dichalcogenides — •Alexander Pearce and Guido Burkard — Department of Physics, University of Konstanz, D-78464 Konstanz, Germany

We present a model of the electronic properties of the monolayer transition-metal dichalcogenides based on a tight binding approach which includes the effects of strain and curvature of the crystal lattice. Mechanical deformations of the lattice offer a powerful route for tuning the electronic structure of the transition-metal dichalcogenides, as changes to bond lengths lead directly to corrections in the electronic Hamiltonian while curvature of the crystal lattice mixes the orbital structure of the electronic Bloch bands. We first present an effective low energy Hamiltonian describing the electronic properties near the K point in the Brillouin zone, then present the corrections to this Hamiltonian due to arbitrary mechanical deformations and curvature in a way which treats both effects on an equal footing. This analysis finds that local area variations of the lattice allow for tuning of the band gap and effective masses, where the application of uniaxial strain decreases the magnitude of the direct band gap at the K point. Additionally, strain induced bond length modifications create a fictitious gauge field but with a coupling that is smaller than seen in related materials like graphene. We also find curvature of the lattice leads to the appearance of both an effective in-plane magnetic field which couples to spin degrees of freedom and a Rashba-like spin-orbit coupling due to broken mirror inversion symmetry. (arXiv:1511.06254).

HL 49.3 Wed 10:15 H16

Observation of charge density wave order in 1D mirror twin boundaries of single-layer MoSe2 — •Sara Barja[1], Sebastian Wickenburg[1], Zhen-Fei Liu[1], Yi Zhang[1], Hyejin Ryu[1], Miguel M. Ugeda[2], Zahid Hussain[1], Zhi-Xun Shen[3], Sung-Kwan Mo[1], Miquel B. Salmeron[1,2], Feng Wang[1,2], Michael F. Crommie[1,2], D. Frank Ogletree[1], Jeffrey B. Neaton[1,2], and Alexander Weber-Bargioni[1] — [1]Lawrence Berkeley National Laboratory, Berkeley, CA, USA — [2]University of California at Berkeley, Berkeley, CA, USA — [3]Stanford Institute of Materials and Energy Sciences, SLAC National Accelerator Laboratory, Menlo Park, CA, USA

Detailed understanding of defect structure in 2D transition metal dichalcogenides may lead to control of the material properties. Here we provide direct evidence for the existence of isolated, 1D charge density waves (CDWs) at mirror twin boundaries (MTBs) in single-layer MoSe2. 4K-STM/STS measurements reveal a substantial bandgap of 60-140 meV opening at the Fermi level in the otherwise one dimensional metallic structure. We find an energy-dependent periodic modulation in the density of states along the MTB, with a wavelength of approximately three lattice constants. The modulations in the density of states above and below the Fermi level are spatially out of phase, consistent with CDW order. In addition to the electronic characterization, we determine the atomic structure and bonding configuration of the 1D MTB by means of high-resolution nc-AFM. DFT calculations reproduce both the gap opening and the modulations of the density of states.

HL 49.4 Wed 10:30 H16

Probing the anisotropic interlayer Raman modes of few-layer ReS_2 — •Philipp Nagler, Gerd Plechinger, Christian Schüller, and Tobias Korn — Institut für Experimentelle und Angewandte Physik, Universität Regensburg, 93040, Regensburg, Germany

ReS_2 has recently emerged as a new member in the rapidly expanding family of two-dimensional materials. Unlike MoS_2 or WSe_2, the optical and electrical properties of ReS_2 are not isotropic due to the reduced symmetry of the crystal. Here, we probe the anisotropic behavior of ReS_2 by Raman spectroscopy in the ultralow frequency regime. Thereby, we are able to access the layer breathing modes (LBM) and shear modes (LSM) of the material which stem from rigid-layer oscillations. The layer dependence of their peak positions enables an easy determination of the layer number of the crystal and can be readily reproduced by means of a monoatomic chain model. By varying the angle between the linearly polarized laser and the in-plane crystal axis, we are able to reveal an energetic shift of the LSM which is directly linked to the in-plane anisotropy of the shear modulus in this material.

30 min. Coffee Break

Invited Talk HL 49.5 Wed 11:15 H16

Enhanced light-matter coupling and single-photon emission of atomically thin semiconductors — •Rudolf Bratschitsch — Westfälische Wilhelms-Universität Münster, Münster, Deutschland

Graphene is known as a prototypical two-dimensional material with unique physical properties. However, the difficulty of creating an optical band gap stimulated the search for other monolayer materials. In my talk I will show that atomically thin transition metal dichalcogenides serve as a promising new material class for opto-electronics and quantum optics [1-3]. In particular, I will explain, how gold nanoantennas may be used to increase the light-monolayer coupling and present single-photon emission from localized excitons in monolayer WSe2.

[1] P. Tonndorf et al., Optics Express 21, 4908 (2013)
[2] J. Kern et al., ACS Photonics 2, 1260 (2015)
[3] P. Tonndorf et al., Optica 2, 347 (2015)

Invited Talk HL 49.6 Wed 11:45 H16

Optical Properties and Carrier Dynamics in Transition Metal Dichalcogenides — •Alexander Steinhoff-List[1], Malte Rösner[1,2], Matthias Florian[1], Michael Lorke[1], Christopher Gies[1], Ji-Hee Kim[3], Deok-Soo Kim[4], Chanwoo Lee[4], Gang Hee Han[3], Mun Seok Jeong[3,4], Tim Wehling[1,2], and Frank Jahnke[1] — [1]Institut für Theoretische Physik, Universität Bremen, P.O. Box 330 440, 28334 Bremen, Germany — [2]Bremen Center for Computational Materials Science, Universität Bremen, 28334 Bremen, Germany — [3]Center for Integrated Nanostructure Physics, Institute for Basic Science, Suwon 440-746, Republic of Korea — [4]Department of Energy Science, Sungkyunkwan University, Suwon 440-746, Republic of Korea

As two-dimensional transition metal dichalcogenides are promising candidates for optoelectronic applications, there is a strong interest in understanding the influence of excited carriers in these materials on optical properties. We present studies of absorption and photoluminescence spectra of monolayer MoS_2 in the presence of excited carriers as well as carrier kinetics, based on material-realistic ab-initio band structures and interaction matrix elements. It is shown that absorption spectra are strongly modified due to band-gap renormalization and screening effects, while the photoluminescence signal can be distinctly influenced by optical excitation above or below the electronic band gap. Moreover, we present results for carrier-carrier Coulomb and carrier-phonon scattering after optical excitation of the monolayer, exhibiting ultra-fast carrier relaxation on the sub-100 fs time scale.

HL 49.7 Wed 12:15 H16

Microscopic modeling of the homogeneous linewidth in absorption spectra of TMDs — •Malte Selig[1], Gunnar Berghäuser[2], Ermin Malic[2], and Andreas Knorr[1] — [1]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Chalmers University of Technology, Department of Physics, SE-412 96 Gothenburg, Sweden

Monolayer transition metal dichalcogenides (TMDs) are direct-gap

semiconductors with strong light-matter and Coulomb interaction. The latter accounts for strongly bound excitons, which dominate the optical spectrum. Here, we investigate the homogeneous linewidth in excitonic spectra induced by radiative coupling and exciton-phonon scattering. In conventional semiconductors, the radiative dephasing / recombination is typically weak in comparison to the electron-phonon scattering which mainly determines the homogeneous linewidth. The situation turns out to be different in atomically thin TMDs. Based on the density matrix formalism combined with the tight-binding approximation, we explicitly calculate the dephasing rates stemming from exciton-radiation interaction and exciton-phonon scattering. We find that in TMDs the radiative coupling is in the range of 1 meV clearly exceeding the exciton-phonon rate. We systematically investigate the resulting homogenous linewidth in absorption spectra of the most prominent TMDs for different temperatures, dopings, and substrates. [1]

[1] Galan Moody et al. Nat Commun 6, 8315 (2015)

HL 49.8 Wed 12:30 H16

Influence of the spin-orbit splitting on the coupled spin-valley-dynamics in monolayer transition metal dichalcogenides — •Gerd Plechinger, Philipp Nagler, Sven Gelfert, Christian Schüller, and Tobias Korn — Institut für Experimentelle und Angewandte Physik, Universität Regensburg, D-93040 Regensburg

Single layers of transition metal dichalcogenides (TMDCs) like MoS_2 and WS_2 can be produced by simple mechanical exfoliation. Offering a direct bandgap at the K-points in the Brillouin zone, they represent promising semiconductor materials for flexible and transparent optoelectronic applications. Due to inversion symmetry breaking together with strong spin-orbit-interaction, the valley and spin degrees of freedom are coupled in monolayer TMDCs. Via circularly polarized optical excitation, an efficient polarization of the K^+ or the K^- valley can be generated. Here, we investigate the dynamics of these coupled spin-valley polarizations in monolayer MoS_2 and WS_2 by means of photoluminescence spectroscopy and time-resolved Kerr rotation (TRKR). The results indicate a maximum achievable spin-valley-lifetime in these materials exceeding one nanosecond at low temperatures. Furthermore, we extract the dependence of the spin-valley lifetime on temperature. By varying the excitation energy, we reveal the excitonic resonances as well as the spin-polarized bandstructure around the K valleys common to monolayer TMDCs.

HL 49.9 Wed 12:45 H16

Ultrafast Coulomb-induced intervalley coupling in atomically thin WS_2 — Robert Schmidt[1], •Gunnar Berghäuser[2], Malte Selig[3], Philipp Tonndorf[1], Ermin Malic[2], Andreas Knorr[3], Steffen Michaelis de Vasconcellos[1], and Rudolf Bratschitsch[1] — [1]Institute of Physics and Center for Nanotechnology, University of Münser, Münster Germany — [2]Chalmers University of Technology, Department of Physics, SE-412 96 Gothenburg, Sweden — [3]Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, TU Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Monolayers of semiconducting transition metal dichalcogenides hold the promise for a new paradigm in electronics by exploiting the valley degree of freedom in addition to charge and spin. For these materials valley polarization can be conveniently initialized and read out by circularly polarized light. However, the underlying microscopic processes governing the valley polarization in these atomically thin equivalents of graphene are still not fully understood. Here, we present a theoretical study on the ultrafast time-resolved intervalley dynamics in monolayer WS_2 [1]. Based on a microscopic theory, we reveal the many-particle mechanisms behind the observed spectral features. We show that Coulomb-induced intervalley coupling explains the immediate and prominent pump-probe signal in the unpumped valley as well as the seemingly low valley polarization degrees typically observed in pump-probe measurements if compared to photoluminescence studies.

[1] R. Schmidt et al, submitted (2015)

HL 50: Gallium Nitride: Fabrication and Characterization

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

HL 50.1 Wed 9:30 H17

Molecular beam epitaxy and characterization of InGaN nanowires on Si (111) — •Saskia Weiszer, Andreas Zeidler, Maximilian Kolhep, and Martin Stutzmann — Walter Schottky Institut and Physics Department, Technische Universität München, Am Coulombwall 4, 85748 Garching, Germany

Multi-junction solar cells have received wide attention as each cell can absorb different wavelengths of the solar spectrum which leads to an increased energy conversion efficiency. InGaN has a variable band gap from 0.7 to 3.4eV that covers nearly the whole solar spectrum. Combined with Si, theoretical considerations show that an InGaN/Si tandem solar cell could be an optimal implementation of a double-junction cell. Especially at an In content of 46%, it is expected that a resonant tunnel junction is formed between both cells. Furthermore, the cell efficiency could be increased by growing nanowires to enhance optical properties and to reduce structural defects, since the lattice mismatch strain can relax through the nanowire sidewalls. As first step towards such an InGaN/Si solar cell, the growth of high quality InN nanowires directly on Si(111) substrates by molecular beam epitaxy was studied. By varying the applied growth parameters, namely substrate temperature and III/V-ratio, different growth regimes were identified and the InN nanowire growth was optimized. As next step towards an InGaN/Si solar cell, the growth of InGaN nanowires with increasing Ga content was investigated. Recent results on the determination of the Ga content by energy dispersive X-ray spectroscopy, Raman spectroscopy and photoluminescence measurements will be presented.

HL 50.2 Wed 9:45 H17

RF sputter deposition of AlN layers on different substrates — •Florian Hörich, Marc Hoffmann, Jürgen Bläsing, Armin Dadgar, and Andre Stritmatter — Otto-von-Guericke-University Magdeburg

We investigated reactive sputtering of AlN by rf-plasma deposition using an Al-Target and varying plasma conditions. The influence of substrate temperature, gas mixture, plasma pressure and magnetron power is discussed for different substrates, like Silicon (111), sapphire, and epitaxially-grown AlN buffer layers on Silicon (111).

The growth of crystalline or amorphous layers depends mostly on the substrate type. Direct growth on Si(111) substrates results in crystalline layers if an Al nucleation layer is used similar to metalorganic vapour phase epitaxy of AlN/Si(111). Epitaxially grown AlN buffer layers can be overgrown without an Al interlayer.

Further analysis performed by high resolution x-ray diffraction (HRXRD) and atomic force microscopy (AFM) will be presented for qualification of the crystalline quality and surface morphology. In particular, the substrate-layer interface is investigated to understand the nucleation processes of the sputtered AlN layers in dependence of process parameters.

HL 50.3 Wed 10:00 H17

Growth of GaN nanowires on crystalline TiN films by molecular beam epitaxy — •David van Treeck, Gabriele Calabrese, Carsten Pfüller, Oliver Brandt, Lutz Geelhaar, and Sergio Fernández-Garrido — Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5–7, 10117 Berlin, Germany

The pronounced tendency of GaN to spontaneously form nanowires (NWs) on many different materials has recently been employed to fabricate GaN NW ensembles on a wide variety of substrates, ranging from amorphous dielectrics to crystalline metals. The use of metallic substrates is particularly appealing for applications because of their excellent electrical and thermal conductivity as well as their high optical reflectivity. We have recently demonstrated the growth of GaN NWs on crystalline TiN films by plasma-assisted molecular beam epitaxy [M. Wölz, et al. Nano Lett. 15, 3743 (2015)]. Here, we study the underlying growth mechanisms in detail. Our substrates consist of a Ti layer sputtered on Al2O3(0001). It is shown that the thickness of the Ti layer has a strong influence on the properties of the resulting NW ensembles. We have also investigated the formation of TiN under different conditions and the impact of the resulting TiN microstructure on the subsequent formation of GaN NWs. The combination of in situ and ex situ analytical tools allowed us to elucidate the nucleation

and growth mechanisms resulting in the formation of long (>1 μm), uncoalesced, and single crystalline GaN NWs. We have found these NWs to be N-polar, and to exhibit a tilt and a comparatively small twist of 2.4° and 0.8°, respectively.

HL 50.4 Wed 10:15 H17

Germanium doping of cubic GaN — •Michael Deppe[1], Jürgen W. Gerlach[2], Dirk Reuter[1], and Donat J. As[1] — [1]Universität Paderborn, Department Physik, Warburger Straße 100, 33098 Paderborn — [2]Leibniz-Institut für Oberflächenmodifizierung e.V., Permoserstraße 15, 04318 Leipzig

Up to now the most commonly used n-type dopant for cubic GaN is silicon. We present a study of germanium as an alternative n-type dopant. The germanium doped cubic GaN films were grown on 3C-SiC/Si (001) substrates by plasma-assisted molecular beam epitaxy. The incorporation of germanium into the GaN films could be verified using secondary ion mass spectrometry (SIMS) and Hall effect measurements revealed the electrical properties of the samples. Films with doping densities above $3 \cdot 10^{18}$ cm^{-3} exhibit n-type conductivity whereas films with lower doping densities are p-type due to electrically active dislocations. A maximum electron concentration of $3.7 \cdot 10^{20}$ cm^{-3} was achieved. From a comparison of SIMS and Hall effect measurements we conclude that in the highest doped sample not all incorporated dopants are electrically active. For doping densities in the order of 10^{19} cm^{-3} and above, a degradation of the crystal quality was observed by high resolution x-ray diffraction (HRXRD). Furthermore, a comparison to silicon doped films reveals no significant differences.

HL 50.5 Wed 10:30 H17

Manipulation of indium incorporation by anisotropic strain in non- and semipolar GaInN/GaN multi quantum well structures — •P. Horenburg[1], U. Rossow[1], R. Buss[1], F. A. Ketzer[1], H. Bremers[1], F. Tendille[2], P. De Mierry[2], P. Vennéguès[2], J. Zuniga-Perez[2], and A. Hangleiter[1] — [1]Institute of Applied Physics, TU Braunschweig, Germany — [2]Centre de Recherche sur l'Hétéro-Epitaxie, Valbonne, France

We demonstrate the effect of anisotropic strain on the In incorporation efficiency in m-plane and (11$\bar{2}$2)-oriented GaInN/GaN multi quantum well (MQW) structures. Inserting a partially relaxed AlInN buffer layer enables manipulation of the strain state in the MQW grown on top. One-dimensional lattice-matching of this AlInN layer to the underlying GaN epilayer induces partial strain relaxation along the perpendicular in-plane direction of the growth surface. This leads to modified lattice constants of the template for the MQW grown subsequently. All samples are grown via low pressure metalorganic vapour phase epitaxy on (11$\bar{2}$2) GaN templates on patterned r-sapphire or commercial m-oriented pseudo-bulk substrates. From structural and optical characterization by X-ray diffraction and photoluminescence measurements, we deduce an impact on the In incorporation efficiency and In concentrations in the quantum wells (QW) up to $x = 40\%$ (semipolar) and $x = 38\%$ (nonpolar) without additional strain energy being accumulated in the QW region. Taking into consideration the reduced quantum-confined Stark effect in such structures, this approach is very encouraging in search for efficient green light-emitting devices.

HL 50.6 Wed 10:45 H17

Epitaxieentwicklung AlN/GaN HEMTs für die Leistungselektronik bei hohen Frequenzen — •Birte-Julia Godejohann, Stefan Müller, Lutz Kirste, Steffen Breuer, Rolf Aidam, Klaus Köhler und Oliver Ambacher — Fraunhofer IAF Tullastraße 72 79180 Freiburg

GaN-Leistungsverstärker ermöglichen im Vergleich zu konventionellen Materialsystemen (GaAs, Si) bei gleichen Betriebsfrequenzen deutlich höhere Leistungsdichten. Dies lässt sich auf die Materialeigenschaften wie hohe Durchbruchfestigkeit, Elektronengeschwindigkeit, Schichtladungsträgerdichten und große Bandlücken der Gruppe III Nitride zurückführen. Um High Electron Mobility Transistoren (HEMT) mit hohen Cut-off Frequenzen realisieren zu können, sind kleine Gatelänge, geringer Kanal-Gate-Abstand sowie eine ausreichend hohe Schichtladungsträgerdichte erforderlich. Hierfür bieten sich im III-Nitrid System grundsätzlich zwei Möglichkeiten an, das gitterangepasste und das verspannte Wachstum einer hoch Al-haltigen Barriere auf GaN; auf das verspannte Wachstum soll hier genauer eingegangen werden. AlN/GaN HEMTs mit variierten Barriere- und Capdicken wurden simuliert und mittels Molekularstrahlepitaxie (MBE) hergestellt um die Schichtladungsträgerdichten beeinflussen zu können. Die elektrische Charakterisierung der Schichten hat Schichtladungsträgerdichten von 7E12 bis zu 3,3E13 cm-2 und Beweglichkeiten von 1040 bis 1580 cm2/Vs ergeben. Entsprechende Strukturen wurden mittels metallorganischer Gasphasenepitaxie (MOCVD) hergestellt und bezüglich ihrer Materialeigenschaften mit den MBE gezüchteten Proben verglichen.

30 min. Coffee Break

HL 50.7 Wed 11:30 H17

MOVPE growth and characterization of GaN based tunnel junctions employing highly Ge-doped GaN — •Silvio Neugebauer, Aqdas Fariza, Marc Hoffmann, Gordon Schmidt, Hartmut Witte, Jürgen Bläsing, Frank Bertram, Armin Dadgar, Jürgen Christen, and André Strittmatter — Institute of Experimental Physics, Otto-von- Guericke-University Magdeburg, Germany

GaN-based p-n tunnel junctions (TJs) are effective means to improve lateral current spreading in surface emitting light-emitting diodes and lasers. Owing to the large bandgap of GaN and the limited achievable acceptor and donor concentration by Mg and Si doping, respectively, the realization of effective TJs by metalorganic vapor phase epitaxy (MOVPE) is challenging. Ultra-high donor concentrations in MOVPE-grown GaN have been recently demonstrated by Ge doping. In this study, we have successfully used different growth sequences to prepare GaN-based TJs. In particular, the growth sequence at the transition from highly p-doped to highly n-doped material is critical for achieving a sufficient tunneling probability. Furthermore, the activation process for the Mg-doped GaN layer has to be optimized. We will compare thermal annealing schemes on mesa structures and unprocessed TJ structures as well as electron beam irradiation for its effective acceptor activation. First results on LED devices will also be presented and the mechanism responsible for the tunneling process will be discussed.

HL 50.8 Wed 11:45 H17

Evaluation and comparison of the intrinsic electric field of semipolar and polar InGaN/GaN QW structures — •Martina Dombrowski, Jan Wagner, Michael Jetter, and Peter Michael — Institut für Halbleiteroptik und Funktionelle Grenzflächen and Research Centers SCoPE and IQST, Universität Stuttgart, Allmandring 3, 70569 Stuttgart, Germany

One of the most promising material systems for green light emitting devices is InGaN/GaN. And still, one of the main issues to achieve high efficiency for light emitting devices is the appearance of piezoelectric fields in the active region. These lead to a tilt in the band structure and therefore to a reduced recombination efficiency. To overcome the effect of this so-called quantum confined Stark effect (QCSE), the active region can be grown on semipolar or nonpolar planes. In this work, we fabricated three-dimensional GaN pyramids by the selective area growth (SAG) method and used their side facets as semipolar GaN templates. To compare the effect of the reduced QCSE, semipolar and c-plane quantum wells (QW) were grown with different thicknesses emitting at the same spectral position. To evaluate the carrier dynamics, recombination efficiency and the strength of the electric field for both semipolar and polar QWs, optical characterizations by time-resolved photoluminescence were performed on these samples.

HL 50.9 Wed 12:00 H17

Capacitance Voltage Spectroscopy of GaN Quantum Dot Ensembles — •Carlo Alberto Sgroi[1], Julien Brault[2], Arne Ludwig[1], and Andreas D. Wieck[1] — [1]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, 44780 Bochum, Germany — [2]CNRS CRHEA, 06560 Valbonne, France

We present a capacitance voltage (CV) measurement of wurtzite GaN quantum dots (QDs) in an $Al_xGa_{1-x}N$ matrix grown by MBE.

GaN and its alloys have excellent properties regarding thermal stability at ambient conditions, high thermal conductivity and wide bandgap energies, thus making it an ideal candidate for high power and high temperature microelectronic and QD devices.

Due to polarization effects in wurtzite GaN/$Al_xGa_{1-x}N$ heterostructure layers induced intrinsically by inversion asymmetry and extrinsically by doping and strain, the band structure is deformed. Band structure simulations were run to calculate a decent tunneling barrier and estimate the quantum dot minimum to be close to the Fermi energy level with a sufficient lever arm to fill and deplete the QDs.

We used the known CV spectroscopy technique adapted to the GaN properties and measured the convoluted s- and p-states of the QDs at room temperature. The coulomb blockade energy is calculated to be

48.81 meV and the s- to p-energy difference is 126.26 meV.

HL 50.10 Wed 12:15 H17

Determination of polarization fields in InAlN/GaN heterostructures by capacitance-voltage-measurements — •Baran Avinc[1], Monir Rychetsky[1], Konrad Bellman[1], Ingrid Koslow[1], Tim Wernicke[1], Michael Narodovitch[1], Michael Lehmann[1], Silvio Neugebauer[2], Andre Strittmatter[2], Bernd Witzigmann[3], and Michael Kneissl[1] — [1]Technische Universität Berlin, Institut für Festkörperphysik, Berlin, Germany — [2]Otto von Guericke University Magdeburg, Institute of Experimental Physics, Magdeburg, Germany — [3]University of Kassel, Computational Electronics and Photonics Group and CINSat, Kassel, Germany

Lattice-matched InAlN/GaN heterostructures exhibit strong spontaneous polarization fields and sheet charges resulting in band bending. In the literature very few publications exist about the exact field strength values for this material system. In this contribution a new approach to determine polarization fields in nearly lattice-matched InAlN/GaN heterostructures based on capacitance-voltage measurements is used. The change of the polarization fields at the heterointerface influences the charge distribution in a PIN junction and consequently the capacitance. In order to enhance the accuracy of the method we compare the depletion width of two PIN junctions: one with an embedded InAlN layer and therefore influenced by the internal polarization fields, and one without it. The results show an internal field strength of 5.5 MV/cm +/- 1.1 MV/cm for a nearly lattice-matched (nearly 18 % In content) InAlN double heterostructure, in good agreement with theoretically predicted values.

HL 50.11 Wed 12:30 H17

Modulation spectroscopy of semipolar InGaN/GaN light emitting diodes — •Stefan Freytag[1], Monir Rychetsky[2], Tim Wernicke[2], Ingrid Koslow[2], Duc V. Dinh[3], Brian Corbett[3], Peter J. Parbrook[3], Martin Feneberg[1], Rüdiger Goldhahn[1], and Michael Kneissl[2] — [1]Institut für Experimentelle Physik, Otto-von-Guericke-Universität, Magdeburg, Germany — [2]Institut für Festkörperphysik, Technische Universität, Berlin, Germany — [3]Tyndall National Institute, University College Cork, Cork, Ireland

Semipolar InGaN/GaN light emitting diodes containing three InGaN quantum well (QWs) were grown on $(20\bar{2}1)$ and $(20\bar{2}\bar{1})$ oriented bulk GaN substrates. The indium content of the QWs was varied between 0.13 and 0.24. Modulation spectroscopy measurements at variable temperatures are employed to investigate electro-optic properties of the devices. By photoreflection we observe free excitons in the GaN matrix and find a very prominent signal from the InGaN quantum wells. The energy position as a function of temperature is compared to photoluminescence data. In polarization dependend measurements we clearly observe a shift of the characteristic quantum well transition energy for different polarization angles attributed to the selection rules of the corresponding valence bands. Excitation density dependent photoluminescence and photoreflection measurements support this explanation. The studies contribute to the understanding of the valence band structure and the quantification of the polarization fields in semipolar InGaN/GaN multi quantum well structures.

HL 50.12 Wed 12:45 H17

Structural characterization and scanning surface potential microscopy (SSPM) of C-doped GaN layers on Sapphire — •Aqdas Fariza, Hartmut Witte, Andreas Lesnik, Jürgen Bläsing, Peter Veit, Armin Dadgar, and Andre Strittmatter — Institute of Experimental Physics, Otto von Guericke University Magdeburg, Magdeburg, Germany

We have compared undoped and C-doped GaN samples with a focus on electrical properties of the material in the vicinity of dislocations. Photoluminescence measurements showed an increase of blue and yellow band emission intensities with increasing carbon concentrations which points to an enhanced incorporation of deep defects. Dislocation densities are estimated from tilt and twist x-ray measurements using omega-scans for the (0002) reflection and grazing incidence in-plane geometry for the (10-10) reflection. Values of skew and edge type dislocation densities are obtained in the range of 10^8 cm^{-2} and 10^9 cm^{-2}, respectively, independent of the carbon content. The type of dislocations in the GaN layer is determined from TEM images. The surface topography and electronic charge state of dislocations are explored by performing atomic force microscopy and scanning surface potential measurements in tapping mode. The charging state of dislocations in unintentionally doped samples is either neutral or negative whereas positively charged surface depressions are also found in highly carbon doped samples.

HL 50.13 Wed 13:00 H17

Investigation of AlInN/GaN heterostructures by scanning tunneling and transmission electron microscopy — •Verena Portz[1], Jean-François Carlin[2], Raphaël Butté[2], Nicolas Grandjean[2], Rafal Dunin-Borkowski[1], and Philipp Ebert[1] — [1]Peter Grünberg Institut, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [2]Institute of Condensed Matter Physics, École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

Ternary III-V semiconductors are of increasing interest for optoelectronic devices. One of the most promising alloys is $Al_{1-x}In_xN$, since it's band gap can be tuned from nearly 0.67 eV to 6.2 eV. Due to the high contrast of the refractive index, alternating layers of GaN and $Al_{1-x}In_xN$ are also commonly used in distributed Bragg reflectors (DBRs) for laser diodes. In these devices, the indium content is tuned to minimize lattice mismatch. Our investigations by scanning tunneling and transmission electron microscopy show that even in $Al_{1-x}In_xN$ layers, nominally lattice matched to GaN, compositional fluctuations can lead to stress and strain. The different strain and compositional effects are discussed.

HL 51: Transport: Graphene (Joint session of DS, DY, HL, MA, O and TT, organized by TT)

Time: Wednesday 9:30–13:15 Location: H22

Invited Talk HL 51.1 Wed 9:30 H22

Ultrafast photo-thermoelectric currents in graphene — •Alexander Holleitner — Walter Schottky Institut and Physics Department, Technical University of Munich, Am Coulombwall 4a, D-85748 Garching, Germany.

We show that photo-thermoelectric currents occur on a picosecond time-scale in graphene [1]. To this end, we apply an on-chip pump/probe photocurrent spectroscopy [2,3] to double-gated junctions of graphene. Our experiments reveal the interplay of photogenerated hot electrons with so-called photovoltaic currents. Moreover, we demonstrate that hot electrons allow to read-out an ultrafast non-radiative energy transfer from fluorescent emitters, namely nitrogen-vacancy centers in nano-diamonds. The non-radiative energy transfer can be exploited as an ultrafast, electronic read-out process of the electron spin in nitrogen vacancy centers in the diamond nanocrystals. The detection gives access to fast energy transfer processes, which have not yet been observed by fluorescence measurements because of quenching of the optical signal for short transfer distances [4].

We thank A. Brenneis, F. Schade, L. Gaudreau, M. Seifert, H. Karl, M.S. Brandt, H. Huebl, J.A. Garrido, F.H.L. Koppens, for a very fruitful collaboration, and the ERC-grant 'NanoREAL' for financial support.

[1] A. Brenneis et al., (2016)
[2] L. Prechtel et al., Nature Comm. **3**, 646 (2012)
[3] C. Kastl et al. Nature Comm. **6**, 6617 (2015)
[4] A. Brenneis et al. Nature Nanotech. **10**, 135 (2015)

HL 51.2 Wed 10:00 H22

Double-logarithmic velocity renormalization at the Dirac points of graphene — •Peter Kopietz, Anand Sharma, and Carsten Bauer — Institut für Theoretische Physik, Universität Frankfurt, Max-von-Laue Str. 1, 60438 Frankfurt

Using a functional renormalization group approach with partial bosonization in the forward scattering channel we reconsider the effect of long-range Coulomb interactions on the quasi-particle velocity v_k close to the Dirac points of graphene. In contrast to calculations based on perturbation theory and field theoretical renormalization group methods, we find that v_k is proportional to $\ln[\kappa_k/k]$ where k is the deviation of the quasiparticle momentum from the Dirac points

and the cutoff scale κ_k vanishes logarithmically for small k. We show that this double-logarithmic singularity is compatible with experiments and with the known three-loop expansion of v_k which contains terms of order $\ln k$ and $\ln^2 k$.

HL 51.3 Wed 10:15 H22

Dirac fermion wave packets in oscillating potential barriers — Walter Pötz[1], Sergey E. Savel'ev[2], Peter Hänggi[3], and •Wolfgang Häusler[3] — [1]Karl Franzens Univ. Graz, Inst. Phys., A-8010 Graz, Austria — [2]Department of Physics, Loughborough University, Loughborough LE11 3TU, United Kingdom — [3]Institut für Physik, Univ. Augsburg, 86135 Augsburg, Germany

We integrate the time-dependent (2+1)D Dirac equation for massless fermions in graphene or topological insulator surfaces. A recently developed staggered-grid leap-frog scheme is employed [1,2]. We consider an initial Gaussian wave packet which moves in the x-direction towards a potential barrier that is homogeneous along y and oscillates periodically in time. As for the x-dependence, we investigate square-well, sinusoidal, and linear-ramp potential profiles. Small transversal momentum components k_y of the wave packet were analyzed analytically [3] and predicted to generate non-zero current densities j_y, even at normal incidence $k_y = 0$ [4]. These findings are consistent with the present numerical studies of particle-, current-, and spin-density. We also investigate massive fermions: regarding some properties they resemble massless fermions, regarding other properties, however, peculiar intrinsic oscillations, reminiscent of Zitterbewegung, appear.

[1] R. Hammer and W. Pötz, PRB **88**, 235119 (2013)
[2] R. Hammer *et al.*, J. Comp. Phys. **265**, 50 – 70 (2014)
[3] S.E. Savel'ev, W. Häusler, and P. Hänggi, PRL **109**, 226602 (2012)
[4] S.E. Savel'ev, W. Häusler, and P. Hänggi, EPJB **86**, 433 (2013).

HL 51.4 Wed 10:30 H22

Electric and magnetic control of electron guiding in graphene — •Ming-Hao Liu and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg

Electrons in graphene are known to behave like massless Dirac fermions, whose transport properties can be best revealed by experiments using ultra-clean graphene. Reliable quantum transport simulations for ballistic graphene is naturally a powerful tool for understanding and predicting high-quality transport experiments. In this talk we show gate-controlled electron guiding along electrically confined channels in suspended graphene, which is a combined work of our transport simulations and the experiment done by the Schönenberger group [1]. We have recently further applied our simulation (Green's function method within the scalable tight-binding model [2]) to revisit the transverse magnetic focusing experiment [3], where the guiding of the electrons is controlled by an external magnetic field, instead of electrical gates. Besides good agreement with the experiments [1,3], our simulations further allow for probing charge flow through an additional scanning probe tip.

[1] P. Rickhaus *et al.*, Nano Lett. **15**, 5819 (2015).
[2] M.-H. Liu *et al.*, Phys. Rev. Lett. **114**, 036601 (2015).
[3] T. Taychatanapat *et al.*, Nat. Phys. **9**, 225 (2013).

HL 51.5 Wed 10:45 H22

Current flow paths in deformed graphene: from quantum transport to classical trajectories in curved space — •Nikodem Szpak[1] and Thomas Stegmann[1,2] — [1]Fakultät für Physik, Universität Duisburg-Essen, Duisburg — [2]Instituto de Ciencias Fisicas, Universidad Nacional Autonoma de Mexico, Cuernavaca

We compare two contrasting approaches to the electronic transport in deformed graphene: a) the condensed matter approach in which current flow paths are obtained by applying the non-equilibrium Green's function (NEGF) method to the tight-binding model with local strain, b) the general relativistic approach in which classical trajectories of relativistic point particles moving in a curved surface with a pseudo-magnetic field are calculated. The connection between the two is established in the long-wave limit via an effective Dirac Hamiltonian in curved space. Geometrical optics approximation, applied to focused current beams, allows us to directly compare the wave and the particle pictures. We obtain very good numerical agreement between the quantum and the classical approaches for a fairly wide set of parameters. The presented method offers an enormous reduction of complexity from irregular tight-binding Hamiltonians defined on large lattices to geometric language for curved continuous surfaces. It facilitates a comfortable and efficient tool for predicting electronic transport properties in graphene nanostructures with complicated geometries, paving the way to new interesting transport phenomena such as bending or focusing (lensing) of currents depending on the shape of the deformation. It can be applied in designing ultrasensitive sensors or in nanoelectronics.

HL 51.6 Wed 11:00 H22

Trigonal Warping in Bilayer Graphene: Energy versus Entanglement Spectrum — •Sonja Predin, Paul Wenk, and John Schliemann — Institute for Theoretical Physics, University of Regensburg, D-93040 Regensburg, Germany

We present a mainly analytical study of the entanglement spectrum of Bernal-stacked graphene bilayers in the presence of trigonal warping in the energy spectrum. Upon tracing out one layer, the entanglement spectrum shows qualitative geometric differences to the energy spectrum of a graphene monolayer. However, topological quantities such as Berry phase type contributions to Chern numbers agree. The latter analysis involves not only the eigenvalues of the entanglement Hamiltonian but also its eigenvectors. We also discuss the entanglement spectra resulting from tracing out other sublattices.

15 min. break

HL 51.7 Wed 11:30 H22

Valley-based Cooper pair splitting via topologically confined channels in bilayer graphene — •Alexander Schroer[1], Peter G. Silvestrov[1], and Patrik Recher[1,2] — [1]Institut für Mathematische Physik, Technische Universität Braunschweig, D-38106 Braunschweig, Germany — [2]Laboratory for Emerging Nanometrology Braunschweig, D-38106 Braunschweig, Germany

Bilayer graphene hosts valley-chiral one-dimensional modes at domain walls between regions of different interlayer potential or stacking order. When such a channel is close to a superconductor, the two electrons of a Cooper pair, which tunnel into it, move in opposite directions because they belong to different valleys related by the time-reversal symmetry. This kinetic variant of Cooper pair splitting requires neither Coulomb repulsion nor energy filtering but is enforced by the robustness of the valley isospin in the absence of atomic-scale defects. We derive an effective normal/superconducting/normal (NSN) model of the channel in proximity to an s-wave superconductor, calculate the conductance of split and spin-entangled pairs, and interpret it as a result of *local* Andreev reflection, in contrast to the widespread identification of Cooper pair splitting with crossed Andreev reflection in an NSN geometry.

HL 51.8 Wed 11:45 H22

The decisive role of stacking faults for understanding transport in bilayer graphene — •Heiko B. Weber[1], Ferdinand Kisslinger[1], Christian Ott[1], and Sam Shallcross[2] — [1]Lehrstuhl für Angewandte Physik, FAU Erlangen-Nürnberg (FAU), Erlangen, Germany — [2]Lehrstuhl für Theoretische Festkörperphysik, FAU Erlangen-Nürnberg (FAU)

Charge transport in bilayer graphene provides rich low-temperature phenomena, often assigned to interaction-driven phase transitions. We will discuss charge transport in bilayer graphene in a single-particle picture, but including stacking faults. Such partial dislocations are unavoidable in bilayer graphene and were recently imaged [1]. Depending on details, partial dislocations can introduce improved conductance, fully insulating behaviour or linear magnetoresistance. The latter is reliably found in transport experiments at elevated temperatures [2].

[1] B. Butz, C. Dolle, F. Niekiel, K. Weber, D. Waldmann, H. B. Weber, B. Meyer, E. Spiecker, Nature **505**, 533 (2014)
[2] F. Kisslinger, C. Ott, C. Heide, E. Kampert, B. Butz, E. Spiecker, S. Shallcross, H. B. Weber, Nature Phys. **11**, 650 (2015).

HL 51.9 Wed 12:00 H22

Linear magnetoresistance in two-dimensional disordered conductors — •Ferdinand Kisslinger[1], Christian Ott[1], Erik Kampert[2], and Heiko B. Weber[1] — [1]Lehrstuhl für Angewandte Physik, FAU Erlangen-Nürnberg (FAU), Erlangen, Germany. — [2]Dresden High Magnetic Field Laboratory, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany.

The recent observation of linear magnetoresistance (MR) in large-area bilayer graphene gives a key to the understanding of this old and barely understood phenomenon [1]. In bilayer graphene, it can be traced back to mosaic-like pattern of a partial dislocation network [2]. In this talk we discuss how linear MR evolves in disordered samples, using a two dimensional resistor network model conceptually introduced by Parish

and Littlewood [3]. This model is in the weak disorder regime dominated by boundary effects. We identified a new regime representing the bulk situation in a disordered conductor. We investigated different possible sources of disorder: mobility, charge carrier density and network structure. The slope of the MR turned out to be simply governed by the Hall resistance and therefore by the inverse of the charge carrier density. An equivalent circuit model finally gives a consistent explanation as to why the magnetoresistance is linear in mosaic like samples.

[1] F. Kisslinger et al., Nature Physics **11**, 650 (2015)
[2] B. Butz et al., Nature **505**, 533 (2014).
[3] M. M. Parish & P. B. Littlewood, Nature **426**, 162 (2003)

HL 51.10 Wed 12:15 H22

Mechanically strained graphene nanojunctions — •Seddigheh Nikipar[1], Dmitry Ryndyk[1], and Gianaurelio Cuniberti[1,2] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, Germany — [2]Dresden Center for Computational Materials Science (DCMS), TU Dresden, Germany

It has been demonstrated recently that mechanically strained graphene presents interesting electrical properties, which have great potential for novel applications in electronic devices. In particular, the strain in graphene nanoribbons can lead to substantial changes in its electronic properties. Besides, it provides a possibility to develop atomic point contacts and break junctions. The main purpose of this work is to investigate theoretically the influence of uniaxial mechanical strains on graphene nanojunctions in order to design graphene point contact.

To this aim, we developed the computational model by combining density functional theory and molecular dynamics methods. First, we investigated the change of the junction shape with increasing strain and the breaking with the formation of the nanogap. As expected, our theoretical model predicts the deformation of the break junction bottleneck into carbon chains before the rupture of the structure. we evaluated the electronic transmission function of graphene quantum junction by employing a coupled tight bonding and nonequilibrium green function methods. Interestingly it is found that graphene point contact can present resonance transmission in contrast to the conventional metallic point contacts with quantized conductance. This might be originated from influence of other parameters on transmission.

HL 51.11 Wed 12:30 H22

Graphene nanoribbons as effective spin ladders — •Cornelie Koop, Manuel J. Schmidt, and Stefan Wessel — Institut für Theoretische Festkörperphysik, RWTH Aachen University

Zigzag edges of graphene nanoribbons host particular, localized edge states. Since the density of states is strongly enhanced near the edges in graphene, interaction effects between the spins of these edge states become important. We can significantly simplify the analysis of such systems by means of an effective model that separates the edge and bulk states. Treating the effective interactions to first order proves sufficient in most cases, while second order corrections do not dramatically change the results. In many cases, the edge system can be reduced to a general spin ladder model, where the decay of the spin-spin interaction is determined by the shape of the edges. We examine these effective spin ladders at finite temperatures by means of quantum Monte Carlo simulations, using the stochastic series expansion method. Thereby, correlation functions and spin structure factors can be determined for realistically large graphene nanoribbons.

HL 51.12 Wed 12:45 H22

Edge State Structure of the $\nu = 0$ quantum Hall State in monolayer Graphene — •Angelika Knothe[1,2] and Thierry Jolicoeur[2] — [1]Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg — [2]Université Paris 11, CNRS, LPTMS, UMR 8626, Orsay 91405 France

Single-layer graphene at neutrality under a magnetic field is a many-body insulator whose phase structure is under intense scrutiny. When tilting the applied magnetic field, there is a phase transition towards a conducting state [1]. A plausible description is to start from a SU(4) spin-valley symmetric quantum Hall ferromagnet and add some lattice-scale anisotropies in valley space [2]. In the manifold of ground states captured by this approach, it has been proposed that graphene undergoes a transition between a canted antiferromagnetic state and a ferromagnetic state. While this picture is clear in the bulk of the system, it remains to understand the effect of this phase change on the current-carrying edge states that are formed a the physical boundaries of a real sample [3]. We use an extended Hartree-Fock approach to describe a finite-size system with a simple model for the edge and extract the one-body spectrum. We then describe the current-carrying edge textures.

[1] A. F. Young et al., Nature (London) 505, 528 (2014) [2] M. Kharitonov, Phys. Rev. B 85, 155439 (2012) [3] M. Kharitonov, Phys. Rev. B 86, 075450 (2012); G. Murthy et al., Phys. Rev. B 90, 241410 (2014) and arXiv:1510.04255; A. Knothe and T. Jolicoeur, Phys. Rev. B 92, 165110 (2015)

HL 51.13 Wed 13:00 H22

Spin lifetimes exceeding 12 ns in graphene non-local spin valves at room temperature — •Christopher Franzen[1], Marc Drögeler[1], Frank Volmer[1], Tobias Pohlmann[1], Maik Wolter[1], Kenji Watanabe[2], Takashi Taniguchi[2], Christoph Stampfer[1], and Bernd Beschoten[1] — [1]2nd Institute of Physics and JARA-FIT, RWTH Aachen University, 52074 Aachen, Germany — [2]National Institute for Materials Science, 1-1 Namiki, Tsukuba, 305-0044, Japan

We present spin transport measurements on graphene non-local spin transport devices by fabricating the electrodes first and subsequently transfer graphene with hexagonal boron nitride on top [1]. We achieve spin lifetimes of 12.6 ns and a spin diffusion length as high as 30 μm at room temperature.
This improvement exceeds all current models for contact-induced spin dephasing which paves the way towards probing intrinsic spin properties of graphene. Furthermore, we investigate the contact properties of our devices using scanning force microscopy (SFM) and conductive SFM. We discuss the importance of using large area hexagonal boron nitride for the transfer process and for achieving such high spin lifetimes and spin diffusion lengths.

[1] M. Drögeler *et al.* Nano Letters **14**, 6050 (2014).

HL 52: Spintronics (incl. quantum dynamics) (Joint session of HL, MA and TT, organized by MA)

Time: Wednesday 9:30–12:15 Location: H32

HL 52.1 Wed 9:30 H32

Valley polarization in magnetically doped single-layer transition-metal dichalcogenides — •Udo Schwingenschlögl, Yingchun Cheng, and Qingyun Zhang — PSE Division, KAUST, Thuwal 23955, Saudi Arabia

We demonstrate that valley polarization can be induced and controlled in semiconducting single-layer transition-metal dichalcogenides by magnetic doping, which is important for spintronics, valleytronics, and photonics devices. As an example, we investigate Mn-doped MoS_2 by first-principles calculations. We study how the valley polarization depends on the strength of the spin orbit coupling and the exchange interaction and discuss how it can be controlled by magnetic doping. Valley polarization by magnetic doping is also expected for other honeycomb materials with strong spin orbit coupling and the absence of inversion symmetry. Reference: Phys. Rev. B **89**, 155429 (2014).

HL 52.2 Wed 9:45 H32

Giant Rashba-type spin splitting in ferroelectric GeTe(111) — •Marcus Liebmann[1], Christian Rinaldi[2], Domenico Di Sante[3], Jens Kellner[1], Christian Pauly[1], Rui Ning Wang[4], Jos Emiel Boschker[4], Alessandro Giussani[4], Stefano Bertoli[2], Matteo Cantoni[2], Lorenzo Baldrati[2], Marco Asa[2], Ivana Vobornik[5], Giancarlo Panaccione[5], Dmitry Marchenko[6], Jaime Sanchez-Barriga[7], Oliver Rader[7], Raffaella Calarco[4], Silvia Picozzi[3], Riccardo Bertacco[2], and Markus Morgenstern[1] — [1]II. Inst. Phys. B, RWTH Aachen University — [2]Politecnico di

Milano, Italy — [3]Consiglio Nazionale delle Ricerche, L'Aquila, Italy — [4]Paul-Drude-Institut für Festkörperelektronik, Berlin — [5]Consiglio Nazionale delle Ricerche, Trieste, Italy — [6]Physikalische und Theoretische Chemie, Freie Universität Berlin — [7]Helmholtz-Zentrum für Materialien und Energie, BESSY, Berlin

The ferroelectric semiconductor GeTe has been proposed to exhibit a giant spin splitting of bulk Rashba bands with spin rotation direction coupled to the dielectric polarization [1]. We probe GeTe(111) grown by MBE using in-situ angular-resolved photoelectron spectroscopy (ARPES). We identify a novel Rashba-split surface band with giant spin splitting and find signatures of the bulk Rashba band by comparison with density functional theory calculations [2]. The ferroelectric polarization, as determined by piezo force microscopy, agrees with the predicted helical spin-momentum relation of the Rashba bands.

[1] D. Di Sante *et al.*, Adv. Mater. **25**, 509 (2013).

[2] M. Liebmann *et al.*, Adv. Mater. 2015, 10.1002/adma.201503459.

HL 52.3 Wed 10:00 H32

Spin Mapping of Surface and Bulk Rashba States in Ferroelectric α-GeTe(111) Films — •H. J. Elmers[1], R. Wallauer[1], M. Liebmann[2], J. Kellner[2], M. Morgenstern[2], R.N. Wang[3], J.E. Boschker[3], R. Calarco[3], O. Rader[4], D. Kutnyakhov[1], S.V. Chernov[1], K. Medjanik[1], C. Tusche[5], M. Ellguth[5], H. Volfova[6], J. Braun[6], J. Minar[6], H. Ebert[6], and G. Schönhense[1] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz — [2]II. Physikalisches Institut B and JARA-FIT, RWTH Aachen — [3]Paul-Drude-Institut für Festkörperelektronik, Berlin — [4]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin — [5]Max Planck Institute for Microstructure Physics, Halle — [6]Department Chemie, Ludwig-Maximilians-Universität München

Ferroelectric semiconductors like GeTe promise a switchable Rashba-parameter for electronic bulk states. A comprehensive mapping of the spin polarization of the electronic bands in α-GeTe(111) films has been performed using a time-of-flight momentum microscope equipped with an imaging spin filter that enables a simultaneous measurement of more than 10.000 data points. In addition to the Rashba type splitting of surface bands we observe a spin splitting of bulk bands with opposite spin helicity of the inner and outer Rashba bands revealing the complex spin texture at the Fermi energy that determines electronic transport.

HL 52.4 Wed 10:15 H32

Optically and thermally driven spin dynamics and quantum Otto cycles on Ni_4 structures — •Stefan Sold[1], Bhaskar Kamble[2], Georgios Lefkidis[1], and Wolfgang Hübner[1] — [1]Departement of physics, University of Kaiserslautern and Research Center OPTIMAS, Germany — [2]Asia Pacific Center for Theoretical Physics, Pohang, Korea

We present two different kinds of combined optical and thermodynamic processes on the chain-like prototypical Ni_4 cluster, described on the basis of high-level quantum chemistry. The one consists of incoherent spin relaxation and thermalization processes, the other one of a nano Otto engine.

First, we model various temperature profiles by coupling to one or two temperature baths. The system dynamics is mathematically described with the Lindblad superoperator [1]. We find that the inhomogeneous temperature profile, giving rise to non-equilibrium mixed states, induces non-uniform spin-density distribution (spin Seebeck effect on the nano scale).

Second, we propose a quantum Otto motor [2], which benefits from the spin degree of freedom and the energy discretization of the cluster, and may thus surpass the efficiency limit of classical Carnot cycles [3].

[1] G. Schaller and T. Brandes, Phys. Rev. A **78**, 022106 (2008)

[2] W. Hübner, G. Lefkidis, C. D. Dong, D. Chaudhuri, L. Chotorlishvili, and J. Berakdar, Phys. Rev. B **90**, 024401 (2014)

[3] C. D. Dong, G. Lefkidis, and W. Hübner, Phys. Rev. B **88**, 214421 (2013)

HL 52.5 Wed 10:30 H32

Theoretical aspects of the Edelstein effect for anisotropic 2DEGs and topological insulators — •Annika Johansson[1,2], Dmitry Fedorov[1,2], Jürgen Henk[2], and Ingrid Mertig[2,1] — [1]Max Planck Institute of Microstructure Physics, Halle, Germany — [2]Martin Luther University Halle-Wittenberg, Halle, Germany

A charge current driven through a two-dimensional electron gas (2DEG) with Rashba spin-orbit coupling [1] generates a spatially homogeneous spin polarization perpendicular to the applied electric field. This phenomenon is the Edelstein effect [2].

For selected model systems, we consider the Edelstein effect within the semiclassical Boltzmann transport theory. Its energy dependence is investigated, in particular the regime below the Dirac point of the 2DEG. In addition to an isotropic 2DEG [1], we analyze systems with anisotropic Fermi contours. We predict that the current-induced spin polarization vanishes if the Fermi contour passes through a Lifshitz transition. In addition, we corroborate that topological insulators provide a very efficient conversion of charge to spin current [3].

Our findings for paradigmatic Rashba systems call for experimental verification.

[1] Y. Bychokov and E. Rashba, J. Phys. C, **17**, 6039 (1984) [2] V. M. Edelstein, Solid State Commun., **73**, 233 (1990) [3] J. C. Rojas Sánchez *et al.*, ArXiv: 1509.02973 (2015)

15 min. break

HL 52.6 Wed 11:00 H32

Spin superfluidity and long-range transport in thin-film ferromagnets — Hans Skarsvåg, •Cecilia Holmqvist, and Arne Brataas — Department of Physics, Norwegian University of Science and Technology, NO-7491 Trondheim, Norway

In ferromagnets, magnons may condense into a single quantum state. Analogous to superconductors, this quantum state may support transport without dissipation. Recent works suggest that longitudinal spin transport through a thin-film ferromagnet is an example of spin superfluidity. Although intriguing, this tantalizing picture ignores long-range dipole interactions; here, we demonstrate that such interactions dramatically affect spin transport. In single-film ferromagnets, "spin superfluidity" only exists at length scales (a few hundred nanometers in yttrium iron garnet) somewhat larger than the exchange length. Over longer distances, dipolar interactions destroy spin superfluidity. Nevertheless, we predict the re-emergence of spin superfluidity in tri-layer ferromagnet-normal metal-ferromagnet films that are ~1 micrometre in size. Such systems also exhibit other types of long-range spin transport in samples that are several micrometers in size.

HL 52.7 Wed 11:15 H32

Ultra-long electron and hole spin lifetimes in monolayer WSe_2 — Sammy Pissinger, •Robin de Winter, Christopher Franzen, Manfred Ersfeld, Sebastian Kuhlen, Christoph Stampfer, and Bernd Beschoten — 2nd Institute of Physics and JARA-FIT, RWTH Aachen University, Germany

There is strong interest in optical generation and detection of valley spin polarizations in transition metal dichalcogenides. We report on time-resolved two color pump probe Kerr rotation measurements on mechanically exfoliated monolayer WSe_2 crystals. We find electron and hole spin lifetimes of up to 100 ns at low temperatures. These values are in good agreement with exciton lifetimes extracted from all-optical time-resolved reflectivity indicating that the spin lifetimes are limited by exciton recombination times in our crystals. Electron spin precession in Voigt geometry furthermore reveals inhomogeneous spin dephasing caused by a large spread in the local g factors.

HL 52.8 Wed 11:30 H32

Bulk Spin-Orbit Torques at finite temperatures in Bulk Half-Metallic Heuslers from First Principle — •Jacob Gayles[1], Libor Šmejkal[2], Jakub Železny[2], Frank Freimuth[3], Zhe Yuan[1], Yuriy Mokrousov[3], Tomas Jungwirth[2], and Jairo Sinova[1] — [1]Institut für Physik, Johannes Gutenberg Universität Mainz, D-55099 Mainz, Germany — [2]Institute of Physics ASCR, v.v.i., Cukrovarnicka 10, 162 53 Praha 6 Czech Republic — [3]Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

We predict bulk spin-orbit torques in the half-metallic Heuslers NiMnSb and PtMnSb, using symmetry arguments in conjunction with first principle calculations. We present under uniaxial growth strain a linear dependence of the even torque and that can be tuned to zero while observing a sizable odd torque is independent of strain. Furthermore, these effects are seen to be two orders of magnitude larger in the PtMnSb. The even torque is strongly dependent on the temperature decreasing by 75% at room temperature where finite temperature is taken into account in the frozen phonon approximation. We show the equivalence of two widely used methods, the Landauer-Bütikker and the Kubo linear response formalism giving confidence in our result

for experimental measurements in bulk magnetic Heusler compounds breaking inversion symmetry.

HL 52.9 Wed 11:45 H32

Dynamics of bound monopoles in artificial spin ice: How to store energy in Dirac strings. — •Elena Vedmedenko — University of Hamburg, Hamburg, Germany

Dirac strings in spin-ices are lines of reversed dipoles joining two quasiparticle excitations. These excitations behave themselves as unbound emergent monopoles if the tension of Dirac strings vanishes. In this work analytical and numerical analysis are used to study dynamics of two-dimensional dipolar spin ices, artificially created analogs of bulk spin-ice, in the regime of bound monopoles. It is shown that in this regime strings rather than monopoles are effective degrees of freedom explaining the finite-width band of Pauling states. A measurable prediction of path-time dependence of endpoints of stretched and then released Dirac string is made and verified via simulations. It is shown that string dynamics is defined by the characteristic tension-to-mass ratio, which is determined by the fine structure constant and lattice dependent parameter. It is proposed to use string tension to achieve spontaneous magnetic currents. A concept of energy storing device on the basis of this principle is proposed and illustrated by an experimental demonstration. A scheme of independent measurement at the nanoscale is proposed.

HL 52.10 Wed 12:00 H32

Spin-orbit torque in antiferromagnets — •Jakub Zelezny[1], Frank Freimuth[2], Yuriy Mokrousov[2], Jacob Gayles[3], Jairo Sinova[3], and Tomas Jungwirth[3] — [1]Institute of Physics of the Czech Academy of Sciences, Czech Republic — [2]Forschungszentrum Julich and JARA, Germany — [3]Institut fur Physik, Johannes Gutenberg Universitat Mainz, Germany

Antiferromagnets are common in nature and just like ferromagnets posses a long-range magnetic order. Unlike ferromagnets though, they have found little practical applications so far, primarily due to their lack of total magnetization. However, development of spintronics opens up ways how they could be used. Antiferromagnets have some advantages over ferromagnets, in particular ultrafast magnetization dynamics and wide range of materials available, including many semiconductors. One of the key problems for application of antiferromagnets in spintronics remains manipulation of the spin-axis. Recently we have predicted that in some bulk antiferromagnets, electrical current can effectively manipulate the magnetic moments [1]. Switching of an antiferromagnet using this method have recently been observed experimentally [2]. The effect is analogous to the spin-orbit torque in ferromagnets. Here we discuss the symmetry of the torques, especially the necessary conditions for their existence and show results of microscopic calculation of the torques in various antiferromagnets.

[1] J. Železný et al., PRL 113 (15), 157201 [2] P. Wadley et al., Science, to be published, arXiv:1503.03765

HL 53: Poster II

Topics: Photovoltaics, Transport properties, Preparation and characterization (Quantum dots and wires and others), Optical properties of quantum dots and wires, Transport properties of quantum dots and wires and others, Devices and Semiconductor lasers

Time: Wednesday 9:30–13:30 Location: Poster A

HL 53.1 Wed 9:30 Poster A

Transport experiments on magneto-electric hybrid lattices — •Karoline Gawenda[1], Jakob Schluck[1], Thomas Heinzel[1], Klaus Pierz[2], Hans Werner Schumacher[2], Julien Chaste[3], and Ulf Gennser[3] — [1]Condensed Matter Physics Laboratory, Heinrich-Heine-Universität, Düsseldorf, Germany — [2]PTB, Braunschweig, Germany — [3]CNRS-LPN, Marcoussis, France

Two-dimensional electron gases in $GaAs/Al_xGa_{1-x}As$ heterostructures are exposed to combinations of periodic electric and magnetic fields. These so-called superlattices are realized with customary lithography methods and are composed of a two-dimensional antidot array and a two-dimensional magnetic lattice. The resulting nontrivial electronic trajectories are expected to manifest themselves in novel magnetoresistivity resonances at cryogenic temperatures. To interpret the experimentally obtained results numerical simulations of the electron dynamics within the semiclassical Kubo formalism are used.

HL 53.2 Wed 9:30 Poster A

Electronic transport properties of polycyclic hydrocarbon and TCNQ derivative based charge transfer dimers — •Simon Liebing, Torsten Hahn, and Jens Kortus — TU Bergakademie Freiberg, Institute for Theoretical Physics, Germany

The realization of high rectification ratios in molecular electronics has been challenge for many years, because of strong coupling of the molecules in the material. As a result even very asymmetric molecules or asymmetric coupling to electrodes showed rather symmetric current-voltage characteristic. Recently, we reported that the molecular system picene-F_4TCNQ [1] is able to act as a molecular rectifier [2]. The rectification mechanism has been explained due to charge transfer between the two molecules effectively creating a molecular pn-junction.

Here we report on our investigations on polycyclic hydrocarbons and TCNQ derivatives in order to elucidate if this rectification mechanism applies there too. The theoretical calculations to obtain electronic and transport properties were performed by means of density functional theory and NEGF transport theory [3,4].

[1] Mahns, B. et al. Crystal Growth & Design (2014). [2] Hahn T., Liebing S., and Kortus J., Nanoscale 6, 14508 (2014). [3] Pederson, M. et al., Phys. Status Solidi b 217, 197. (2000). [4] Enkovaara, J. et al., JOP: Condensed Matter 22, 253202 (2010).

HL 53.3 Wed 9:30 Poster A

Commensurability effects of magnetic barriers in 2D electron gases — •Andreas Leuschner, Mihai Cerchez, and Thomas Heinzel — Heinrich Heine University Düsseldorf, Universitätsstr. 1 D-40225 Düsseldorf

Localized magnetic fields (magnetic barriers) in 2D electron gases lead to a magnetoresistance with a number of classical and quantum implications [1,2]. The simultaneous superposition of a variable homogeneous perpendicular magnetic field gives rise in addition to commensurability effects. These are explained in terms of the interplay between transverse snake orbit electrons, with variable cyclotron radii and the finite size of the sample.

[1] S. Hugger, M. Cerchez, H. Xu, and T. Heinzel, Phys. Rev. B 76, 195308 (2007) [2] B. Schüler, M. Cerchez, Hengyi Xu,, J. Schluck, T. Heinzel, and A. D. Wieck, Phys. Rev. B 90, 201111(R) (2014)

HL 53.4 Wed 9:30 Poster A

low temperature magneto-transport behavior in the phase change compound Sn1Sb2Te4 — •Zhe Yang[1,2], Hanno Volker[1], Nicholas P. Breznay[3], and Matthias Wuttig[1] — [1]Department of Physics, RWTH Aachen University, Aachen, Germany — [2]School of Optical and Electronic Information, Huazhong University of Science and Technology, Wuhan, China — [3]Department of Physics, University of California, Berkeley, Berkeley, United States

Disorder is a critical parameter to tailor the transport properties of phase change materials for an improved performance in memory devices. In this work, we have investigated crystalline Sn1Sb2Te4 samples where the disorder is tuned via annealing. Both the temperature dependence of the resistivity and the magnetoresistance have been studied. Hopping transport is observed in the strongly disordered state, while Boltzmann transport is found for the weakly disordered state. Our samples show a metal-insulator transition, which coincides with the divergence of the localization length. From magnetoresistance measurements at low temperature, we calculate the dephasing length induced by electron-electron scattering dephasing processes at the metallic side and derive its evolution near the MIT.

HL 53.5 Wed 9:30 Poster A

low temperature magneto-transport behavior in the phase

change compound $Sn_1Sb_2Te_4$ — •Zhe Yang[1,2], Hanno Volker[1], Nicholas P. Breznay[3], and Matthias Wuttig[1] — [1]Department of Physics, RWTH Aachen University, Aachen, Germany — [2]School of Optical and Electronic Information, Huazhong University of Science and Technology, Wuhan, China — [3]Department of Physics, University of California, Berkeley, Berkeley, United States

Disorder is a critical parameter to tailor the transport properties of phase change materials for an improved performance in memory devices. In this work, we have investigated crystalline $Sn_1Sb_2Te_4$ samples where the disorder is tuned via annealing. Both the temperature dependence of the resistivity and the magnetoresistance have been studied. Hopping transport is observed in the strongly disordered state, while Boltzmann transport is found for the weakly disordered state. Our samples show a metal-insulator transition, which coincides with the divergence of the localization length. From magnetoresistance measurements at low temperature, we calculate the dephasing length induced by electron-electron scattering dephasing processes at the metallic side and derive its evolution near the MIT.

HL 53.6 Wed 9:30 Poster A

Electrical transport in γ-CuI crystals and thin films and usage in bipolar γ-CuI/ZnO-heterodiodes with high rectification ratio — •Max Kneiss, Chang Yang, José Barzola-Quiquia, Michael Lorenz, and Marius Grundmann — Universität Leipzig, Institut für Exp. Physik II, Germany

The interest in γ-CuI has increased recently, as it is an intrinsically p-conducting transparent semiconductor with a high excitonic binding energy of 62 meV and fairly high hole mobility making it a promising alternative for usage in transparent optoelectronics [1]. We investigated γ-CuI crystals and thin films grown with various techniques via temperature dependent Hall-Effect-, I-V- and magnetoresistance measurements. We modeled the temperature dependent resistance and I-V-curves and found evidence for a tunneling process dominating the transport at low temperature in both crystals and thin films. A change from semiconducting to metallic behaviour with increasing temperature is observable only for thin films, where a power law is characterizing the resistance at higher temperature, which is in agreement with the high carrier concentrations in our thin films ($\approx 10^{19}$-10^{20} cm^{-3}). Magnetoresistance furthermore suggests a weak antilocalization effect for crystals at low temperatures. Finally we were able to grow CuI thin films epitaxially on a ZnO-layer via reactive sputtering thus producing transparent γ-CuI/ZnO-heterodiodes with even higher rectification ratios (up to 9 orders of magnitude) than previously reported [2].

[1] Grundmann et al., Phys. Status Solidi A **210**, 1671 (2013)
[2] Schein et al., Appl. Phys. Lett. **102**, 092109 (2013)

HL 53.7 Wed 9:30 Poster A

The influence of nanopatterning on the electrical conductivity of boron-doped silicon nanowires — •Maximilian Kockert[1], Stefan Weidemann[1], Danny Kojda[1], Zhi Wang[2], Michael Kröner[2], Peter Woias[2], Klaus Rademann[3], Martin Albrecht[4], and Saskia F. Fischer[1] — [1]Novel Materials Group, Humboldt-Universität zu Berlin, D-12489 Berlin — [2]Laboratory for Design of Microsystems, University of Freiburg - IMTEK, D-79110 Freiburg — [3]Institut für Chemie, Humboldt-Universität zu Berlin, D-12489 Berlin — [4]Leibniz-Institut für Kristallzüchtung, D-12489 Berlin

Investigations of silicon nanowires (SiNWs) have shown, that nanopatterning affects the thermal conductivity of SiNWs, because of the reduced phonon contribution [1]. In this work, the resistivity ρ of bulk silicon and porous SiNWs was investigated to determine the influence of nanopatterning on the electrical properties. Van der Pauw measurements of bulk silicon show $\rho_{\mathrm{bulk}} = (1.60\pm0.01)\cdot10^{-2}\,\Omega$cm. SiNWs were prepared from that highly boron-doped bulk silicon using the two-step metal-assisted chemical etching method [2]. SiNWs were contacted by means of electron beam-induced deposition. Two-terminal measurements of SiNWs show $\rho_{\mathrm{SiNWs}} = (1.1 \pm 0.2) \cdot 10^3\,\Omega$cm. The difference between the resistivity of bulk silicon and silicon nanowires indicates a consumption of the dopant boron during the etching process.

[1] A. I. Hochbaum *et al.*, Nature **451**, 163 (2008).
[2] S. Weidemann *et al.*, Journal of Nanomaterials **2015**, 672305 (2015).

HL 53.8 Wed 9:30 Poster A

Enhancing current-voltage characterisation utilising complementary immittance analysis — •Julian Alexander Amani, Tristan Koppe, Hans Hofsäss, and Ulrich Vetter — II. Physikalisches Institut der Georg-August-Universität Göttingen, Deutschland

Current-voltage characterisation is the standard method of determining underlying conduction mechanisms. Usually performed by measuring the stationary currents under different environmental conditions, mostly at different temperatures, it can be used to identify the conduction processes in single homogeneous pieces of material as well as in heterogeneous systems consisting of multiple materials.

It is almost inevitable that parasitic resistances, e. g. at the contacts, or alternate pathways, for example along surfaces, influence the measurement of the current-voltage characteristics. Identification or removal of the distortions caused by these parasitic contributions, solely using current-voltage measurements, can be complicated.

Complementary immittance spectroscopy can be used to identify and remove the parasitic contributions, often even without the need to understand the specific parasitic processes in detail. We will present a strategy to remove and, if desired, identify parasitic contributions with little overhead. Although not limited to specific contact arrangements, we will show certain geometries that simplify the complementary immittance measurement process. Finally, we discuss whether immittance spectroscopy can replace conventional current-voltage characterisation altogether.

HL 53.9 Wed 9:30 Poster A

Growth of Site-Controlled InAs Quantum Dots by MOVPE — •Marc Sartison, Mauro Bono, Leonard Spira, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen and Research Centers SCoPE and IQST, Universität Stuttgart, Allmandring 3, 70569 Stuttgart, Germany

In the last decade, it has been demonstrated, that semiconductor quantum dots (QDs) have the potential to be excellent light sources for the application in single-photon devices. Stranski-Krastanov grown QDs with a high optical quality and structrual purity can be obtained self-assembled with a low spatial density. Hence, it is a challenging task to integrate QDs into optical circuits on chip, a precise control of the QD position is essential. It also has been shown, that the surface potential can be locally modified to create sites of higher nucleation probability by prepatterning the substrates. In this contribution, we present two approaches of the site-controlled growth of InAs QDs on prepatterned GaAs substrates. To create nucleation sites, the substrate is structured with a hexagonal hole pattern, which is etched by a combination of wet and dry chemical etching. Afterwards, the templates are overgrown with either GaAs buffer structures or with a burried strain iducing InGaAs layer. The nucleation behavior of the following deposited InAs QDs material is monitored by AFM and SEM measurements. To reveal the optical characteristics, the QDs were capped with a GaAs layer and micro-photoluminescence measurements were carried out.

HL 53.10 Wed 9:30 Poster A

Metamorphic buffer layers on GaAs for the deposition of InGaAs quantum dots — •Julian Kluge, Matthias Paul, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und funktionelle Grenzflächen, University Stuttgart and Research Centers Scope and IQST, Allmandring 3, Universität Stuttgart

The interest in In(Ga)As semiconductor quantum dots (QDs) as sources for entangled or indistinguishable photons has increased in the last years due to a need for non-classical light generation in quantum information or quantum cryptography. For an implementation in fiber-coupled networks, emission wavelengths in the telecommunication bands at 1.31 μm or 1.55 μm are desirable to minimize absorption losses. The high strain in InAs QDs directly deposited on GaAs leads to emission wavelengths below 1 μm. A shift to wavelengths above 1.3 μm is possible by depositing the QDs on InP substrates, thus, decreasing the lattice mismatch. InGaAs metamorphic buffer (MB) layers can substitute InP substrates. We grow MB layers on GaAs substrates for the deposition of In(Ga)As QDs with emission in the range of the telecommunication bands. The Indium content in the MB is increased gradually to adjust the lattice constant and decrease the lattice mismatch between the QDs and the growth surface. In X-ray diffraction experiments, the residual strain on the surface and the Indium content is determined with the help of reciprocal space maps of the symmetrical (004) and asymmetrical (224) reflexes. The surface roughness of the partially relaxed buffers is investigated by atomic force microscopy (AFM). A smooth surface is a prerequisite for the deposition of QDs.

HL 53.11 Wed 9:30 Poster A

Capacitance-Voltage Spectroscopy of InAs Quantum Dots Under External Applied Strain — •Sascha René Valentin[1], Arne Ludwig[1], Andreas D. Wieck[1], and Dirk Reuter[2] — [1]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum — [2]Arbeitsgruppe Optoelektronische Materialien und Bauelemente, Universität Paderborn

Self-assembled InAs quantumdots (QDs) are integrated in a variety of interesting optical and electronical devices and are also highly interesting from a fundamental point of view. Electric fields are often used to tune the optical and electronical properties of QDs. Recently it has been shown that external applied strain can reversibly shift the optical emission energy of QDs. Theoretical calculations indicate that the shift in the emission energy originates in the changed coulomb interaction between the charge carriers as well as in the shift of the energy levels themselves. In this project we want to measure the dependence of the interaction energies of the carriers on externally applied strain using capacitance voltage (CV) spectroscopy. In the device we present, a thin electrically contacted CV-membrane is bonded to a PMNPT-piezoelectric actuator. This allows to apply strain to the QDs and at the same time it enables electrical and optical measurements on a QD ensemble.

HL 53.12 Wed 9:30 Poster A

Huge thermal shift of the excitonic charging featured energy in self-assembled quantum dots — •Fabian Brinks, Patrick Labud, Andreas Wieck, and Arne Ludwig — Ruhr-Universität Bochum, Lehrstuhl für Angewandte Festkörperphysik

It has been shown that excitons of different charge can be detected in self-assembled InAs quantum dots (QD) by means of capacitance-voltage (C(V)) spectroscopy [1]. Above bandgap illumination of QDs embedded in a Schottky diode induces electron hole-pairs, while eventually the built-in electric field separates them before recombining. Electrons flow to the back-contact and holes get trapped in the quantum dots. Reducing the built-in field by applying forward bias to the diode, electrons tunnel from a highly n-doped back contact into the quantum dots and form excitonic complexes before recombining. The associated tunnel current can be measured by C(V)-spectroscopy and light induced, well resolved charging peaks appear at lower gate voltages than by tunnelling into the single electron s-states.

Rising the temperature, these light induced peaks shift to significantly lower voltages, whereas the non-light induced s-peaks charging voltage basically stays unaltered.

In our presentation we will discuss various possible origins of this effect.

[1] P. Labud et al., *Physical Review Letters* **112**, 46803 (2014).

HL 53.13 Wed 9:30 Poster A

Focused ion beam induced growth of single III/V nanowires on arbitrarily arranged sites — •Rüdiger Schott, Sven Scholz, Arne Ludwig, and Arndreas D. Wieck — Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum

Semiconductor nanowires (NWs) are used as building blocks for a new generation of advanced devices intended for different applications in the field of nanoelectronics, nanophotonics and nanomechanics. NWs are near one-dimensional structures that typically have a high length-to-width ratio. This is the base of fascinating structural properties. Heterostructures of highly lattice mismatched materials can be combined without dislocations and metastable phases, unattainable in bulk materials like wurtzite GaAs, are feasible. We present focused ion beam (FIB) induced molecular beam epitaxy (MBE) grown single III/V nanowires from site selectively deposited Au seeds [1]. The possibility of maskless patterning makes focused ion beam lithography a powerful tool and an alternative to conventional lithography based methods in semiconductor processing. With an FIB system, equipped with an ExB filter and a liquid metal alloy ion source (LMAIS), most of the elements of the periodic table are accessible for ion implantation and patterning. Structural and optical properties of the nanowires are investigated by secondary electron microscopy, transmission electron microscopy, cathodoluminescence and photoluminescence spectroscopy.

[1] G. Bussone et al., *J. Appl Crystallogr.* **46**, 887-892 (2013).

HL 53.14 Wed 9:30 Poster A

Silicon incorporation in III/V-Nanowires - Comparison of growth and catalyst doping — •Marcel Schmidt, Rüdiger Schott, Sven Scholz, Andreas D. Wieck, and Arne Ludwig — Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum

Semiconductor Nanowires (NWs) have a big potential in the aim of further miniaturization of future nanoscale devices. A prerequisite for the fabrication of functional nanowire devices is their electrical doping. We investigate doping of nanowires due to implant doped metal seeds like gold silicon (AuSi) for catalyst assisted molecular beam epitaxy (MBE) growth of GaAs NWs. A focused ion beam system equipped with an ExB filter and a liquid metal alloy ion source (LMAIS) is used to implant the metal seeds. We will present first results, comparing Au and AuSi catalysed GaAs NWs.

HL 53.15 Wed 9:30 Poster A

Fabrication of sub-50 nm silicon nanowires using inductively coupled plasma etching — •Muhammad Bilal Khan, Dipjyoti Deb, Yordan M. Gieorgiev, and Artur Erbe — HZDR, Bautzner Landstraße 400, 01328 Dresden, Germany

Development of an etching process for fabrication of ultrathin silicon nanowires (SiNWs) with inductively coupled plasma (ICP) source and C4F8/SF6 mixed gas recipe at 18 oC is reported. Etch selectivity of silicon (SOI) to hydrogen silsesquioxane (HSQ), a negative tone electron beam resist and selectivity of silicon (SOI) to SiO2 are investigated to identify suitable process window. Effects of ICP power, RF power, chamber pressure, flow rates and ratio of C4F8/SF6 on etch rate, selectivity and surface roughness are examined. Atomic force microscopy (AFM) is used for identifying surface roughness of the plain silicon (SOI) substrates after etching. Thereafter etching of HSQ patterned substrates is performed. Scanning electron microscopy is performed to observe the etch profile. Parameters such as flow rates of C4F8/SF6 are optimized to attain sub-50 nm SiNWs with smooth and vertical sidewalls.

HL 53.16 Wed 9:30 Poster A

Impact of plasma parameters on the growth of InGaN nanowire heterostructures by plasma-assisted molecular beam epitaxy — •Pascal Hille[1], Felix Walther[1], Philip Klement[1], Jörg Schörmann[1], Vanessa Dahmen[2], Nils Rosemann[2], Sangam Chatterjee[2], Philomela Komninou[3], and Martin Eickhoff[1] — [1]I. Physikalisches Institut, Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, 35392 Gießen, Germany — [2]Faculty of Physics and Materials Science Center, Philipps Universität Marburg, Renthof 5, 35032 Marburg, Germany — [3]Physics Department, Aristotle University of Thessaloniki, GR-54124 Thessaloniki, Greece

Its tunable direct bandgap (UV to IR) renders (In,Ga)N nanowires a promising material platform for nano-opto electronic devices. However, the large lattice mismatch between the two binaries as well as the low decomposition temperature of InN compared to GaN leads to structural degradation of the grown material with increasing In content. Preventing InN dissociation during growth by bond stabilization might increase the material quality. For metal rich growth conditions theory predicts that an increase of the nitrogen flux should achieve such a bond stabilization and also yield an increase of the incorporated In fraction [1]. Here, we varied the nitrogen flux and the applied forward plasma power for the growth of InGaN/GaN nanowire heterostructures (NWHs) and studied the influence these variations have on the morphological and optical properties of the NWHs.

[1] Turski et al., J. Cryst. Growth 367, 115–121 (2013)

HL 53.17 Wed 9:30 Poster A

Luminescence and photoconductivity properties of hybrid Carbon-nanodot/ZnO nanostructures — •Kseniia Sergeeva[1], Angelina Vogt[1], Rene Gorny[1], Frank Dissinger[2], Sebastian Resch[2], Siegfried Waldvogel[2], and Tobias Voss[1] — [1]TU Braunschweig, Institut für Halbleitertechnik, Germany — [2]Johannes Gutenberg-Universität Mainz, Institut für Organische Chemie, Germany

Carbon nanodots (C-Dots) have attracted tremendous attention due to their low-cost manufacturing processes, low toxicity, tuneable photoluminescence and absorption properties, and photochemical stability. All these properties make C-Dots well-suited candidates for LED and gas-sensing technologies. In this work, hydrothermally synthesized C-Dots (as-grown or in a reduced state) were attached electrostatically and covalently to the surface of ZnO nanowires. The C-Dots show a strong blue (reduced particles) or green (as-grown particles) luminescence under irradiation with UV-light (365nm). Models which were

recently published in the literature suggest that the luminescence properties of C-Dots can be related to different species of polycyclic aromatic molecules (PAH) which form the core of the dot. Their tuneable luminescence and absorption properties may also be related to varying size-distribution of the synthesised C-dots. The structural properties of the C-Dots together with their polymeric shell were characterized with Raman spectroscopy and FTIR. Photoconductivity measurements of ZnO/C-Dot hybrid structures were carried out to study the electron transfer dynamics from the dots to the oxide material.

HL 53.18 Wed 9:30 Poster A

Intense Intrashell Luminescence of Eu-Doped ZnO Nanowires — •Torsten Lindemann[1], Sebastian Geburt[1], Michael Lorke[2], Andreia Luisa da Rosa[2], Thomas Frauenheim[2], Robert Röder[1], Tobias Voss[3], and Carsten Ronning[1] — [1]Institute of Solid State Physics, Friedrich-Schiller-University Jena, Germany — [2]Bremen Center for Computational Materials Science (BCCMS), University of Bremen, Germany — [3]Institute of Semiconductor Technology, University of Technology Braunschweig, Germany

Semiconductor nanowires (NW) have been proposed as route towards the miniaturization of light sources and solid-state lasers. Doping of materials with rare earth (RE) elements enables new optical properties. If these elements are incorporated into host matrices, optical intra-4f transitions become possible, which consequently show long lifetimes and are therefore spectrally very sharp. Successful doping and excellent optical activation of Eu^{3+} ions in single crystalline zinc oxide (ZnO) NWs is realized using the ion implantation approach subsequently to growth. The origin of the intense intra-4f luminescence of Eu^{3+} ions in ZnO is assigned by first-principles calculations to the formation of Eu-Oi complexes within the lattice. These complexes are formed during the nonequilibrium ion implantation process and subsequent annealing at 700 °C in air. Our targeted defect engineering resulted in intense intrashell luminescence of single ZnO:Eu nanowires even at room temperature. The high intensity enabled us to study the luminescence of single ZnO nanowires in detail, their behaviour as a function of excitation power and waveguiding properties.

HL 53.19 Wed 9:30 Poster A

Speeding up a single quantum dot pump-probe experiment — •Gerhard Johannes Schäfer, Christian Dicken, and Markus Lippitz — Experimental Physics III, University of Bayreuth, Germany

We recently showed [1], that it is possible to measure transient reflection on single semiconductor quantum dots in the far field.

Here we show how to improve those measurements. We decrease the integration time by using a high repetition rate laser (1 GHz instead of 76 MHz). At the same time, we also increase the spectral rate to 120 kHz.

[1] *C. Wolpert et al, Nano Lett., 2012, 12 (1), pp 453-457.*

HL 53.20 Wed 9:30 Poster A

Spatio-temporal propagation of nonclassical light in a coupled quantum dot-waveguide system — •Kilian Kuhla and Marten Richter — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, EW 7-1, Technische Universität Berlin, Hardenbergstrasse 36, 10623 Berlin, Germany

Caused by the need for new quantum technologies, propagation of nonclassical light in an optical waveguide interacting with embedded semiconductor quantum dots (QDs) constitutes a focus of current experimental and theoretical research.

In this contribution, we study the time- and space-resolved characteristics of the waveguide-QD-system in the few-photon-limit, e.g. for single photon and (entangled) photons pairs.

To describe an open system dynamics, we propose a density matrix formalism, based on spatial dependent photon operators, specifically suitable for the few photon limit.The approach allows to include relevant pumping and dissipation mechanisms in a phenomenological Lindblad formalism. Overall the framework provides a closed set of equation of motion for the excitons in the quantum dot as well as the photon traveling in the waveguide.

HL 53.21 Wed 9:30 Poster A

Hybrid density matrix approach as a factorization scheme for many-body systems — •Sandra Kuhn and Marten Richter — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, EW 7-1, Germany

Semiconductor quantum dots coupled to an embedding bulk, quantum well or wetting layer carrier reservoir play a significant role in a variety of applications. These structures represent an important example of a hybrid system, which consist of a subsystem with localized, discrete states and a subsystem with quasi continuous states. However, both systems (quantum dot and carrier reservoir) constitute many-body systems with different properties, which requires a description including different approximations. We developed a theoretical factorization scheme to describe interactions between those hybrid many-body systems. The used projection operator technique combines the advantages of conventional correlation expansions and an exact diagonalization scheme. In particular, the approach allows a dynamical treatment of the continuum and is capable of including Non-Markovian effects. Thus, the presented hybrid density matrix approach goes beyond the Markovian approximation typically used in Lindblad formalism to describe scattering processes. The method is illustrated on the example of Coulomb scatterings between quantum dot and surrounding bulk material. However, the approach is also applicable to other systems and interactions mechanisms such as electron-phonon interactions [1].

[1] S.C. Kuhn and M. Richter, PRB **91**, 155309 (2015).

HL 53.22 Wed 9:30 Poster A

Semiconductor quantum dots interfaced with cesium: Mollow triplet and a Faraday filter — •Simone L. Portalupi[1], Matthias Widmann[2], Cornelius Nawrath[1], Sang-Yun Lee[2], Michael Jetter[1], Joerg Wrachtrup[2], Ilja Gerhardt[2], and Peter Michler[1] — [1]Institut für Halbleiteroptik und Funktionelle Grenzflächen, University of Stuttgart, Germany — [2]3. Institute of Physics, University of Stuttgart, Germany

Quantum dots (QDs) are nowadays the brightest source of single photons, allowing for high indistinguishability, photonic entanglement generation, and their use as "flying qubits" for quantum communication. A long lasting quantum memory could be realized using the highly coherent properties of atoms. Quantum hybrid systems, which realize spectral superposition of QDs and atoms, have been recently attracting a lot of attention. Atomic vapors have shown their potential in efficient filtering, based on the Faraday rotation. The so called "Faraday anomalous dispersion optical filter" is realized placing an atomic vapor cell in a magnetic field and between two crossed polarizers. It displays the complete rejection of the optical spectrum, except for wavelengths close and on the atomic transitions. Transmission efficiency close to unity makes them ideal filters for practical applications. Here we present the filtering of QDs emission in the vicinity of the Cs D1 line. The QD is resonantly driven in the so called dressed state regime, resulting in the Mollow triplet spectrum. The spectrum can be tuned to have both sidebands resonant with the atomic filter, and hence transmitted, while the Rayleigh peak as well as the scattered laser, is strongly suppressed.

HL 53.23 Wed 9:30 Poster A

Polarization dependent coherent photocurrent spectroscopy of single InAs quantum dots at 1500 nm — •Simon Gordon[1], Matusala Yacob[2], Yves Alexander Leier[1], Mohamed Benyoucef[2], Johann Peter Reithmaier[2], and Artur Zrenner[1] — [1]CeOPP, Universität Paderborn, Paderborn, Germany — [2]INA, Universität Kassel, Kassel, Germany

For long distance quantum communication it is essential to use flying qubits in the telecom wavelength bands. Quantum emitters or detectors in this wavelength regime can be realized with InAs quantum dots (QDs) on InP substrate. In this work, such InAs QDs are investigated by low-temperature photocurrent spectroscopy. Suitable p-i-n diode structures with self-assembled QDs have been grown by molecular beam epitaxy on InP(100) substrates. The layer sequence of the diodes consists of an n-InP back contact, an intrinsic region of lattice-matched InAlGaAs, which contains the QDs – elongated in [0-11] direction –, and a p-InP front contact. The QDs are coherently excited by an optical parametric oscillator. By changing the applied reverse voltage the resonance energy of the QD is tuned by the quantum confined Stark effect to the energy of the light pulse. By increasing the power of the excitation light pulses, we observe a clear signature of Rabi oscillations in the photocurrent. To investigate the fine structure splitting of the exciton, we also performed polarization dependent photocurrent measurements, which reveal a polarization alignment along the [0-11] and the [011] crystal axis. We are further able to estimate the Rabi frequencies of the two ground state transitions.

HL 53.24 Wed 9:30 Poster A

Hybrid approach towards fast electronic control of quantum dot — •Alex Widhalm[1], Amlan Mukherjee[1,2], Nandlal Sharma[1], Dirk Reuter[1,3], Andreas Thiede[2,3], and Artur Zrenner[1,3] — [1]Department Physik, Universität Paderborn, Warburger Str. 100, 33098 Paderborn, Germany — [2]Höchstfrequenzelektronik, Universität Paderborn, Warburger Str. 100, 33098 Paderborn, Germany — [3]Center for Optoelectronics and Photonics Paderborn (CeOPP), Universität Paderborn, Warburger Str. 100, 33098 Paderborn, Germany

A hybrid approach to coherent manipulation of transitions in a quantum dot using combinations of electric and optical pulses promises possibilities of new quantum devices. In this work, we intend to demonstrate a technique for nonlinear and coherent control of transitions within the coherence time in InGaAs quantum dot photodiodes by ultrafast electric fields. The new functional structure comprises of a SiGe hetero-bipolar electronic circuit which generates picosecond electric fields to drives a single quantum dot photodiode. While the amplitude of excited states can be coherently controlled with optical pulses, the coherent phase and resonance conditions for exciton and biexciton transitions can be manipulated by ultrafast Stark effect tuning. Here we present the room temperature characteristics of the first generation picosecond pulse circuit designed. Also, we report the progress in the system integration and design of fast quantum dot photodiode.

HL 53.25 Wed 9:30 Poster A

Improving the indistinguishability of single-photons from resonantly excited single semiconductor quantum dots — •Jonas H. Weber, Eva Schöll, Jan Kettler, Markus Müller, Simone L. Portalupi, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen, Universität Stuttgart, Germany

Single-photons from single semiconductor quantum dots are promising candidates for a number of applications within quantum information technology. As a key feature in various implementations, e.g. linear optical quantum computation, maximum photon indistinguishability is needed and therefore an important goal of on-going research. Two-photon interference in an optimised Hong-Ou-Mandel-like experiment was used to determine the degree of indistinguishability. On the way towards Fourier-limited photons, requirement for perfect indistinguishability, different excitation methods were investigated in order to minimise dephasing mechanisms in the quantum emitter. In contrast to above-band excitation, resonant pumping of the exciton state excites single electron-hole pairs, thereby reducing spectral diffusion. Another promising excitation scheme relies on the use of two-photon excitation to prepare the biexciton state. That simplifies the photon detection due to the spectral separation of pump beam and signal, improving the signal-to-noise ratio. In future experiments, we will focus on several approaches for the stabilisation of the two-level system. With an applied magnetic field, it is possible to compensate for the Overhouser field. Furthermore, an electric field can be applied to stabilise the Fermi level, also enabling slight tuning of the emission line.

HL 53.26 Wed 9:30 Poster A

Analysis of the energy transfer in Mn doped CdS/ZnS quantum dots funtionalized with organic dye molecules — •Mikko Wilhelm[1], Uwe Kaiser[1], Luise Rost[1], Carolina Carrillo-Carrion[1], Nadeem Sabir[1], Pablo Del Pino[2], Wolfgang Parak[1], and Wolfram Heimbrodt[1] — [1]Philipps-University Marburg, Germany — [2]CIC Biomagune, San Sebastian, Spain

The luminescence and energy transfer characteristics of colloidal core shell CdS/ZnS quantum dots doped with manganese in the ZnS shell are investigated. Next to a luminescence band around 430nm from the CdS core a luminescence band typical for the manganese around 580nm can be observed after successful doping. Moreover, the quantum dots are functionalized with an organic dye. Time resolved measurements are used to investigate the Förster resonance energy transfer in the system and show a dye lifetime in the millisecond range, compared to a lifetime of a few nanoseconds for the pure dye. This is due to the quantum dot and manganese states acting as donors for the dye states. These properties are furthermore studied in dependence of the temperature. The quantum dots are therefore transferred from solution via drop casting on a quartz substrate. A change in the intensity and the lifetime of the different luminescence band is observed at low temperatures. Furthermore the manganese ions provide a magnetic moment to the system and the influence of a magnetic field on the luminescence is discussed.

HL 53.27 Wed 9:30 Poster A

Coherence time analysis of long-wavelength InAs quantum dots — •Fabian Olbrich, Jan Kettler, Matthias Paul, Simone Luca Portalupi, Michael Jetter, and Peter Michler — Universität Stuttgart, Institut für Halbleiteroptik und Funktionelle Grenzflächen, Allmandring 3, 70569 Stuttgart

One promising light source for applications in quantum communication, e.g. quantum cryptography or quantum computation is given by semiconductor quantum dots. Since properties like single-photon emission ensuring secure data transfer and indistinguishability providing low error computation are essential requirements for many communication protocols, they have to be deeply investigated and improved.

Dephasing plays an important role for these characteristics and one can gather information about this effect considering linewidth and coherence time studies.

Therefore we compared the PL spectra and coherence times of our MOVPE-grown In(Ga)As/GaAs quantum dots, placed in a planar cavity structure under non-resonant excitation. Their emission wavelengths are varying from 1 micron to the telecom O-band (1.3 micron).

Furthermore, first two-photon interference measurements under non-resonant and (quasi-)resonant excitation will be discussed.

HL 53.28 Wed 9:30 Poster A

Micro-Photoluminescence Spectroscopy and CCD-Imaging of Optically Coupled Microdisk Dimer-Structures — •Simon Seyfferle[1], Fabian Hargart[1], Matthias Paul[1], Michael Jetter[1], Tsung-Li Liu[2], Evelyn Hu[2], and Peter Michler[1] — [1]Institut für Halbleiteroptik und Funktionelle Grenzflächen, Universität Stuttgart, Allmandring 3, 70569 Stuttgart — [2]School of Engineering and Applied Sciences, Harvard University, 29 Oxford Street, Cambridge, MA 02138

The coupling of optical microcavities forming photonic molecules allows for interesting cQED devices, e.g. low threshold lasers and single-photon sources. Providing high Q-factors and small mode volumes microdisk structures put themselves forward for the investigation of optically coupled photonic molecules.

We investigate two adjacent GaInP-based microdisks coupled via the evanescent field of their whispering-gallery modes. Each 5 μm diameter disk houses an active layer of InP semiconductor quantum dots. Additionally to the already successfully established temperature tuning approach by local laser heating that brings uncoupled modes into resonance, we search for disk pairs displaying already coupled modes by means of μ -PL spectroscopy scans applying a $4f$-setup.

Furthermore, we undertake efforts in real space CCD-imaging of the dimer structures mode profile to obtain additional evidence of optically coupled disk pairs.

HL 53.29 Wed 9:30 Poster A

Electrical Properties of Single As-Grown Semiconductor Core-Shell Nanowires — •Danial Bahrami[1], Genziana Bussone[2], Jovana Colvin[3], Hanno Küpers[4], Ryan B Lewis[4], Rainer Timm[3], Lutz Geelhaar[4], and Ullrich Pietsch[1] — [1]University of Siegen, Solid State Physics department , Siegen, Germany — [2]Deutsches Elektronen-Synchrotron, Hamburg, Germany — [3]Lund University, NanoLund and division of Synchrotron Radiation Research, Lund, Sweden — [4]Paul Drude Institut für Festkörperelektronik, Berlin, Germany

Core-shell nanowire (NW) heterostructures have been employed in device applications including photonics, sensors, and electronics. Understanding and control of electrical properties, e.g. resistivity and mobility, in these NWs is necessary for their integration into the respective devices. For conventional conductivity studies, the NW is removed from the substrate, deposited horizontally and contacted with electrodes in as-called field-effect transistor geometry. Here, we report on conductivity measurements at single NWs in their as-grown geometry onto the substrate by means of FIB/SEM and AFM systems. Using either a tungsten nano-manipulator probe installed inside the FIB/SEM or a sharp metallic tip of a conductive AFM, the I-V characteristics of selected GaAs/InGaAs core-shell NWs grown by MBE onto Silicon (111) have been measured. The I-V characteristic always shows a nonlinear behavior with different slope comparing different NWs grown on the same substrate. The data can be analyzed in terms of thermoionic emission theory.

HL 53.30 Wed 9:30 Poster A

Ray Optics with Ballistic Electrons — •Jaan Freudenfeld[1], Sergey Platonov[1,2], Vladimir Umansky[3], and Stefan Ludwig[1,2] — [1]Center for NanoScience & Fakultät für Physik, LMU-Munich,

80539 München, Germany — [2]Paul-Drude-Institut für Festkörperphysik Hausvogteiplatz 5-7 10117 Berlin, Germany — [3]Weizmann Institute of Science, Rehovot 76100, Israel

Precise control of the motion of ballistic electrons on the nanoscale would be a major step towards the realization of integrated electronic quantum circuits. We explore the feasibility of ray optics with ballistic electrons in a high mobility two-dimensional electron system to reach this goal. Our device contains two gate defined quantum point contacts coupled either via parabolic mirrors or an electrostatic lens. A lens for electron diffraction works by modulation of the Fermi velocity just as light is diffracted if its velocity is modulated [1,2]. We present first experiments of the coupled conductance of two QPCs in series, where the QPCs are located in the focus points of a lens in between.

[1] J. Spector et al., Appl. Phys. Lett. 56, 1290 (1990)
[2] U. Sivan et al., Phys. Rev. B 41, 7937(R) (1990)

HL 53.31 Wed 9:30 Poster A

Ambipolar transport in GaAs/InSb core/shell nanowires — •Johanna Janssen[1,3], Patrick Zellekens[1,3], Franz Josef Hackemüller[1,3], Fabian Haas[1,3], Torsten Rieger[1,3], Nataliya Demarina[2,3], Mihail Lepsa[1,3], Detlev Grützmacher[1,3], Hans Lüth[1,3], and Thomas Schäpers[1,3] — [1]Peter Grünberg Institute 9 — [2]Peter Grünberg Institute 2, Forschungszentrum Jülich, 52425 Jülich, Germany — [3]JARA - Fundamentals of Future Information Technologies

Modern epitaxial growth technology of semiconductor nanowires allows the formation of complex axial and radial heterostructures and the combination of materials comprising a large lattice mismatch. In this context, nanowires constituted by a GaAs core and a surrounding InSb shell are very interesting systems. They combine the large g-factor and carrier mobility of InSb and the possibility of band engineering by changing the diameter of the GaAs core.

In this contribution, we present field-effect measurements of GaAs/InSb core/shell nanowires at room temperature. For InSb shells with a thickness smaller or equal to 10 nm, we observe a hole dominated ambipolar transport behavior. By increasing the thickness of the InSb shell, the p-type branch of the gate-dependent conductance is suppressed until the nanowires become purely n-type for shell thicknesses larger than 30 nm. This result agrees well with theoretical calculations which predict a diameter-dependent semiconductor-to-semimetal transition for GaAs/InSb core/shell nanowires due to the formation of a type-III, i.e. broken, band alignment.

HL 53.32 Wed 9:30 Poster A

Imaging of Condensed Quantum States in the Quantum Hall Effect Regime — Josef Oswald[1] and •Rudolf A. Römer[2] — [1]Leoben University, Franz Josef Str. 18, A-8700 Leoben, Austria — [2]University of Warwick, Coventry CV4 7AL, UK

It has been proposed already some time ago that Wigner crystallization in the tails of the Landau levels may play an important role in the quantum Hall regime. Here we use numerical simulations for modelling condensed quantum states and propose real space imaging of such highly correlated electron states by scanning gate microscopy (SGM). The ingredients for our modelling are a many particle model that combines a self-consistent Hartree-Fock calculation for the steady state with a non-equilibrium network model for the electron transport. If there exist condensed many particle quantum states in our electronic model system, our simulations demonstrate that the response pattern of the total sample current as a function of the SGM tip position delivers detailed information about the geometry of the underlying quantum state. For the case of a ring shaped dot potential in the few electron limit it is possible to find regimes with a rigid (condensed) charge distribution in the ring, where the SGM pattern corresponds to the probability density of the quantum states. The existence of the SGM image can be interpreted as the manifestation of an electron solid, since the pattern generation of the charge distribution requires certain stability against the moving tip potential.

HL 53.33 Wed 9:30 Poster A

Optical and magnetic studies of MBE-grown ferromagnetic CrSe and CrS layers in zincblende structure — •Johannes Röder[1], Nico Hofeditz[1], Richard T Moug[2], Kevin A Prior[2], Dana Vieweg[3], Hans-Albrecht Krug von Nidda[3], Alois Loidl[3], and Wolfram Heimbrodt[1] — [1]Department of Physics and Material Science Center, Philipps University, Marburg, Germany — [2]Institute of Photonics and Quantum Sciences, SUPA, School of Engineering and Physical Sciences, Heriot-Watt University, Edinburgh, UK — [3]Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, Germany

Theoretical calculations predicted Chromium chalcogenides in the zinc blende (ZB) structure to be promising candidates for half-metallic spin-aligner at room temperature. Unfortunately, the thermodynamically stable phase of CrSe and CrS is the hexagonal NiAs-structure. Different approaches have been tested to stabilize the ZB state. Most promising were CrSe layers grown on GaAs substrates with either ZnSe or ZnSe/MgS as buffer layers and CrS-layers embedded between ZnMgS layers. All samples have been grown by MBE. We investigated the ferromagnetic properties and magnetic phase transitions and the respective optical properties of these films by temperature dependent SQUID and photoluminescence measurements. Ferromagnetic phase transitions have been found. The highest yet observed Curie temperature was at 255 K. Optical measurements revealed excitonic transitions, which will be discussed in detail.

HL 53.34 Wed 9:30 Poster A

Towards bright electrically driven single-photon sources in the red spectral range using In-Situ Lithography — •Marc Sartison, Simone Luca Portalupi, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen and Research Centers SCoPE and IQST, Universität Stuttgart, Allmandring 3, 70569 Stuttgart, Germany

Semiconductor quantum dots (QDs) have high potential as single-photon light sources in quantum information technologies. Usually, high quality QDs are deposited in Stranski-Krastanov growth mode resulting in a random distribution in position on the sample and in size. Moreover, also the emission energies and the linewidth of single QDs vary due to this deposition scheme. For the fabrication of an efficient bright single-photon source, it is necessary to place the QD at the proper position inside a micro-cavity device. We present a method to find a suitable QD and process the fitted device around the selected QD with an optical lithography method. For this, a sample with resist is placed into the cryostat for optical inspection at 4K. After optical identification of the right QD, the resist is exposed by a green laser to form the mask for the device. Then, the usual semiconductor processing steps including further in-situ lithography form the target electrical resonant cavity LED.

HL 53.35 Wed 9:30 Poster A

Hydrogen sensing with sub-micrometer Pt/TiO2 sensors — Svenja Herbertz, •Mihai Cerchez, and Thomas Heinzel — Heinrich Heine University Düsseldorf, Universitätsstr. 1, D-40225 Düsseldorf

Pt/TiO2 hydrogen sensors are technically well established although the underlying physics is still at debate due to incomplete understanding of the interplay between oxygen vacancies, titanium interstitials, and hydrogen incorporation in disordered systems. In addition, operational voltages required may lead to electroforming effects [1]. Here we present a submicrometer lateral sensor produced by local anodic oxidation of a Ti thin layer evaporated on an insulating layer. A brief Pt evaporation produces clusters of Pt at the TiO2 without shortcutting the lateral contacts [2]. We discuss the sensing and the influence of oxygen and humidity as well as electroforming effects.

[1] M. Strungaru, M. Cerchez, S. Herbertz, T. Heinzel, M. El Achhab, and K. Schierbaum, Appl. Phys. Lett. 106, 143109 (2015)
[2] S. Herbertz, M. Cerchez and T. Heinzel, Sensors and Actuators B 221, 401 (2015)

HL 53.36 Wed 9:30 Poster A

GaAs nanowire photodetectors with avalanche multiplication — •Stepan Shvarkov[1], Wadim Quiring[2], Artur Zrenner[2], and Dirk Reuter[1] — [1]Optoelektronische Materialien und Bauelemente, Universität Paderborn, Warburgerstr.100, 33098, Paderborn, Germany — [2]Optoelektronik und Spektroskopie an Nanostrukturen, Universität Paderborn, Warburgerstr.100, 33098, Paderborn, Germany

Efficient single photon detectors (SPD) working at the telecom wavelength (1.5 um) are essential for the establishment of fiber-based quantum communication networks. GaAs-based heterostructures are in principle suited for this task. In this contribution, we present a SPD design based on a lateral p-i-n-junction within a nanowire. This should allow for efficient absorption of the photons and avalanche multiplication of the photo-generated carriers. The GaAs nanowires based detectors are fabricated using combination of optical and electron beam lithography. The formation of n- and p-type regions is realized by ion

beam implantation through a hard mask. The non-implanted region of about 10 um separates n- and p-type areas. After post-implantation rapid thermal annealing and contacts fabrication the wires of a different thickness are fabricated using electron beam lithography and reactive ion etching. The devices show rectifying current-voltage characteristics typical for p-i-n junctions. The reverse biased nanowires show very low dark currents and are very sensitive to illumination which is attributed to the avalanche multiplication of the photo-generated electron-hole pairs.

HL 53.37 Wed 9:30 Poster A

Design of single-mode waveguides with integrated quantum dots for on-chip single-photon operations — •Ulrich Rengstl, Mario Schwartz, Thomas Herzog, Matthias Paul, Simone Luca Portalupi, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen (IHFG), Research Center SCoPE and IQST, Universität Stuttgart, Allmandring 3, D-70569 Stuttgart

The future use of linear optics quantum computation depends on a miniaturization and therefore a full integration of single-photon sources, beamsplitters and detectors on single chips. III-V semiconductors are promising candidates for the realization of such devices due to the simple implementation of quantum dots (QDs) as single-photon sources.

We present the integration of QDs in rib-type GaAs/AlGaAs waveguides. The design of the waveguides was optimized for the exclusive propagation of the fundamental TE- and TM-mode using frequency-domain simulations to obtain the mode profiles and dispersion diagrams. Time-domain simulations and measurements of propagation losses around 2.6 dB/mm depict the coupling of the QDs to low-loss propagation modes. The single-mode TE operation of our device is shown by the high degree of polarization of the propagating light.

An additional on-chip evanescent field coupler forms a 50:50 beamsplitter as fundamental operation on single photons. The purity of our integrated single-photon source is verified by cross-correlation measurements on the output arms of the beamsplitter.

HL 53.38 Wed 9:30 Poster A

Tunable lasing from hexagonal ZnO micro wires at room temperature — Tom Michalsky, •Marcel Wille, Evgeny Krüger, Helena Franke, Marius Grundmann, and Rüdiger Schmidt-Grund — Institut für Experimentelle Physik II, Universität Leipzig, Linnéstraße 5, D-04103 Leipzig, Germany

We demonstrate a hexagonal ZnO micro wire resonator (MW) whose emission wavelength can be finely tuned. Furthermore one can switch between single- or dual mode operation. For that we use a slightly tapered MW with a diameter range (∼resonator length) that allows only one or two whispering gallery modes (WGMs) to be amplified by gain from an electron-hole plasma. The emission wavelength as well as single- or dual mode operation can be set by choosing the matching wire diameter and thus resonator length by slightly changing the position of the excitation spot on the wire in micro photoluminescence experiments. It turnes out that the modes in lasing operation are purely TE polarized. We also present an approach to increase the WGMs' quality factor (∼lifetime) by a factor of five by sandwiching the hexagonal wire resonator between two planar distributed Bragg reflectors.

HL 53.39 Wed 9:30 Poster A

Coexistence of strong and weak coupling in ZnO nanowire cavities — Tom Michalsky[1], Helena Franke[1], •Oliver Herrfurth[1], Robert Buschlinger[2], Ulf Peschel[2], Marius Grundmann[1], and Rüdiger Schmidt-Grund[1] — [1]Institut für Experimentelle Physik II, Universität Leipzig, Linnéstraße 5, D-04103 Leipzig, Germany — [2]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

We present a high quality two dimensional cavity structure based on concentrically Bragg reflector coated ZnO nanowires acting as active material. The spatial mode distribution allows for the simultaneous appearance of the weak and strong exciton-photon coupling regime even at room temperature which is shown experimentally by photoluminescence measurements as well as reproduced by FDTD simulations. The high quality ZnO core nanowires uniquely allow for the observation of middle polariton branches between the A- and B-exciton ground state resonances in ZnO. Further, lasing emission is observed by excitation dependent PL measurements up to room temperature.

HL 53.40 Wed 9:30 Poster A

Sub-Monolayer-Control in Epitactic Growth of Quantum Cascade Lasers — •Michael Kwiatek[1], Negar Hekmat[2], Arne Ludwig[1], Nathan Jukam[2], and Andreas D. Wieck[1] — [1]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum — [2]AG Terahertz-Spektroskopie und Technologie, Ruhr-Universität Bochum

A quantum cascade laser (QCL) consists of multiple vertically stacked semiconductor modules including several well-dimensioned quantum wells. In QCLs intersubband transitions in the conduction band generate the laser light. Due to QCL's cascading structure, one electron generates multiple photons. The production of good QCLs sets high demands on the fabricating process, especially on the layer quality of the quantum wells and barriers, why QCL fabrication is often performed with Molecular Beam Epitaxy (MBE). A known problem in MBE is the shutter transient of the effusion cells (EC). When the EC-shutter is closed, the heat of the EC is reflected back in itself. If the shutter is opened, more power is needed to stabilize the temperature and hence the material flux of the EC. For QCLs very thin material layers of only a few monolayers with high precision are crucial. The time the EC needs to stabilize leads to a change in the growth rate for those thin layers. Our goal is the reduction of the shutter transient effect and other growth related errors on the QCL's layer structure.

HL 53.41 Wed 9:30 Poster A

Towards Nanowire Lasers Integrated onto Silicon Waveguides — •Daniel Ruhstorfer, Thomas Stettner, Bernhard Loitsch, Julian Treu, Benedikt Mayer, Gerhard Abstreiter, Gregor Koblmüller, and Jonathan Finley — Walter Schottky Institut and Physik Department, TU München, Garching, Germany

III-V semiconductor nanowires (NW) have been shown to be a highly promising candidate for the monolithic integration of nanoscale lasers on silicon [1,2]. In this work we present our progress towards the growth and demonstration of III-V NW lasers on low-order mode waveguides.

We investigate the coupling of GaAs/AlGaAs core shell NW lasers with shallow silicon ridge waveguides. Our FDTD simulations show a tunable optical coupling efficiency of up to 20% while at the same time preserving high modal reflectivities required for NW lasing.

In our design we use <111> silicon on insulator (SOI) substrates in which the waveguides are patterned using electron beam lithography and reactive ion etching. The SOI substrates provide the advantage of strong modal confinement by high refractive index contrast while its thick buried oxide also provides a high reflectivity at the substrate interface. By thermal oxidation of the silicon surface, the waveguides are covered with a thin protective layer of silicon oxide. We further delineate the entire fabrication scheme of GaAs/AlGaAs core-shell NW lasers on SOI by employing molecular beam epitaxial growth on predefined nucleation sites directly on the silicon ridge waveguides.

[1] B. Mayer, et al. Nature Comm. 4, 2961 (2013).
[2] B. Mayer, et al. Nano Lett. 15, just accepted (2015).

HL 53.42 Wed 9:30 Poster A

THE INVESTIGATION OF PRESSURE EFFECT ON THE OPTICAL PROPERTIES, SPONTANEOUS POLARIZATION AND EFFECTIVE MASS OF BaHfO3: AB INITIO STUDY — •azahaf chaimae — aculté des Sciences, 4 Avenue Ibn Battouta B.P. 1014 RP, Rabat

Through first principles calculations, the optical properties, spontaneous polarization and the effective mass of the cubic perovskite BaHfO3 under pressure effect have been investigated, using the Full Potential Linearized Augmented Plane Wave (FP-LAPW) method implemented in the WIEN2K code, in connection with the Generalized Gradient Approximation (GGA). During this study, the effect of pressure is seen on the electronic and optical properties such as: The band gap value (Eg) of the perovskite BaHfO3 is reduced and it becomes indirect instead of direct band gap as pressure increased. From the band structure we have also computed the variation of effective masse (m*) which increases to the same effect as the pressure. The results of the optical study, shows that the absorption coefficient increases and the spontaneous polarization (Ps) increases in a quasi-linear behavior as pressure increases. Our conclusion is that BaHfO3 is a piezoelectric material; also this material could be applicable in optoelectronic applications.

HL 54: Frontiers of Electronic Structure Theory: Focus on Topology and Transport II

Time: Wednesday 10:30–13:00 Location: H24

HL 54.1 Wed 10:30 H24

Coupled-Cluster approach for both molecules and solids in the numeric atom-center orbital framework — •Tonghao Shen, Arvid Conrad Ihrig, Igor Ying Zhang, and Matthias Scheffler — *Fritz-Haber-Institut der MPG, Berlin.*

For a quantitative prediction of material properties, an advanced description of electronic correlation is crucial. As the "gold standard" correlation method in quantum chemistry, the coupled-cluster (CC) ansatz with singles, doubles and perturbative triples (CCSD(T)) is starting to gain attention in materials science[1]. At present, the CCSD(T)-quality description of the correlation effects in solids can be achieved by either studying the cluster-size convergence toward the bulk in real space[1] or implementing CCSD(T) for extended systems in reciprocal space[2]. In order to investigate and compare these approaches on an equal footing, it is essential to have a computational platform that enables CCSD(T) simulations to be carried out using both cluster and periodic models in a single computational environment. In this report, we present a CCSD(T) implementation for both molecules and solids in the all-electron full-potential code FHI-aims[3] with numeric atom-center orbital(NAO) basis sets. A special memory-distribution strategy is designed to significantly reduce the inter-CPU communication, which is the main challenge for the parallelization of wave-function methods. The accuracy and efficiency are demonstrated for a group of molecules, 1D-, 2D- and 3D-periodic materials. [1] C. Müller, *et al.*, PCCP. **14**, 7605 (2012); [2] A. Grüneis, *et al.*, JCTC **7**, 2780 (2011); [3] V. Blum, *et al.*, CPC **180**, 2175-2196 (2009).

HL 54.2 Wed 10:45 H24

Surface adsorption energetics at the "gold standard": Small molecule binding to TiO_2(110) — •Daniel Berger[1,2], A. Kubas[3], D. Manganas[3], H. Oberhofer[1], F. Neese[3], and K. Reuter[1] — [1]TU München — [2]University of California, Los Angeles — [3]MPI für chemische Energiekonversion, Mülheim an der Ruhr

Adsorption energies at oxide surfaces are central quantities required for catalysis, energy and a multitude of other application areas. At present, the by far dominant computational method to obtain such energetics is density-functional theory (DFT). Unfortunately, systematic benchmarking of such energetics against accurate reference numbers from correlated wave-function theory as known from molecular systems is scarce, largely owing to the fact that the latter techniques are often not available for standard periodic boundary condition supercell calculations.

We address this situation with a solid-state QM/MM embedded cluster approach, in which the adsorbate and immediate surrounding surface atoms are described quantum mechanically, while the long-range electrostatic interactions are accounted for through a polarizable force field. This yields a numerically highly efficient approach that enables use of the recently developed domain-based local pair natural orbital coupled cluster method with single-, double- and perturbative triple-excitations (DLPNO-CCSD(T)) in the quantum region. We exploit corresponding "gold standard" adsorption energies for a set of prototypical small molecules interacting with the rutile TiO_2(110) surface for a systematic benchmark of DFT numbers.

HL 54.3 Wed 11:00 H24

Water adsortpion on surfaces form many-body perturbation theory — •Theodoros Tsatsoulis and Andreas Grüneis — Max-Planck-Institute for Solid State Research, Stuttgart

The accurate description of the interaction of molecules with surfaces is of crucial importance for a wide range of phenomena. While Kohn-Sham density functional theory is one of the most widely-used methods for describing the electronic structure of surfaces, many local and semi-local functionals are often not able to produce accurate molecular adsorption energies. Quantum chemical wave-function based methods such as Møller-Plesset perturbation theory (MP2) and coupled-cluster methods promise controllable accuracy, however, at much higher computational costs. Large part of the latter is due to the number of virtual states. We consider an approach whereby the occupied orbitals are converged in a plane wave basis, whereas the virtual space is then constructed using pseudized Gaussian orbitals expanded in plane waves, leading to reduced computational cost. In particular we study water adsorption on bulk LiH and h-BN sheets at the level of MP2 theory within the projector-augmented-wave method as implemented in VASP [1]. The results are compared to state-of-the-art methods such as hybrid functionals and diffusion Monte Carlo [2].

[1] Marsman et al., The Journal of Chemical Physics, 130, 184103 (2009)

[2] Al-Hamdani et al., The Journal of Chemical Physics, 142, 181101 (2015)

HL 54.4 Wed 11:15 H24

Photo-isomerization in azobenzene-functionalized self-assembled monolayers: The impact of many-body effects — •Caterina Cocchi and Claudia Draxl — Institut für Physik und IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany

Self-assembled monolayers (SAMs) of azobenzene-functionalized alkanethiols on gold suffer from hindered photo-isomerization, as observed experimentally [1]. While this behavior is generally ascribed to strong intermolecular coupling, a clear microscopic understanding of this phenomenon is still missing. In order to address this question, we perform a first-principles study of the excited-state properties of azobenzene-functionalized SAMs. In the framework of many-body perturbation theory (GW approximation and Bethe-Salpeter equation), as implemented in the all-electron full-potential code exciting [2], we investigate the optical absorption spectra of these materials, inspecting the influence of packing density and functionalization of the azobenzene molecules with different end groups. Through a systematic analysis of the character of the excitations, we clarify the role and interplay of screening and local-field effects, which strongly impact light absorption and hence photo-isomerization in these systems.

[1] C. Gahl et al. J. Am. Chem. Soc. 132, 1838 (2010). [2] A. Gulans et al. J. Phys.: Condens. Matter 26, 363202 (2014).

HL 54.5 Wed 11:30 H24

Laplace-transformed MP2 with localized Resolution of Identity -efficient in-memory MP2 for large systems — •Arvid Conrad Ihrig[1], Patrick Rinke[2], Igor Ying Zhang[1], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]Aalto University, Helsinki, Finland

A well-known problem in local and semi-local density functional approximations and to a lesser extend also in hybrid functionals is the one-electron self-interaction error, which can lead to a qualitatively wrong description for applications like charge-transfer systems. One possible remedy is the 2nd order Møller-Plesset perturbation theory (MP2), which does not suffer from this error. However, the time and memory requirements for MP2 prevent it routine-use for large molecular and periodic systems. The Laplace-transformed MP2 (LT-MP2) [1] can significantly reduce the computational time, but requires the usage of intermediate variables stored on disk, resulting in an inefficient usage of computational resources. In this work we combine the LT-MP2 with our localized Resolution of Identity (RI-LVL) [2] approach to eliminate the disk-storage bottleneck and fully exploit massive parallelization strategies. RI-LVL expands the basis function pairs in the electron repulsion integrals in local auxiliary basis sets. For the example of water clusters, we demonstrate the favourable memory scaling (at worst N^2) of our new MP2 implementation, which facilitates the in-memory calculation of large systems at high accuracies.

[1] P. Ayala et al., J. Chem. Phys. 110, 3660 (1999)

[2] Ihrig et al., New J. Phys. 17, 093020 (2015)

HL 54.6 Wed 11:45 H24

***GW* singles contributions for the random phase approximation correlation energies** — •Jiri Klimes[1], Merzuk Kaltak[2], Emanuele Maggio[3], and Georg Kresse[3] — [1]J. Heyrovský Institute of Physical Chemistry, Prague, Czech Republic — [2]Department of Physics and Astronomy, Stony Brook University, Stony Brook, NY — [3]University of Vienna, Faculty of Physics, Vienna, Austria

The random phase approximation (RPA) to the correlation energy yields often very accurate results for condensed matter systems. However, a general tendency to underbind has been observed for systems such as molecular solids or for adsorption. One of the ways that have been proposed to improve the accuracy of RPA are the so-called singles corrections of Ren and coworkers [1]. We present our derivation of the singles corrections using the assumption that the electron density

changes when going from the reference to the interacting system [2]. This leads to a very compact expression for the corrections. Moreover, the singles formula can be easily modified to account for screening effects, giving the *GW* singles. We assess the effect of both the original and modified singles on covalently and metallically bonded systems as well as on simple weakly bonded systems. Finally, we show that adding the singles corrections leads to considerably improved adsorption energies and lattice energies of molecular solids.

[1] Ren, Tkatchenko, Rinke, Scheffler, Phys. Rev. Lett **106**, 153003 (2010).

[2] Klimeš, Kaltak, Maggio, Kresse, J. Chem. Phys. **143**, 102816 (2015).

HL 54.7 Wed 12:00 H24

Long-range corrected DFT meets *GW*: Vibrationally resolved photoelectron spectra from first principles — •Thomas Körzdörfer — Institut für Chemie, Universität Potsdam, D-14476 Potsdam

We introduce an entirely non-empirical and computationally efficient scheme to calculate highly reliable vibrationally resolved photoelectron spectra for molecules from first principles.[1] To this end, we combine non-empirically tuned long-range corrected hybrid functionals with non-self-consistent many-body perturbation theory in the G_0W_0 approximation and a Franck-Condon multi-mode analysis based on DFT-calculated frequencies. The vibrational analysis allows for a direct comparison of the GW-calculated spectra to gas-phase ultraviolet photoelectron measurements of neutral and anionic molecules, respectively. In addition, vertical IPs and EAs were benchmarked against other *GW* methods and basis-set extrapolated CCSD(T) results for a recently introduced test set of 24 molecules frequently used in organic electronics.[2] G_0W_0@LRC-DFT yields mean absolute errors on the order of 0.1 eV for IPs, EAs, and fundamental gaps, clearly outperforming commonly used G_0W_0 approaches as well as partially and fully self-consistent *GW* methods.

[1] L. Gallandi and T. Körzdörfer, JCTC **11**, 5391 (2015).
[2] L. Gallandi, N. Marom, P. Rinke, and T. Körzdörfer, JCTC *accepted for publication* (2015).

HL 54.8 Wed 12:15 H24

LDA-1/2 as a starting point for G_0W_0 calculations — •Ronaldo Rodrigues Pela[1,2], Ute Werner[1], Dmitrii Nabok[1], and Claudia Draxl[1] — [1]Humboldt-Universität zu Berlin, Institut für Physik and IRIS Adlershof, Berlin, Germany — [2]Instituto Tecnológico de Aeronáutica, São José dos Campos, Brazil

For many semiconductors and insulators, LDA represents a bad starting point for G_0W_0 calculations. Hybrid functionals improve upon LDA, but at the price of increasing computational cost of about 2 orders of magnitude. An alternative starting-point for the single-shot G_0W_0 can be the LDA-1/2 method [1], because it approximately includes the self-energy of quasi-particles within a generalized Kohn-Sham scheme, leading to improved band-gaps over the LDA ones, but without being computationally more involved. In this work, we systematically compare 3 starting-points for G_0W_0 calculations: LDA, PBE0, and the LDA-1/2 method. A selection of semiconductors (C, Si, SiC, AlP, LiF, MgO, Ne, Ar, GaN, GaAs, CdS, ZnS, and ZnO) is chosen for this benchmark. We demonstrate that LDA-1/2 is a good choice in most cases, reducing the root mean square error in band-gap predictions by 50% when compared to G_0W_0 on top of LDA or PBE0. With the exception of large band gap materials, LDA-1/2 predictions are already close to the experimental band gaps, and thus G_0W_0 has minor effects.

Reference [1]: Phys. Rev. B 78, 125116 (2008).

Acknowledgements: "Coordenação de Aperfeiçoamento de Pessoal de Nível Superior" (CAPES) and "Alexander von Humboldt Stiftung".

HL 54.9 Wed 12:30 H24

DFT+U within a numeric atom-centered orbital basis — •Matthias Kick, Harald Oberhofer, and Karsten Reuter — Technische Universität München

Materials like transition metal oxides (TMOs) still challenge a description through first-principles density-functional theory (DFT). Appropriately capturing the electron localization in TMOs generally requires at least hybrid exchange-correlation functionals. Such higher-rung functionals come with appreciable computational cost, which limits their use in large supercell calculations. For such applications effective and numerically less intense approaches are therefore still a much sought alternative.

One such method is the DFT+U approach, where the on-site Coulomb correlation effects are treated using a model Hamiltonian, while remaining interactions are treated on the level of semi-local DFT. Full DFT+U functionality including nuclear gradients (forces) has been implemented in the electronic structure code *FHI-aims*. We account for three common occupation matrix representations, differing in the way how the occupations of the correlated subspaces are determined. We critically discuss their performance and differences in the context of the numeric atomic orbital basis sets employed in *FHI-aims*. The established numerically efficient framework is finally used to address neutral and charged oxygen vacancies at the TiO_2(110) surface within a solid-state embedding approach.

HL 54.10 Wed 12:45 H24

High-throughput Screening and Statistical Learning for Design of Transparent Conducting Oxides — •Christopher Sutton, Luca M. Ghiringhelli, and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft

Transparent conducting oxides (TCOs) represent a class of well-developed and commercialized wide-bandgap semiconductors that are crucial for many electronic devices. Ternary Al, Ga, and In-based sesquioxides are investigated as alternative wide-bandgap semiconductors motivated by very intriguing recent experimental work that has demonstrated bandgap engineering in (GayIn1-y)2O3 from 3.8 eV to ca. 5 eV[1] and ca. 5 eV to 7.5 eV for (Al1-xGax)2O3.[2]

New ternary oxides with the chemical structure of (AlxGayIn1-x-y)2O3 have been identified using cluster expansion (CE) models combined with fast stochastic optimization techniques (e.g., Wang-Landau and diffusive nested sampling) in order to efficiently search potential (ordered and disordered) configurations within a given lattice and for different temperatures. Wang-Landau and diffusive nested sampling has also allowed for a consideration of the effect of entropy on the relative stability of ternary oxides. Statistical learning has also been used to identify a structure-property relationship to efficiently identify new wide-band gap TCOs to improve the fundamental chemical and physical properties (e.g., conductivities, mobilities, and optical transparency) by investigating the parameters that control these properties.

[1] F Zhang, et al., Solid State Communications 2014, 186, 28. [2] H Ito, et al., Japanese Journal of Applied Physics 2012, 51, 100207.

HL 55: Photonics and Nanooptics I: Nonlinear Response

Time: Wednesday 10:30–13:15 Location: S051

HL 55.1 Wed 10:30 S051

Nonlinear Plasmonic Sensing — •Martin Mesch, Bernd Metzger, Mario Hentschel, and Harald Giessen — 4th Physics Institute and Research Center SCoPE, University of Stuttgart, Germany

We introduce the concept of *nonlinear* plasmonic sensing, relying on third harmonic generation from simple plasmonic nanoantennas. Due to the nonlinear conversion process we observe a larger sensitivity upon a local change in the refractive index as compared to the commonly used linear localized surface plasmon resonance sensing. Refractive index changes as small as 10^{-3} can be detected. In order to determine the spectral position of highest sensitivity, we perform linear and third harmonic spectroscopy on plasmonic nanoantenna arrays, which are the fundamental building blocks of our sensor. Furthermore, simultaneous detection of linear and nonlinear signals allows quantitative comparison of both methods, providing further insight into the working principle of our sensor. While the signal-to-noise ratio is comparable, nonlinear sensing gives about seven times higher signal levels. Our scheme can be extended to other nonlinear processes such as second harmonic generation and sum frequency generation. This opens a new avenue in plasmonic sensing.

HL 55.2 Wed 10:45 S051

Investigation of Plasmonic Modes of Gold Tapers — •Surong

Guo[1], Nahid Talebi[1], Wilfried Sigle[1], Christian Knipl[1], Martin Esmann[2], Simon Becker[2], Ralf Vogelgesang[2], Christoph Lienau[2], and Peter van Aken[1] — [1]Max Planck Institute for Solid State Research , Heisenbergstraße 1, D-70569 Stuttgart, Germany — [2]Carl von Ossietzky Universität Oldenburg, Ammerländer Heerstraße 114-118, D-26129 Oldenburg, Germany

Plasmonic tapers have been studied intensively due to the ability of adiabatically coupling the propagating surface plasmon polaritons along their shaft to the nanolocalized plasmons at their apex. Therefore, they can find applications in the fields of sub-diffraction-limit nanofocusing, ultrafast photoemission, and near-field optical microscopy.

We investigate the plasmonic modes of three-dimensional single crystalline gold tapers by means of electron energy loss spectroscopy and numerical calculation. We observe discrete higher-order azimuthal plasmonic modes of the gold taper with an opening angle of ˜45° with energy dispersions roughly proportional to the inverse local radius. The importance of phase-matching between electron field and radiative taper modes in mesoscopic structure is demonstrated [1]. We further systematically study the changes in the dispersion of higher-order plasmonic modes of gold tapers versus the opening angle of the taper, both experimentally and theoretically.

[1] N. Talebi et al, ACS Nano, 2015, 9 (7), 7641-7648.

HL 55.3 Wed 11:00 S051

Nonlinear Emission of Electrons in a Strong Plasmonic Field — Daniel Podbiel[1], Philip Kahl[1], Bettina Frank[1], Harald Giessen[2], and •Frank Meyer zu Heringdorf[2] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, 47048 Duisburg, Germany — [2]4th Physics Institute and Research Center SCoPE, University of Stuttgart, 70550 Stuttgart, Germany

Observing surface plasmon polaritons (SPPs) in a photoemission electronmicroscope (PEEM) is possible via nonlinear photoemission if ultra-short laser pulses (<20fs) of a suitable wavelength are directed onto the surface of a plasmonic material. We study the time-resolved propagation and interaction of SPPs by means of a direct conceptual visualization of the SPPs in a "normal incidence geometry". This experimental setup allows us to observe transient phenomena that exist for only a few femtoseconds during the coherent interaction of the ultrashort SPP pulses. In focusing structures for SPPs we find an unexpected time-signature of the nonlinear photoemission signal at the focus point that must be explained by emission of electrons from the SPP alone. The energy distribution of these 'plasmoelectrons' shows that the SPP fields are sufficiently high to make nonlinear photoemission pathways of higher orders the dominant contribution to the PEEM signal.

HL 55.4 Wed 11:15 S051

Coherent control of photoemission from a single nanotip in a two-color scheme — •Michael Förster[1,2], Timo Paschen[1], Michael Krüger[1,2], Florian Libisch[3], Christoph Lemell[3], Georg Wachter[3], Thomas Madlener[3], Joachim Burgdörfer[3], and Peter Hommelhoff[1,2,4] — [1]Department Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Staudtstrasse 1, 91058 Erlangen — [2]Max-Planck Institut für Quantenoptik, Hans-Kopfermann-Str. 1, 85748 Garching — [3]Institute for Theoretical Physics, Vienna University of Technology, Wiedner Hauptstr. 8-10/E136, 1040 Wien — [4]Max-Planck Institut für die Physik des Lichts, Günther-Scharowsky-Str. 1/Geb. 24, 91058 Erlangen

We discuss coherent control of photoemission from a tungsten tip in a Brumer-Shapiro scheme. We observe that photoemission from the nanotip induced by a femtosecond laser displaying many multiphoton orders can be strongly enhanced or reduced by the presence of a weak second harmonic, depending on the phase between the laser pulses. With optimized parameters the phase-dependent contrast in the total emitted current can exceed 90%. Time-resolved data shows that emission takes place on femtosecond time scales. With the help of spectrally-resolved measurements and density functional theory calculations we interpret our observations in terms of interfering emission pathways.

HL 55.5 Wed 11:30 S051

Above threshold ionization of Rydberg electrons localized to a gold nanotip — •Jörg Robin[1], Jan Vogelsang[1], Benedek J. Nagy[2], Petra Gross[1], and Christoph Lienau[1] — [1]Carl von Ossietzky Universität, 26129 Oldenburg — [2]Wigner Research Centre for Physics, H-1121 Budapest

Metallic nanotips are model systems to study nanometre and femtosecond electron dynamics and provide the possibility for ultrafast electron microscopy. Evidence of strong-field phenomena has been observed by one-colour photoemission of electrons from metallic nanotips [1-3], while two-colour photoemission has established the existence of surface states on metallic films [4]. Here, we report femtosecond two-colour photoemission of electrons from a gold nanotip. We observe long-lived wave packets of Rydberg electrons bound to their own image potential. These intermediate bound states facilitate above-threshold ionization similar to atomic systems and give access to a cold, ultrafast, nanolocalized electron source. [1] Krüger, M. et al. Nature 475, 78 (2011) [2] Herink, G. et al. Nature 483, 190 (2012) [3] Piglosiewicz, B. et al. Nat. Photon. 9, 37 (2014) [4] Höfer, U. et al. Science 277, 1480 (1997)

HL 55.6 Wed 11:45 S051

Third harmonic efficiency scaling with plasmonic antenna length — •Maxim Nesterov, Mario Hentschel, Bernd Metzger, Harald Giessen, and Thomas Weiss — 4th Physics Insitute and Research Centre SCoPE, University of Stuttgart, 70550 Stuttgart, Germany

Nonlinear interaction of light with plasmonic structures leads to higher-order harmonic generation, such as second-order harmonics in non-centrosymmetric media, and third-order harmonics in centrosymmetric systems. Metallic antennas are characterized by a high field concentration at resonances, resulting in a relatively strong nonlinear optical response. The enhancement of higher-order harmonic generation depends on the size and shape of antenna, and a strong nonlinear signal can be achieved with a proper design.

We study scaling of the third harmonic generation with rod antenna length numerically for a single antenna, as well as for array configurations. The third-harmonic intensity is found to be increasing as a twelfth power of an antenna length in the model based on Miller's rule. We discuss applicability of the Miller's rule in the context of the origin of the nonlinear susceptibility in the metals. An analytical model has been developed to support the numerical results.

HL 55.7 Wed 12:00 S051

Nonlinear chiral plasmonics: Quantitative modeling of the third-harmonic response of 3D chiral plasmonic nanoantennas — •Lili Gui, Xinghui Yin, Mario Hentschel, and Harald Giessen — 4th Physics Institute and Research Center SCoPE, University of Stuttgart, 70569 Stuttgart, Germany

Optical activity exists generally in nature, as many biomolecules such as proteins are chiral. Chiral plasmonic nanostructures are highly interesting since they are potentially ideal and sensitive platforms for biosensing due to the strong superchiral near fields and their own giant chiroptical effects. Exploration of nonlinear chiroptical effects in chiral plasmonic structures is even more desired since the nonlinear chiroptical effects are typically orders of magnitude higher than the linear optical counterparts. Here we study the third-order nonlinear chiroptical effects of 3D chiral structures consisting of corner-stacked gold nanorods. Compared to second-order effects, third-order effects are more immune to fabrication defects and surface roughness. We experimentally investigate the third-harmonic spectroscopy with left- and right-circularly polarized fundamental light, respectively. The third-order chiroptical responses can be well understood when we utilize a coupled anharmonic oscillator model considering the phase retardation of light interaction with the 3D gold nanorods. This model is instructive to guide a practical design of plasmonic chiral structures for a giant third-harmonic-generation circular dichroism (THG-CD) effect.

HL 55.8 Wed 12:15 S051

Shaping the Nonlinear Near-Field of Single Gold Nanostructures — •Daniela Wolf[1,2], Julian Obermeier[1], Thorsten Schumacher[1], and Markus Lippitz[1] — [1]Experimental Physics III, University of Bayreuth, Universitaetsstr. 30, 95447 Bayreuth, Germany — [2]Max Planck Institute for Solid State Research, Heisenbergstr. 1, 70569 Stuttgart, Germany

Light scattering at plasmonic nanoparticles and their assemblies has led to a wealth of applications in metamaterials and nanooptics. While the shaping of fields around nanostructures is widely studied, the influence of the field inside the nanostructures is often overlooked. The linear field distribution inside the structure taken to the third power causes third-harmonic generation, a nonlinear optical response of matter. Here we demonstrate by a far-field Fourier imaging method how this simple fact can be used to shape fields around already a single particle alone. We employ this scheme to switch the third-harmonic

emission from a single point source to two spatially separated but coherent sources, as in Young's double slit assembly. Finally, we present some recent results on more advanced structures combining nonlinear plasmonics and waveguiding.

HL 55.9 Wed 12:30 S051

An ultrafast nanotip electron gun triggered by grating-coupled surface plasmons — •Benjamin Schröder, Murat Sivis, Reiner Bormann, Sascha Schäfer, and Claus Ropers — 4th Physical Institute - Solids and Nanostructures, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

We present recent results on the photoelectron emission from metal nanotips induced by propagating surface plasmon polaritons (SPPs) excited in a grating-coupler on the tip shaft [1-3]. Nanofocusing of the SPPs induces multiphoton photoemission with high efficiency. The nanostructure is inserted in a modified field-emitter electron gun geometry controlling the electrostatic environment of the tip. In this way, a site-selective control of the electron emission is achieved, and we can disentangle electrons emitted from the apex from those originating at the grating or shaft. Both the control of the transverse beam properties and the local extraction fields enabled by the gun design will be beneficial in future ultrafast transmission electron microscope applications [4].

[1] C. Ropers, C.C. Neacsu, T. Elsaesser, M. Albrecht, M.B. Raschke, and C. Lienau, Nano Lett. 7, 2784 (2007).

[2] S. Berweger, J.M. Atkin, X.G. Xu, R.L. Olmon, and M.B. Raschke, Nano Lett. 11, 4309 (2011).

[3] J. Vogelsang, J. Robin, B.J. Nagy, P. Dombi, D. Rosenkranz, M. Schiek, P. Groß, and C. Lienau, Nano Lett. 15, 4685 (2015).

[4] B. Schröder, M. Sivis, R. Bormann, S. Schäfer, and C. Ropers, accepted for puplication in Appl. Phys. Lett. (2015).

HL 55.10 Wed 12:45 S051

Plasmon dynamics on nanoporous gold particles revealed by strong field photoemission — Germann Hergert[1], •Jan Vogelsang[1], Jörg Robin[1], Petra Gross[1], Dong Wang[2], Peter Schaaf[2], Erich Runge[2], and Christoph Lienau[1] — [1]Carl von Ossietzky Universität, Oldenburg, Germany — [2]Technische Universität Ilmenau, Ilmenau, Germany

Nanoporous gold particles or "nanosponges" are particles with a diameter of hundreds of nanometers, perforated with randomly arranged pores with diameters in the 10-nm range. They have recently attracted attention as templates for surface-enhanced Raman sensing as they combine several advantageous properties, such as multiple plasmon resonances in the visible or NIR spectral range, a high surface-to-volume ratio, and a high density of catalytic sites [1].

Here we investigate the plasmon dynamics of such particles using ultrafast photoemission microscopy. When using 14-fs excitation pulses at 1600 nm for excitation of single nanosponges, we observe long-lived plasmon oscillations as a function of the pulse delay. Introducing a new model for the optical properties of these particles, we show that our results reveal the existence of long-lived plasmon hotspots with lifetimes of several tens of fs on the surface of the sponge. This plasmon localization could be of key importance for enhancing the sensing capability of such particles.

[1] C. Vidal et al, ACS Photonics 2, 1436 (2015)

HL 55.11 Wed 13:00 S051

Suppression of radiative damping and enhancement of second harmonic generation in bull's eye nanoresonators — •Vladimir Smirnov[1], Jue-min Yi[1], Xianji Piao[2], Jiho Hong[2], Heiko Kollmann[1], Martin Silies[1], Wei Wang[1], Petra Gross[1], Ralf Vogelgesang[1], Namkyoo Park[2], and Christoph Lienau[1] — [1]University of Oldenburg, Germany — [2]Seoul National University, Korea

Bull's eye (BE) nanoresonators, consisting of a central aperture in an Au film surrounded by a series of concentric circular grooves, are highly interesting structures in the context of manipulating light propagation [1] and also optimizing the coupling to quantum emitters [2]. Using broadband linear spectral interferometry and ultrahigh time resolution spectroscopy, we study the temporal response and the local field enhancement of such BE nanoresonators. We find surprisingly long lifetimes of the extended resonator eigenmodes of more than 35 fs [3]. Furthermore, by replacing the central circular hole with an annular ring void, we obtain 50-times higher second harmonic generation efficiency, illustrating the efficient field enhancement and confinement possible in BE nanoresonators. The combination of spatial light concentration with high quality factors has high potential for sensing and coherent control of light-matter interactions on the nanoscale.

[1] H. J. Lezec et al., Science 297, p. 820 (2002); [2] A. G. Curto et al., Science 329, p. 930 (2010); [3] J. Yi et al, submitted to ACS Nano (2015)

HL 56: 2D Materials: Growth

Time: Wednesday 10:30–13:00 Location: S053

HL 56.1 Wed 10:30 S053

Growth and electronic structure of epitaxial single-layer WS_2 on Au(111) — •Maciej Dendzik, Matteo Michiardi, Charlotte Sanders, Marco Bianchi, Jill A. Miwa, Signe S. Grønborg, Jeppe V. Lauritsen, Albert Bruix, Bjørk Hammer, and Philip Hofmann — Department of Physics and Astronomy, Interdisciplinary Nanoscience Center, Aarhus University, 8000 Aarhus C, Denmark

Single-layer WS_2 is a promising alternative to the widely studied MoS_2, because of the larger size of the spin-splitting and the lower effective mass of the valence band maximum. Here we present a detailed study of the electronic structure of the large-area single-layer WS_2 grown epitaxially on Au(111) using evaporation of W atoms in a low pressure H_2S atmosphere. The growth process is characterized by means of scanning tunneling microscopy, low-energy electron diffraction and core-level spectroscopy. The electronic band structure of the single-layer WS_2 is determined by angle-resolved photoemission spectroscopy. The valence band maximum at $\bar{K}$ is found to be significantly higher than at $\bar{\Gamma}$. The observed dispersion around $\bar{K}$ is in good agreement with density functional theory calculations for a free-standing monolayer, whereas the bands at $\bar{\Gamma}$ are found to be hybridized with states originating from the Au substrate. Strong spin-orbit coupling leads to a large spin-splitting of the bands in the neighborhood of the $\bar{K}$ points, with a maximum splitting of 419(11) meV. The valence band dispersion around $\bar{K}$ is found to be highly anisotropic with spin-branch dependent effective hole masses of $0.40(02)m_e$ and $0.57(09)m_e$ for the upper and lower split valence band, respectively.

HL 56.2 Wed 10:45 S053

Synthesis of high quality TaS_2 monolayer using molecular beam epitaxy — •Arlette S. Ngankeu, Charlotte E. Sanders, Marco Bianchi, Maciej Dendzik, and Philip Hofmann — Department of Physics and Astronomy, Aarhus University, 8000 Aarhus C, Denmark

The transition metal dichalcogenide TaS_2 has been intensively studied in its bulk form due to the rich properties arising from the interplay of electronic instabilities. As in many other materials, the electronic properties of TaS_2 might change in interesting ways in the thickness limit of a single layer. However, finding a good method for the production of high quality single layer TaS_2 is still a big challenge, and the thinnest crystals of TaS_2 obtained so far (by exfoliation of the TaS_2 bulk) actually have thicknesses of a few monolayers. In this talk, we report the first successful preparation of single- and few-layered TaS_2 on the Au(111) substrate by molecular beam epitaxy. Scanning tunneling microscopy, low energy electron diffraction and angle resolved photoemission spectroscopy have been used to probe the surface topography and electronic properties of TaS_2/Au.

HL 56.3 Wed 11:00 S053

2D Heterojunctions from Non-local Manipulations of the Interactions — Malte Rösner[1,2], •Christina Steinke[1,2], Michael Lorke[1], Christopher Gies[1], Frank Jahnke[1], and Tim O. Wehling[1,2] — [1]Institut für Theoretische Physik, Universität Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany — [2]Bremen Center for Computational Materials Science, Universität Bremen, Am Fallturm 1a, 28359 Bremen, Germany

We propose to create lateral heterojunctions in homogeneous two-

dimensional materials based on non-local manipulations of the Coulomb interaction using structured dielectric substrates. By means of ab-initio calculations for MoS_2 as well as generic semiconductor models, we show, that changes in the dielectric environment can induce sizeable band-gap modulations. The Coulomb interaction induced self energy corrections in real space are sufficiently non-local, to be manipulated externally, and are clearly localized within a radius of a few unit cell at the same time. This allows to induce spatially sharp interfaces within a single homogeneous monolayer and thus to form a heterojunction by the external manipulation of the Coulomb interaction via structured dielectric substrates. Hence, new kinds of heterojunctions can be constructed by placing semiconducting 2d materials on appropriately structured substrates: For a laterally structured dielectric environment, we find a type-II heterojunction with a sharp band-gap crossover within less than 5 unit cells. By establishing four perpendicular interfaces a band gap modulation reminiscent of a quantum dot can be realised.

HL 56.4 Wed 11:15 S053

TFT Fabrication Based on Liquid Exfoliated MoS_2 Flakes — •Xiaoling Zeng[1], Sonia Metel[2,3], Valeria Nicolosi[2,3,4], and Veit Wagner[1] — [1]Jacobs University Bremen, Campus Ring 1, 28759 Bremen, Germany — [2]School of Chemistry, Trinity College Dublin, Ireland — [3]CRANN, Trinity College Dublin, Ireland — [4]School of Physics, Trinity College Dublin, Ireland

There is a large interest in establishing cheap, scalable processes for producing low dimensional semiconducting dichalcogenide films for electronic application. In this work, well exfoliated MoS_2 dispersions were prepared through two step liquid phase exfoliation process with N-methyl-pyrrolidone (NMP) and Isopropanol (IPA). The obtained exfoliated MoS_2 flakes were characterized by microscopy (TEM and SEM), Uv - Vis and Raman spectroscopy.

Bottom gate thin film transistors (TFTs) based on exfoliated MoS_2 film were fabricated by using spray coating techniques. The deposition process was optimized to get uniform and percolated MoS_2 film with different thicknesses. Transistors show only minor conductivity directly after layer deposition. However, depositing additional PMMA layer on top shows large improvement in electrical characteristics, i.e. switching behavior with changing gate voltage. Interpretation is that the PMMA layer brings the initially separated flakes into contact and enables proper percolation. Further investigation found that the thickness of PMMA influences the electrical properties. This low-cost and scalable solution-based fabrication process will promote the application of dichalcogenides in future nanoelectronic devices.

HL 56.5 Wed 11:30 S053

Novel Deposition Approach of Semiconducting MoS2 Thin Films and Their Application for Electronic Devices — •Francis Oliver Vinay Gomes[1,2], Marko Marinkovic[1], Jochen Brendt[1], Torsten Balster[2], and Veit Wagner[2] — [1]Evonik Resource Efficiency GmbH, Paul-Baumann-Strasse 1, 45764 Marl, Germany — [2]Jacobs University Bremen, Department of Physics & Earth Science, Campus Ring 1, 28759 Bremen, Germany

In this work, MoS2 films obtained from precursor solution via spin-coating on various substrates were investigated. Molybdenum(V) chloride dissolved in 1-methoxy-2-propanol was used as precursor solution. The MoS2 films obtained from the Mo-precursor upon sulfurization during annealing were analyzed for surface morphology and roughness, chemical composition and crystallinity. In addition, comparison of silicon and sapphire substrates were studied. Our approach focuses on novel deposition technique compared to the current state-of-the-art chemical vapour deposition.

The thickness of the MoS2 films was controlled in the process, and film thicknesses between 2 and 27 nm were obtained. The thickness of the films linearly scaled with precursor concentration. SEM/EDX measurements indicate that the surface morphology and film composition is strongly dependent on the annealing temperature and processing environment. Electrical measurements demonstrate a film conductivity of 0.27 S/cm while XRD confirms the formation of semiconducting 2H-MoS2 films. The future steps will lead towards applying fabricated films in electronic devices such as thin film transistors.

HL 56.6 Wed 11:45 S053

Growing graphene underneath hBN on Rh(111) — •Uta Schlickum[1], Daniel Rosenblatt[1], Sebastian Koslowski[1], and Klaus Kern[1,2] — [1]Max-Planck-Institute for Solid State Research, 70569 Stuttgart, Germany — [2]École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

The stable hexagonal monolayer of hBN is an insulator with excellent dielectric properties. It can be grown on a large variety of transition metal surfaces like Rh(111) on which it shows a hexagonal Moire super-lattice. We grow a single layer of hBN on Rh(111) by chemical vapor deposition and found beside the well known hexagonal structure a new periodic pattern resembling a lattice of a "spoked wheel" (SW). For small coverages this new phase appears at the intersection of the rims connecting three valleys of the Moire lattice, and forms large islands for higher coverage. Atomic resolution topographic images reveal that the phase boundaries do not disturb the atomic lattice periodicity of the hBN. Depending on the preparation parameters, the relative coverage of the two phases can be tuned at will. The crucial parameter determining the relative coverage is the time, the sample stays at about $600°C$ after the exposure to borazine at $800°C$. It is well known that at $600°C$, C impurities segregate and accumulate at the surface. This together with the fact that the hBN lattice itself remains intact crossing a phase boundary, leads us to conclude that the SW phase consists of an additional graphene layer below the hBN layer. Various experimental details, like high resolution spectroscopy, support this interpretation.

HL 56.7 Wed 12:00 S053

Prediction of metastable two-dimensional compounds in the C/Si system using global optimization techniques, and investigation of their electronic properties — •Johann Christian Schön and Rico Gutzler — MPI for Solid State Research, Heisenbergstr. 1, D-70569 Stuttgart

We employ the global energy landscape exploration package G42+[1,2] to predict (meta)stable two-dimensional crystalline polymorphs in the carbon/silicon system for a range of compositions: C:Si = 1:0, 3:1, 2:1, 1:1, 1:2, 1:3, and 0:1.[1] During the global search (energy function: DFT), both atom positions and cell parameters in the xy-plane were allowed to vary freely. The global optimization method used was basin-hopping-simulated annealing, with two consecutive local optimizations - the first keeping the atoms restricted to the z = 0 plane, while the second one also permitted relaxation in the z-direction. For all compositions, the lowest energy 2D-structures exhibited a graphene-like super-structure with 6-membered rings, but many quite stable competing minimum structures containing a variety of rings of size 4 - 12 were also observed. Deviations from planarity occurred most frequently for structures where a high local concentration of the Si-atoms was present. Complementing geometric structure prediction, we performed band-structure calculations to investigate the effect of geometry and C:Si ratio on the electronic properties of these 2D-materials.

[1] J. C. Schön, Proc. Appl. Ceram. 9:157-168 (2015); [2] J. C. Schön, G42+ Manual, www.chemie.uni-bonn.de/ac/schoen/forschung/g42-manual, (2015)

HL 56.8 Wed 12:15 S053

Tuning the physical properties of MoS_2 membranes by organophosphonate interfacial chemistry — •Susanne Schwarzwälder[1], Réka Csiki[1], Eric Parzinger[1], Jeffrey Schwartz[2], Alexander Holleitner[1], Martin Stutzmann[1], Ursula Wurstbauer[1], and Anna Cattani-Scholz[1] — [1]Walter Schottky Institut and Physik Department, Technische Universität München, Germany — [2]Princeton University, New Jersey, USA

One of the most prominent members of the 2D material family is the transition metal dichalcogenide MoS_2, due to its natural occurrence and its promising potential applications in nanoelectronic and optoelectronic devices [1]. Interfacial chemistry strongly influences the interaction of molecularly thin semiconducting membranes with the underlying substrate, hence a suitable silicon surface functionalization can be employed for improving the performance of MoS_2-based devices [2]. Our work focuses on the investigation of surface functionalization using homogeneous organophosphonate self-assembled monolayers (SAMs) covalently bonded to SiO_2. In particular, the interaction of single layer (SL) MoS_2 with SAMs based on four different aromatic phosphonic acids are investigated. Modulation of the intrinsic n-type doping of SL-MoS_2 via charge transfer with aromatic SAMs is suggested by a shift in the Raman-active out-of plane vibrational mode A_{1g}, emphasizing the importance of interfacial interactions in MoS_2-based nanodevices.

[1] R. Ganatra, Q. Zhang, ACS Nano 8, 4074 (2014).
[2] S. Najmaei et al., Nano Lett. 14, 1354 (2014).

HL 56.9 Wed 12:30 S053

Structural analysis of one monolayer of hBN on Cu(111) via NIXSW and SPA-LEED — •Timo Heepenstrick[1], Christine Brülke[1], Ina Krieger[1], Sergey Subach[2], Simon Weiss[2], Niklas Humberg[1], and Moritz Sokolowski[1] — [1]Institut für Physikalische und Theoretische Chemie der Universität Bonn, Wegelerstraße 12, 53115 Bonn, Germany — [2]Peter Grünberg Institut, Forschungszentrum Jülich, 52452 Jülich, Germany

We present a detailed structural analysis of hBN on Cu(111) with normal incidence x-ray standing waves (NIXSW) supported by spot profile analysis low energy electron diffraction (SPA-LEED). hBN forms an incommensurate structure on Cu(111) with a lattice mismatch of 2.3% corresponding to the unstrained hBN layer. The NIXSW experiments show that the hBN layer is weakly bonded with a distance of 3.23 Å (for the nitrogen) and 3.26 Å (for the boron) and shows little buckling. We also present an analysis for the topmost Cu(111) layer with and without a monolayer of hBN.

HL 56.10 Wed 12:45 S053

Nanotents - 2 nm void-formation and self-healing in 2D monolayers on metals — •Huanyao Cun[1], Marcella Iannuzzi[2], Adrian Hemmi[1], Silvan Roth[1], Jürg Osterwalder[1], and Thomas Greber[1] — [1]Physik-Institut, Universität Zürich, Winterthurerstrasse 190, CH-8057 Zürich, Switzerland — [2]Chemistry-Institut, Universität Zürich, Winterthurerstrasse 190, CH-8057 Zürich, Switzerland

At room temperature, it is quite challenging to immobilize single atoms. However, with the single layers of hexagonal boron nitride (h-BN) or graphene, site-selective immobilization of atoms at surfaces becomes feasible. The h-BN nanomesh is a corrugated structure that consists of two regions, the 'pores' with 2 nm diameter and the surrounding 'wire' regions.

In the present study, we demonstrate that the h-BN nanomesh, which acts as thin "rainfly", can trap atoms at distinct subsurface sites and form so-called "nanotents" structure. Remarkably, annealing to 900 K induces the "can-opener" effect: h-BN flakes at pore sites are cut out from the h-BN monolayer and 2 nm voids form on the h-BN surface. We assign the "can-opener" effect to the vacancy defects generated during the Ar+ penetration. Higher temperature annealing leads to the "self-healing" of the h-BN monolayer. Systematic measurements reveal that the entire process, including nanotent formation, "can-opener" effect and nanomesh "self-healing", is well controlled and repeatable. The reported effects are robust and quite general: they are also observed in graphene on ruthenium, for neon and rubidium atoms.

HL 57: Quantum Dots and Wires: Quantum Optics II

Time: Wednesday 12:15–13:00 Location: H15

HL 57.1 Wed 12:15 H15

Photon Statistics Excitation Spectroscopy of a Single Two Level System — •Max Strauss[1], Marlon Placke[1], Sören Kreinberg[1], Christian Schneider[2], Martin Kamp[2], Sven Höfling[2,3], Janik Wolters[1], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, TU Berlin, Germany — [2]Technische Physik, Universität Würzburg, Germany — [3]SUPA, School of Physics and Astronomy, University of St. Andrews, UK

The interaction of a coherent light wave with a fermionic two level system (TLS) is one of the corner stones of modern quantum optics. Interestingly, its inherent nonlinearity makes it also an ideal probe for the photon statistics of the interacting light field. In recent years this exciting field of quantum optics has been extended from atomic systems to semiconductor nanostructures, e.g. to the coherent control of self-assembled quantum dots (QDs). Here, we address a so far unexplored regime of resonance fluorescence in which the QD is excited not with a laser but with a narrowband chaotic light source. By analysing the resonantly scattered emission of the TLS, we find that the photon statistics of the excitation source greatly influences the TLS's dynamics in quantitative agreement with theoretical predictions.

HL 57.2 Wed 12:30 H15

Optical Counting Statistics of Single Electron Tunneling into a Single Self-Assembled Quantum Dot — Annika Kurzmann[1], Arne Ludwig[2], Andreas D. Wieck[2], Axel Lorke[1], and •Martin Geller[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany — [2]Chair of Applied Solid State Physics, Ruhr-Universität Bochum, Universitätsstr. 150, 44780 Bochum, Germany

We demonstrate here an optical detection scheme to observe single electron tunneling into a single self-assembled quantum dot (QD). The detection scheme is based on driving the excitonic transition into resonance fluorescence [1]. It allows us to use optical counting statistic [2] to reveal the interactions and correlations between excitons and electrons.

The single QD is embedded in a diode structure with a 3D charge reservoir, which allows the controlled charging and discharging of the QD. The time-resolved resonance fluorescence of the exciton is measured, while tunneling between the charge reservoir and the QD is possible. In the generated telegraph-noise we directly observe quantum jumps of the electrons tunneling into and out of the QD, which gives access to the distribution of the fluctuations, i.e. shot noise and Fano factor. A reduced Fano factor is observed for equal tunneling rates into and out of the QD, due to an enhanced correlation in the current fluctuation.

[1] C. Matthiesen et al., Phys. Rev. Lett. **108**, 093602 (2012).
[2] L. S. Levitov et al., J. Math. Phys. **37**, 4845 (1996).

HL 57.3 Wed 12:45 H15

Creation of a squeezed photon distribution using artificial atoms with broken inversion symmetry — •Martin Koppenhöfer and Michael Marthaler — Karlsruhe Institut of Technology, Karlsruhe, Germany

We consider a two level system with both a transversal and a longitudinal coupling to the electromagnetic field of a resonator. Using a polaron transformation, this Hamiltonian can be mapped onto a Jaynes-Cummings Hamiltonian with generalized field operators acting on the electromagnetic field in the resonator. In contrast to the usual ladder operators a and $a^\dagger$, these operators exhibit a non-monotous coupling strength with respect to the number n of photons in the resonator. Especially, there are roots of the coupling between qubit and resonator at certain photon numbers n_0. We show that this effect can be exploited to generate photon-number squeezed light, characterized by a Fano factor $F \ll 1$, with a large number of photons (e.g. of the order of 10^4).

HL 58: Organic Photovoltaics and Electronics

Time: Wednesday 14:45–18:30 Location: H2

Invited Talk HL 58.1 Wed 14:45 H2

Ultrafast excitonic and charge transfer dynamics in nanostructured organic polymer materials — •Irene Burghardt[1], Robert Binder[1], Matthias Polkehn[1], and Hiroyuki Tamura[2] — [1]Institute for Physical and Theoretical Chemistry, Goethe University Frankfurt, Germany — [2]WPI-Advanced Institute for Material Research, Tohoku University, Japan

We present first-principles quantum dynamical studies of ultrafast photoinduced exciton migration and dissociation in functional organic materials, in view of understanding the key microscopic factors that lead to efficient charge generation in photovoltaics applications. The talk will specifically address (i) exciton dissociation and free-carrier generation in donor-acceptor materials, including models for P3HT-PCBM heterojunctions [1] as well as highly ordered thiophene-perylene diimide assemblies [2], (ii) exciton migration [3] and formation of charge-

transfer excitons in oligothiophene H-aggregates, and (iii) exciton multiplication by singlet fission in acene materials [4]. Special emphasis is placed on the critical role of exciton and charge delocalization which are a sensitive function of molecular packing.

[1] H. Tamura, I. Burghardt, J. Am. Chem. Soc. 135, 16364 (2013), M. Huix-Rotllant, H. Tamura, I. Burghardt, J. Phys. Chem. Lett. 6, 1702 (2015). [2] T. Roland et al., Phys. Chem. Chem. Phys. 14, 273 (2012), J. Wenzel, A. Dreuw, I. Burghardt, Phys. Chem. Chem. Phys. 15, 11704 (2013). [3] J. Wahl, R. Binder, I. Burghardt, Comput. Theor. Chem. 1040, 167 (2014). [4] H. Tamura et al., Phys. Rev. Lett. 115, 107401 (2015).

HL 58.2 Wed 15:15 H2

Non-Equilibrium Charge Carrier Dynamics in Organic Disordered Semiconductors — •Andreas Hofacker[1], Jan Oliver Oelerich[2], Alexey Nenashev[3], Florian Gebhard[2], and Sergei Baranovskii[2] — [1]Institute of Applied Photophysics, Dresden University of Technology, D-01069 Dresden — [2]Department of Physics and Materials Science Center, Philipps-University, D-35032 Marburg — [3]Institute of Semiconductor Physics, 630090 Novosibirsk, Russia

Time-dependent processes in organic semiconductors dominated by non-equilibrium physics are subject of current debate in the scientific community. The understanding of these processes promises fundamental insights into transport and recombination dynamics of charge carriers in organic semiconductor devices such as organic solar cells, and can therefore reveal possibilities for further efficiency enhancement.

Based on an analytical model developed for inorganic disordered semiconductors by Orenstein and Kastner in 1981, we formulate a description of carrier thermalization and recombination in organic disordered semiconductors. For this purpose we extend the very transparent approach of Orenstein and Kastner to enable the description of low recombination rates and applicability of the approach to arbitrary density of tail states (DOS) functions. We predict that the behavior of systems with a Gaussian DOS, which organic semiconductors are commonly believed to be, is distinctively different from systems with an exponential DOS. This fact could be used to experimentally distinguish whether a given sample possesses an exponential or a Gaussian DOS by performing a time-dependent carrier density measurement.

HL 58.3 Wed 15:30 H2

Mobility-limited recombination models for organic solar cells — •Alexander Wagenpfahl and Carsten Deibel — Institut für Physik, Technische Universität Chemnitz, 09126 Chemnitz, Germany

Recent results of kinetic Monte Carlo simulations indicate that recombination of charge carriers in organic semiconductor blends show a strong dependence on the domain size of neat material phases [1]. Consequently, the Langevin recombination model does not generally apply and has to be modified by the geometric mean of the charge carrier mobilities. Here, we present drift–diffusion simulations to reveal the influence of such a recombination model in comparison to the Langevin theory. We discuss differences in the quality of the solar cell current–voltage characteristics and distinguish the different processes which lead to a reduction of the observed recombination rate [2].

[1] Phys. Rev. Lett. 114, 136602 (2015)
[2] Phys. Rev. B 80, 075203 (2009)

HL 58.4 Wed 15:45 H2

Energy-Gap Law of Non-Radiative Voltage Losses in Organic Solar Cells — •Johannes Benduhn[1], Kristofer Tvingstedt[2], Fortunato Piersimoni[3], Olaf Zeika[1], Donato Spoltore[1], Dieter Neher[3], and Koen Vandewal[1] — [1]IAPP, TU Dresden, Germany — [2]EP VI, Julius-Maximillian University of Würzburg, Germany — [3]IPA, University of Potsdam, Germany

The open-circuit voltage of organic solar cells is low as compared to their optical gap, indicating large energy losses per absorbed photon. These losses arise from the necessity of an electron transfer from an electron donor to an electron acceptor to dissociate the excitons, and furthermore from the recombination of the resulting free charge carriers. It has been shown that the energy loss in the electron transfer event can be below 0.1 eV, while radiative recombination losses are in principle unavoidable.

In this work, we investigate the remaining voltage losses due to non-radiative decay of charge carriers. We find that the non-radiative voltage losses increase when the energy difference between charge transfer (CT) state and ground state decreases. This behaviour is consistent with the "energy gap law for non-radiative transitions", which implies that internal conversion from CT state to ground state is facilitated by molecular vibrations. With this work, we identify a possibly intrinsic loss mechanism, which until now has not been thoroughly considered for organic photovoltaics, and which is different in its very nature as compared to the commonly considered inorganic photovoltaic loss mechanisms of defect, surface, and Auger recombination.

HL 58.5 Wed 16:00 H2

Development of a photocapacitor based on printed solar cells and supercapacitors — •Katrin Anneser[1], Lukas Hörlin[2], Stephan Braxmeier[1], Andreas Baumann[1], Gudrun Reichenauer[1], and Vladimir Dyakonov[1,2] — [1]Bavarian Center for Applied Energy Research (ZAE Bayern), 97074 Würzburg — [2]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg

The main drawbacks of renewable energy sources such as wind and solar energy are unpredictable power fluctuations presenting a major challenge to stability and efficiency of the grid. With increasing fraction of these intermittent energy sources it is necessary to smooth the power before feeding it into the grid without just cutting off the fluctuations. We are following the few previous research activities aiming at combining a fast energy storage device, a supercapacitor, and a solar cell. Rather than developing a modular system our objective is an integrated layered system provided by printing the components from solution processed precursors. Those combined cells will provide a more constant power output compared to stand-alone photovoltaic systems and thus allow feeding into storage units with far slower kinetics (e.g. batteries) or the grid. We present the concept and the related boundary conditions and problems to be solved. Furthermore, we show experimental data from solar cells measured at a high frequency (every second) and derive the basic requirements in terms of power and energy density required for the storage unit per m^2 of the integrated system from these data.

HL 58.6 Wed 16:15 H2

Passivation and modification of silicon nanowires towards hybrid solar cells — •Jessica Hänisch[1], Carola Klimm[1], Marc A. Gluba[1], Karsten Hinrichs[2], Iver Lauermann[3], Wolfram Calvet[3], Norbert H. Nickel[1], and Jörg Rappich[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Institut für Silizium-Photovoltaik, Berlin, Germany — [2]ISAS e.V. - Leibniz-Institut für Analytische Wissenschaften, Berlin, Germany — [3]BESSY, Berlin, Germany

Hybrid solar cells combine inorganic and organic materials to benefit from both areas, particularly in terms of production costs and material consumption. The inorganic-organic interface needs to be well passivated, especially if nanowires with a high surface area are implemented to enhance light absorption. The silicon nanowires were prepared by metal assisted chemical etching (MACE). The etching procedure leads to surface damaging and thereby generates surface defects. These defects reside in the band gap and act as recombination centers. As a consequence, the amount of collected charge carriers is reduced and therefore, the power conversion efficiency decreases. We applied electropolishing procedures to the silicon surface to minimize the amount of surface defects. Changes in the density of surface defects were directly monitored by in-situ photoluminescence measurements. To preserve the improved surface passivation obtained after the electropolishing process we used (electro-)chemical grafting of small molecules and investigated the surfaces by infrared spectroscopy, x-ray photoelectron spectroscopy and photoluminescence measurements.

30 min. Coffee Break

HL 58.7 Wed 17:00 H2

Vertical Organic Field-Effect Transistors - Functional Principles and Applications — •Alrun Aline Günther[1], Michael Sawatzki[1], Christoph Hossbach[2], Petr Formánek[3], Daniel Kasemann[1,4], Johannes Widmer[1], Johann W. Bartha[2], and Karl Leo[1,5] — [1]Institut für Angewandte Photophysik, TU Dresden, Germany — [2]Institut für Halbleiter- und Mikrosystemtechnik, TU Dresden, Germany — [3]Leibniz-Institut für Polymerforschung Dresden e.V., Germany — [4]currently: CreaPhys GmbH, Dresden, Germany — [5]Fellow of the Canadian Institute for Advanced Research, Toronto (ON), Canada

Vertical organic field-effect transistors (VOFETs) are a means to overcome the limitations of conventional organic field-effect transistors

(OFETs). At present however, they often suffer from two major drawbacks: performance limitation by contact effects and limitation to certain materials and processing techniques, making a controlled shift of parameters such as the transistor threshold voltage difficult. Here, we present p- and n-type VOFETs operating in the accumulation and inversion regimes. By introducing contact doping, we are able to increase the transconductance and On/Off ratio of VOFETs by an order of magnitude. We further show that the realisation of inversion VOFETs is possible and can shift the threshold voltage in a controlled manner, while reducing the Off state current of VOFETs through reduction of the source-drain leakage current.

HL 58.8 Wed 17:15 H2

Vertical Organic Light Emitting Transistors for Investigation of Charge Transport in VOFETs — •Franz Michael Sawatzki[1], Alrun Günther[1], Duyhai Doan[2], Christoph Hossbach[3], Petr Formánek[4], Daniel Kaseman[1,5], Johannes Widmer[1], Thomas Koprucki[2], and Karl Leo[1,6] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, Germany — [2]Weierstraß-Institut für Angewandte Analysis und Stochastik, Leibniz-Institut im Forschungsverbund Berlin e. V., Germany — [3]Institut für Halbleiter- und Mikrosystemtechnik, Technische Universität Dresden, Germany — [4]Leibniz-Institut für Polymerforschung Dresden e.V., Germany — [5]currently: CreaPhys GmbH, 01257 Dresden, Germany — [6]Fellow of the Canadian Institute for Advanced Research (CIFAR), Toronto, Ontario M5G 1Z8, Canada

The vertical organic field effect transistor (VOFET) offers many technological advantages due to its very short geometric channel length. However, in contrast to the standard lateral organic field effect transistor (OFET), the basic physics and working principles are not yet well known. Here, we compare results regarding the charge transport obtained from simulations with measured charge carrier density distributions. The latter ones are obtained from the light emission of vertical organic light emitting transistors (VOLETs). These devices are a combination of an organic light emitting diode (OLED) and a VOFET, which allow to locally resolve the current path. We show the dependence of the channel size and geometry on the gate-source voltage, the drain-source voltage, and the source geometry.

HL 58.9 Wed 17:30 H2

Ultra-High Current Densities in Organic Transistors — •Markus P. Klinger, Axel Fischer, Felix Kaschura, Daniel Kasemann, Johannes Widmer, and Karl Leo — Institut für Angewandte Photophysik, Technische Universität Dresden, George-Bähr Str. 1, 01069 Dresden

Organic transistors are considered for flat panel or flexible displays, radio identification systems, and sensor arrays. Much effort has been spent to optimize the charge carrier mobility and to reduce the channel length of organic field-effect transistors (OFETs). Likewise, new device concepts have been introduced based on charge transport perpendicular to the substrate utilized in so-called vertical organic transistors. One representative is the high-performing organic permeable-base transistor (OPBT) [1,2]. Here, we show that this device is determined by space-charge limited current (SCLC) in the on-state. Thus, OPBTs can drive as much current as possible for a certain thickness of semiconducting material. Using C_{60} with a low charge carrier mobility of about $0.025\,\mathrm{cm^2\,V^{-1}s^{-1}}$ in the vertical direction, current densities of more than $600\,\mathrm{A\,cm^{-1}}$ are reached at voltages below 6 V. This performance can be achieved as the total thickness of the device is in the range of 100 nm. With that, OPBTs can easily outperform OFETs in terms of current per footprint area.

[1] M. P. Klinger et al., Adv. Mater. (2015), 27(47);
[2] A. Fischer et al., Appl. Phys. Lett. (2012), 101, 213303

HL 58.10 Wed 17:45 H2

Controlling the electronic properties in liquid crystal conjugated small molecules for application in electronics — •Nadine Tchamba Yimga[1], Holger Borchert[1], Peer Kirsch[3], Jürgen Parisi[1], and Elizabeth von Hauff[2] — [1]Department of Physics, University of Oldenburg, Germany — [2]Department of Physics and Astronomy, VU University Amsterdam, The Netherlands — [3]Merck KGaA, Liquid Crystals R&D Chemistry, Germany

Organic semiconductors offer numerous advantages for electronics. However, carrier mobilities in organic semiconductors are generally orders of magnitude lower than in inorganic semiconductors. This is a major bottle neck for device efficiency. The electrical properties are additionally dependent on thin film morphology which is challenging to control in solution deposited films. We studied structure-function relationships in a novel liquid crystal molecule. The molecular films demonstrate phase changes from crystalline to nematic to isotropic phases at temperatures of 140 C, 165 C and 250 C, respectively. We demonstrate the influence of temperature on the structure of solution processed films with cross polarized microscope (CPM) and X-ray diffraction (XRD). Current-voltage measurements and impedance spectroscopy were performed on films annealed to temperatures above the crystalline - nematic phase change and subsequently cooled. The mobility increases from 10^{-4} cm^2 V^{-1} s^{-1} to 10^{-3} cm^2 V^{-1} s^{-1}. We demonstrate that controlled structural manipulation of the film can be used to reduce electronic disorder. These results show the potential of liquid crystal conjugated materials in electronic applications.

HL 58.11 Wed 18:00 H2

Photodetectors Based on an Anilino Squaraine for Efficient Detection of Light in the 700 nm Region — •Andre Pries[1], Matthias Schulz[2], Arne Lützen[2], Jürgen Parisi[1], and Manuela Schiek[1] — [1]Institute of Physics, Energy and Semiconductor Research Laboratory, Oldenburg, Carl von Ossietzky University, Germany — [2]Kekulé Institute of Organic Chemistry and Biochemistry, Bonn, Rheinische Friedrich-Wilhelms-University, Germany

In this work the squaraine derivative 2,4-bis[4-(N,N-diisobutylamino)-2,6-dihydroxyphenyl] squaraine (SQIB) is analyzed in a conventional bulk-heterojunction photodiode architecture, Glass/ITO/MoO_3/SQIB:PCBM/LiF/Al. This architecture shows a power conversion efficiency of ≈2.5 % and a peak external quantum efficiency (EQE) of ≈50 % at 700 nm, making the device highly sensitive in the red wavelength region. In order to even further increase the EQE a negative bias voltage is used. Next the time-dependent response of the device is measured, to find, e.g. the rise- and fall time. Finally, the bandwidth of the device is determined and the cut-off frequency.

[1] G. Chen et. Al, Optical and electrical properties of a squaraine dye in photovoltaic cells, Applied Physics Letters, Vol. 101, No.8 2012, 083904

[2] M.Binda et. Al, Fast and air stable near-infrared organic detector based on squaraine dyes, Organic Electronics, 2009, Vol. 10, Issue 7, p. 1314-1319

HL 58.12 Wed 18:15 H2

First results of an implementation of GW of reduced complexity for organic semiconductors — •Saber Gueddida and Dietrich Foerster — LOMA, Université de Bordeaux, France

We have implemented a GW algorithm of reduced complexity (N^3 rather than N^4) for crystals containing N»1 atoms in their unit cell. The main ideas of the algorithm and first results of its implementation will be given. Our code aims at contributing to optimizing organic solar cells by predicting the bands and gaps of their constituents.

HL 59: Optical Properties II

Time: Wednesday 14:45–18:30 Location: H10

HL 59.1 Wed 14:45 H10

Electro-optical polariton transistor switch — •Holger Suchomel[1], Sebastian Brodbeck[1], Timothy Liew[2], Martin Klaas[1], Sebastian Klembt[1], Martin Kamp[1], Sven Höfling[1,3], and Christian Schneider[1] — [1]Technische Physik and Wilhelm-Conrad-Röntgen-Research Center for Complex Material Systems, Universität Würzburg, D-97074 Würzburg, Am Hubland, Germany — [2]Division of Physics and Applied Physics, Nanyang Technological University, 63737 Singapore, Singapore — [3]SUPA, School of Physics and Astronomy, University of St. Andrews, St. Andrews, KY 16 9SS, United Kingdom

We study the propagation of an optically injected exciton-polariton condensate along a one dimensional wire under the influence of a local,

electrical gate. Applying a gate voltage, results in a general redshift of the emission along the wire superimposed by a local potential dip underneath the contact. Tuning of the trap depth and taking advantage of the detuning gradient along the wire is sufficient to block the polariton flow through the contact. As a consequence of the switching process and increased field ionization of excitons, the device shows a negative differential resistance and features a pronounced bistability in the probed photocurrent.

The combination of lithographic and electro-optical potential landscape engineering results in a compact device. It works as a polariton transistor switch which is operated by an external electric field rather than a control laser beam. This makes the approach suitable for on-chip applications and complex polariton circuits.

HL 59.2 Wed 15:00 H10

Probing the carrier reservoir across the polariton condensation and photon lasing transitions in a quantum well microcavity — •Sebastian Brodbeck[1], Holger Suchomel[1], Matthias Amthor[1], Theresa Steinl[1], Martin Kamp[1], Christian Schneider[1], and Sven Höfling[1,2] — [1]Technische Physik, Physikalisches Institut and Wilhelm Conrad Röntgen-Research Center for Complex Material Systems, Universität Würzburg, Am Hubland, 97074 Würzburg — [2]SUPA, School of Physics and Astronomy, University of St. Andrews, St. Andrews, KY 16 9SS, United Kingdom

We monitor the free carrier reservoir in a GaAs-based quantum well microcavity under non-resonant pulsed optical pumping by measuring the photocurrent between lateral contacts deposited directly on the quantum wells that are partially exposed by wet chemical etching. We identify two clear thresholds in the input-output characteristic of the photoluminescence signal which can be attributed to polariton condensation and photon lasing, respectively. The power dependence of the probed photocurrent shows a distinct kink at the threshold power for photon lasing due to increased radiative recombination of free carriers as stimulated emission into the cavity mode sets in. At the polariton condensation threshold on the other hand, the nonlinear increase of the luminescence is caused by stimulated scattering of exciton-polaritons to the ground state which do not contribute directly to the photocurrent. In the strong coupling regime, the system can be described by a rate equation model which includes field ionization related losses.

HL 59.3 Wed 15:15 H10

Investigation of the binding energy of $Al_xGa_{1-x}As/Al_yGa_{1-y}As$ quantum wells for high temperature polariton lasers — •Stefanie Kreutzer[1], Holger Suchomel[1], Sebastian Brodbeck[1], Maciej Pieczarka[2], Grzegorz Sęk[2], Christian Schneider[1], and Sven Höfling[1,3] — [1]Technische Physik, Physikalisches Institut and Wilhelm Conrad Röntgen-Research Center for Complex Material Systems, Universität Würzburg, Am Hubland, 97074 Würzburg — [2]Institute of Physics, Wroclaw University of Technology, Wybrzeze Wyspianskiego 27, 50-370 Wroclaw, Poland — [3]SUPA, School of Physics and Astronomy, University of St. Andrews, St. Andrews KY16 9SS, United Kingdom

We study the exciton binding energy in $Al_xGa_{1-x}As/Al_yGa_{1-y}As$ quantum wells for various aluminium concentrations in well and barrier as well as well widths. Binding energies are determined by comparing calculated transition energies to experimental values obtained from photoluminescence and photoreflectance studies. We find a strong enhancement of the binding energy compared to $GaAs/Al_xGa_{1-x}As$ quantum wells with increasing transition energy until the type I-type II-transition crossover with values exceeding 25 meV.

When integrating these quantum wells into microcavities, we observe a normal mode splitting between excitons and photons. Strong coupling persists at elevated temperatures with a measured Rabi splitting of 5meV at 230K.

HL 59.4 Wed 15:30 H10

InP-based photonic crystal microcavities embedded with InAs quantum dots for telecom wavelengths — •Andrei Kors, Matusala Yacob, Johann P. Reithmaier, and Mohamed Benyoucef — Institute of Nanostructure Technologies and Analytics (INA), CINSaT, University of Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany

Self-assembled semiconductor quantum dots (QDs) embedded in photonic crystals can be used as building blocks for future quantum information processing. Here, we report on the fabrication and optical characterization of InP-based photonic crystal microcavities embedded with InAs/InP QDs. Medium InAs/InP QD density emitting at the telecom wavelengths is grown by solid source molecular beam epitaxy. Using special capping technique and temperature processing after the dot formation, density of about 10^9 cm^{-2} is obtained. L3 photonic crystal air-bridge cavities are fabricated by electron beam lithography, inductively coupled plasma reactive ion etching and wet etching technique. Optical properties of microcavities such as polarization, emission wavelengths and quality factors are determined by micro-photoluminescence measurements. Results reveal sharp cavity modes at telecom wavelengths.

HL 59.5 Wed 15:45 H10

Carrier density driven lasing dynamics in ZnO nanowires — •Marcel Wille[1], Chris Sturm[1], Tom Michalsky[1], Robert Röder[2], Carsten Ronning[2], Rüdiger Schmidt-Grund[1], and Marius Grundmann[1] — [1]Institut für Experimentelle Physik II, Universität Leipzig, Linnéstraße 5, 04103 Leipzig — [2]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena

The laser on-time of semiconductor nanowires was currently found to be in the range of 1 - 3 ps [1]. However, the emission onset characteristics of lasing semiconductor nanowires is not yet understood in detail because of the high demand on the temporal and spatial resolution of the detection technique. We report on the lasing dynamics of CVD grown ZnO nanowires from cryogenic temperatures up to room temperature using time-resolved micro-photoluminescence (μ-PL) technique. Our studies focus on the investigation of the temperature dependent emission onset-time (t_{on}). It turns out that t_{on} depends strongly on the excitation power and becomes smallest in the lasing regime, with values below 5 ps. Furthermore, we observed a red shift of the dominating lasing modes in time, which was described by a carrier density induced change of the refractive index dispersion after the optical excitation. For the qualitative analysis of the observed phenomena, we extended an existing model to calculate the carrier density dependent refractive index as well as the extinction coefficient for different temperatures. [1] T.P.Sidiropoulos et al., Nature Phys. 10, 870 (2014)

Invited Talk HL 59.6 Wed 16:00 H10

Discontinuous Galerkin Methods in Nano-Photonics — •Kurt Busch — Humboldt Universität zu Berlin, Institut für Physik, AG Theoretische Optik & Photonik, 12489 Berlin and Max-Born-Institut, 12489 Berlin, Germany

Discontinuous Galerkin (DG) methods facilitate efficient computations of nano-photonic systems [1] by combining the flexibility of finite element approaches with efficient time-stepping capabilities. While the former allows for an accurate representation of complex geometries, the latter requires material models that are amenable to auxiliary differential equations techniques. This latter aspect specifically includes material models for magneto- [2] and/or nonlinear-optical properties. In this talk, the present state of Discontinuous Galerkin Time-Domain (DGTD) approaches to nano-photonic systems is presented. This includes (i) methodic aspects such as convergence properties of DGTD computations with regards to the above-mentioned material models as well as (ii) selected applications such as the computation electron energy loss spectra [3,4] and modified emission dynamics [5], and the nonlinear-optical properties of plasmonic nanostructures [6,7].

[1] K. Busch et al., Laser Photon. Rev. **5**, 773 (2011)
[2] C. Wolff et al., Opt. Express **21**, 12022 (2013)
[3] F. von Cube et al., Nano Lett. **13**, 703 (2013)
[4] B. Schröder et al., Phys. Rev B **92**, 085411 (2015)
[5] A.W. Schell et al., Nano Lett. **14**, 2623 (2014)
[6] A. Hille et al., J. Phys. Chem. C, in press
[7] D. Huynh et al., Appl. Phys. B, in press

30 min Coffee Break

HL 59.7 Wed 17:00 H10

Radiative modes in anisotropic planar microcavities — •Steffen Richter, Tom Michalsky, Chris Sturm, Helena Franke, Marius Grundmann, and Rüdiger Schmidt-Grund — Universität Leipzig, Institut für Experimentelle Physik II, Linnéstr. 5, 04103 Leipzig, Germany

We present dispersions and polarizations of modes in microcavities with optically uniaxial cavity material, as e.g. wide gap oxides.

Using a 4×4 transfer matrix ansatz we compute mode energies and broadenings, i.e. lifetimes, as matrix poles. In contrast to the separation into transversal electric (TE) and transversal magnetic (TM)

polarization, which is commonly done for the isotropic case, we can obtain the mode polarizations without any prior restriction. We show that an optical anisotropic cavity material does not change the number of eigenmodes compared with an isotropic one, i.e. two for a $\lambda/2$ cavity. Most strikingly, in non-trivial anisotropic configurations the modes are no longer orthogonally polarized to each other but tend both to TM polarization with increasing in-plane wavevectors $k_{||}$. Further, for configurations with the propagation direction almost, but not exactly, parallel or perpendicular to the optical axis of the cavity layer, circular polarization contributions of more than 90% can occur at large $k_{||}$.

HL 59.8 Wed 17:15 H10

Raman Tensor Formalism for Anisotropic Crystals — •Christian Kranert, Chris Sturm, Rüdiger Schmidt-Grund, and Marius Grundmann — Universität Leipzig, Institut für Experimentelle Physik II, Semiconductor Physics Group, Leipzig, Germany

In optically anisotropic materials, the polarization of incident and scattered radiation changes within the crystal along the propagation direction due to birefringence. Consequently, the polarization state at an individual scattering event varies. This prohibits the direct application of the "standard" Raman tensor formalism and causes experimental Raman intensities to generally depend on specifics of the experiment such as focus depth and depth resolution. Therefore it was assumed that the Raman intensities for polarizations, which are not parallel to a principal axis of the dielectric indicatrix, cannot be analytically described. If done anyway, the polarization dependence was modeled using ad-hoc complex phase parameters for the individual Raman tensor elements without connection to a physical property.

We present a modified Raman tensor formalism which allows to model the Raman intensity in dependence on the polarization configuration for any crystal symmetry. It further establishes the complex phase parameters as special case for uniaxial crystals and explains their physical meaning. We explain that for an integration over a sufficiently large depth range, which is fulfilled for bulk samples and typical experimental setups, the depth dependence vanishes. We further discuss the case of an integration over a smaller depth range which is for example required for thin films.

HL 59.9 Wed 17:30 H10

Theory for the edge-state optical absorption in two-dimensional transition metal dichalcogenide flakes — •Maxim Trushin — University of Konstanz, Konstanz, Germany

The edge states provide electrical conductivity in quantum Hall systems and other two-dimensional (2d) topological insulators. Their role in optical and transport properties of other 2d materials, like 2d transition metal dichalcogenides [1], still remains illusive. There are indications that the optical absorption in MoS_2 at excitation energies below the band gap could be due to the edge states [2]. Here, we elaborate this problem from the theoretical point of view. We model the border between semiconductor and vacuum by means of the spatially dependent band gap: It is finite within the semiconducting region but infinite outside [3]. This model neglects the detail of the edge at the atomic level, but offers an analytical formula for the linear as well as saturable absorption. We show that the relative absorption of a single 50 nm-size MoS_2 flake is of the order of 0.01 % that corresponds to the absorption of a MoS_2-enriched polymer film of a few percent. We also find that at high radiation intensities the edge-state electron temperature can reach a few thousands Kelvin, whereas the bulk electrons and holes remain at lattice temperature. Our outcomes can be directly utilized for understanding of the subgap absorption in MX_2 flakes [2] and pave the way towards application of MS_2-based optoelectronic devices. [1] K.F. Mak et al. Phys. Rev. Lett. **105**, 136805 (2010). [2] R. I. Woodward et al. Photon. Res. **3**, A30 (2015). [3] M.V. Berry and R.J. Mondragon. Proc. R. Soc. (London) A **412**, 53 (1987).

HL 59.10 Wed 17:45 H10

Optical constants of Ge and GeO2 from ellipsometry — T. Nathan Nunley, Nalin Fernando, Jaime Moya, and •Stefan Zollner — New Mexico State University, Las Cruces, NM, USA

We studied the optical constants of GeO2 and Ge using spectroscopic ellipsometry. Ge substrates were prepared for oxidation by ozone cleaning at 150C for 90 minutes, followed by an ultrasonic clean in DI water, and then in isopropanol. The samples were then annealed in ultra high purity oxygen at 550C at a pressure of 25 psi at a flow rate of 1 l/min. The ellipsometric angles and depolarization were measured using a rotating analyzer ellipsometer with a computer controlled Berek waveplate compensator from 0.5-6.6 eV. X-ray reflectance with Cu radiation was performed to obtain thickness, roughness, and electron density independently. Measurements of the optical phonons were performed at CINT Sandia using FTIR ellipsometry. Samples with 0.1-200 nm GeO2 on Ge were studied, and it was found that the oxidation rate at this pressure was more than twice that previously reported in the literature. The optical constants of GeO2, assumed to be independent of thickness, and the Ge substrate are decoupled by varying the oxide thickness allowing for an optical constant optimization of both the film and the substrate. Using this method we have been able to obtain the optical constants for thermal GeO2 and Ge in the mid infrared and from 0.5-6.6 eV. These data sets will be crucial for the design of Ge based optoelectronic devices and for thickness measurements of thin films on Ge substrates.

HL 59.11 Wed 18:00 H10

Determination of optical and electronic structure properties of Sr2Si5N8:Eu2+ and Ce3+ phosphors — •sikander azam[1] and jan minar[2] — [1]New Technologies-Research Center, University of West Bohemia, Univerzitni 8, 306 14 Pilsen, Czech Republic — [2]Dept. of Chemistry, University of Munich, Germany

Upon doping with lanthanide ions (e.g. Eu2+, Ce3+), a number of nitridosilicates and oxonitridosilicates emerged as highly efficient luminescent materials (phosphors) that found considerable industrial application in white light emitting diodes (LEDs). It is found that the nitride (alumo) silicates *Sr2Si5N8:Eu2+* found broad industrial application as highly efficient red-emitting phosphor materials in pc-LEDs [1-3]. Using density functional theory (DFT) within the GGA+U form we investigated the structural, electronic and optical properties of Eu2+ and Ce3+ doped Sr2Si5N8. The total energy has been optimized as a function of the unit cell volume. Electronic structure like e.g. the density of state (DOS), the band structure and the linear optical susceptibility are calculated for the relaxed structure applying the optimized lattice constant. It will be shown that for the calculation of optical properties, which are closely related to the corresponding electronic structure our results are in very good agreement with experimental data. Concerning calculations we have to discuss it in a detail. References [1] Martin Zeuner, Peter J. Schmidt, Wolfgang Schnick, Chem. Mater., Vol. 21, No. 12, 2009 [2] Zeuner, M.; Schmidt, P. J.; Schnick, W. Chem. Mater. 2009, 21,2467. [3] Zeuner, M.; Pagano, S.; Schnick, W. Angew. Chem., Int. Ed. 2011, 50, 7754

HL 59.12 Wed 18:15 H10

THE INVESTIGATION OF PRESSURE EFFECT ON THE OPTICAL PROPERTIES, SPONTANEOUS POLARIZATION AND EFFECTIVE MASS OF BaHfO3: AB INITIO STUDY — •chaimae azahaf — Laboratory of Magnetism and High Energy Physics (URAC 12), Faculty of Sciences, Mohammed V University, B.P. 1014, Rabat, Morocco

Through first principles calculations, the optical properties, spontaneous polarization and the effective mass of the cubic perovskite BaHfO3 under pressure effect have been investigated, using the Full Potential Linearized Augmented Plane Wave (FP-LAPW) method implemented in the WIEN2K code, in connection with the Generalized Gradient Approximation (GGA). During this study, the effect of pressure is seen on the electronic and optical properties such as: The band gap value (Eg) of the perovskite BaHfO3 is reduced and it becomes indirect instead of direct band gap as pressure increased. From the band structure we have also computed the variation of effective masse (m*) which increases to the same effect as the pressure. The results of the optical study, shows that the absorption coefficient increases and the spontaneous polarization (Ps) increases in a quasi-linear behavior as pressure increases. Our conclusion is that BaHfO3 is a piezoelectric material; also this material could be applicable in optoelectronic applications.

HL 60: III-V Semiconductors (no Nitrides)

Time: Wednesday 14:45–17:15 Location: H13

HL 60.1 Wed 14:45 H13

Electronic Transport Properties of Novel Superlattice GaAs/AlAs Nanowire Heterostructures — •Jakob Seidl[1], Dominik Irber[1], Jonathan Becker[1], Stefanie Morkötter[1], Bernhard Loitsch[1], Daniel Rudolph[1], Julia Winnerl[1], Markus Döblinger[3], Nari Jeon[2], Max Bichler[1], Matthew Grayson[4], Lincoln J. Lauhon[2], Gregor Koblmueller[1], Jonathan J. Finley[1], and Gerhard Abstreiter[1] — [1]Walter Schottky Institut and Physik Department, TU München, Garching, Germany — [2]Department of Materials Science and Engineering, Northwestern University, Evanston, U.S.A. — [3]Department of Chemistry, LMU München, Munich, Germany — [4]Department of Electrical Engineering and Computer Science, Northwestern University, Evanston, U.S.A.

This work focuses on recent developments of GaAs/AlAs superlattice shell Nanowire MODFETs. We present a new design based on multiple alternating MBE-grown GaAs/AlAs layers around a GaAs core, promising enhanced electronic properties. The high structural quality of the device is confirmed using both STEM and APT techniques. Electrical transport measurements probing the FET characteristics reveal low resistance ohmic contacts and outstanding top gate performance at ambient temperature, as well as 4.2K, without the need for illumination. At RT, we obtained contact resistances of $R = 1\,k\Omega$, subthreshold swings of about $SS = 70\,mV/dec$ and mobilities up to $\mu = 700\,cm^2/Vs$. The transfer characteristics at 4.2 K show steplike features related to a discrete electronic subband structure in very good agreement with numerical simulations performed using nextnano.

HL 60.2 Wed 15:00 H13

Next generation gating: Prepatterned back gates implemented into the growth of ultra-high mobility GaAs/AlGaAs heterostructures — •Matthias Berl[1], Lars Tiemann[1], Werner Dietsche[1], Werner Wegscheider[1], and Helmut Karl[2] — [1]ETH Zürich, 8093 Zürich, Switzerland — [2]Universität Augsburg, 86159 Augsburg, Germany

Electrostatic gating of semiconductors is of fundamental interest, because it allows to modify the inherent electrical properties of the semiconducting material. Typically evaporated top gates are used after the heterostructure growth, because their processing is more flexible and can be adjusted at will. However, top gates are not always the best solution. Due to the Schottky barrier, top gates are often limited in the gating range and they can be obstructive for optical penetration.

We have developed a method to implement patterned back gate structures into the growth of high mobility MBE heterostructures. The back gate structures are defined by local oxygen implantation into a silicon doped GaAs epilayer grown on top of the insulating substrate. The oxygen implantation suppresses the conductance without affecting the surface quality, allowing for high quality heterostructure growth. First measurements have demonstrated a wide range of tunability ($2*10^{10}$ cm^{-2} to $4.4*10^{11}$ cm^{-2}) for a two-dimensional electron gas grown on an implantation patterned substrate with mobilities exceeding $20*10^{-6}$ cm^2/Vs.

HL 60.3 Wed 15:15 H13

Heat flow and noise measurements in etched semiconductor quantum wire structures — •Christian Riha[1], Olivio Chiatti[1], Sven S. Buchholz[1], Christoph Kreisbeck[1], Dirk Reuter[2], Andreas D. Wieck[3], Tobias Kramer[4], and Saskia F. Fischer[1] — [1]Novel Materials Group, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — [2]Optoelektronische Materialien und Bauelemente, Universität Paderborn, 33098 Paderborn, Germany — [3]Angewandte Festkörperphysik, Ruhr-Universität Bochum, 44780 Bochum, Germany — [4]Konrad-Zuse Zentrum für Informationstechnik Berlin, 14195 Berlin, Germany

Low-dimensional transport in semiconductor meso- and nanostructures is a topical field of fundamental research with potential applications in future quantum devices. However, thermal non-equilibrium may destroy phase-coherence and remains to be explored experimentally. In the limit of non-interacting charge carriers the heat and charge transport are coupled, as given by the Wiedemann-Franz relation between the electrical and thermal conductivity. Here, we present effects of thermal non-equilibrium in narrow quasi-two-dimensional (2D) channels, quasi-one-dimensional (1D) waveguide networks, quantum rings (QRs) and single 1D constrictions such as quantum point contacts (QPCs) using current heating and noise thermometry [1]. Therefrom, we determine and discuss electron-energy loss rates, electron-phonon interaction and heat transport processes.

[1] C. Riha *et al.*, Appl. Phys. Lett. **106**, 083102 (2015);

HL 60.4 Wed 15:30 H13

Mapping of an electron wave function by a local electron scattering probe — •Christian Reichl — Labor für Festkörperphysik, ETH Zürich, Schweiz

We developped a technique which allows for the detailed mapping of the electronic wave function in two-dimensional electron gases with low-temperature mobilities up to $15{\cdot}10^6$ cm^2/Vs.

Thin ("delta") layers of aluminium are placed into the regions where the electrons reside. This causes electron scattering which depends very locally on the amplitude of the electron wave function at the position of the Al delta-layer. By changing the distance of this layer from the interface we map the shape of the wave function perpendicular to the interface. Despite having a profound effect on the electron mobiliy, the delta-layers do not cause a widening of the quantum Hall plateaus.

30 min. Coffee Break

HL 60.5 Wed 16:15 H13

Probing the Dynamics of Self-Localised Exciton-Polariton Condensates in Moving 2D Lattices — •Jakov V. T. Buller[1], Raul E. Balderas-Navarro[2], Klaus Biermann[1], Edgar A. Cerda-Méndez[1], and Paulo V. Santos[1] — [1]Paul-Drude-Institut für Festkörperelektronik, 10117 Berlin, Germany — [2]Instituto de Investigación en Comunicación Óptica, 78000 San Luis Potosí, México

Microcavity exciton-polaritons are bosonic half-light half-matter quasiparticles which result from the strong coupling between light and excitons. Their low effective mass enables their condensation at low particle densities and high temperatures in comparison to atomic systems. Additionally, by introducing a periodic spatial modulation exciton-polariton gap solitons (GS), i.e. self-localised exciton-polariton condensates, can be created at excitation powers close to or above the condensation threshold.

In this contribution, we report on the temporal dynamics of GS in moving acoustic square lattices generated by surface acoustic waves (SAWs). Beside the observation of the temporal evolution of the GS wave function, we find that the GS photoluminescence (PL) shows periodic variations of its intensity at harmonics of the SAW frequency. These variations can reach up to tens of percent of the average PL intensity and depend on the power as well as on the FWHM of the excitation laser spot. Possible explanations will be addressed in the talk. Our results enhance the fundamental understanding of the self-localised exciton-polariton condensates and may be relevant for their implementation of polaritonic devices.

HL 60.6 Wed 16:30 H13

CXDI as tool for real structure analysis — •Arman Davtyan[1], Alexander Seel[1], Otmar Loffeld[1], Sebastian Lehmann[2], Dominik Kriegner[3], Mohammad Kashani[1], Ali Al Hassan[1], and Ullrich Pietsch[1] — [1]NT faculty, University of Siegen, Siegen, Germany — [2]Department of Physics and The Nanometer Structure Consortium, Lund University, P.O. Box 118, 22 100 Lund, Sweden — [3]Department of Condensed Matter Physics, Charles University in Prague, Ke Karlovu 5, 121 16 Prague 2, Czech Republic

The distribution of planar stacking faults and twins within single semiconductor GaAs nanowires (NWs) has been studied using the Coherent x-ray diffraction imaging (CXDI) technique at ID1 beamline at ESRF. CXDI probes the defect structure of the certain segment along the nanowire growth direction at asymmetric geometry with grazing exit condition. CXDI pattern from the segment of the NW shows a clear periodicity around the (10-15) WZ reflection indicating that the segment of the NW which is being illuminated with coherent X-rays has only few stacking faults. The electron density distribution in real space can be inverted from the diffraction pattern. We demonstrate the feasibility of phase retrieval algorithms in case of low density planar defects along the NW growth direction following the approach demonstrated for the NWs with high density of stacking faults. Here, we present also

a novel approach to retrieve the arrangement of twin domains within single GaAs nanowires based on Kalman filter and L1 minimization.

HL 60.7 Wed 16:45 H13

Terahertz magneto-optical activity of III-V semiconductors — •Jan Chochol[1,2], Kamil Postava[1], Michael Čada[2], Mathias Vanwolleghem[3], Dominique Vignaud[3], Martin Mičica[1,3], and Jaromír Pištora[1] — [1]VŠB - Technical University of Ostrava, Czech Republic — [2]Dalhousie University, Halifax, Canada — [3]Université Lille 1, Villeneuve-d'Ascq, France

The recent advances in terahertz technology have put a demand for new materials and devices capable of operating with submillimeter waves. One of the desired properties is the non-reciprocity, which is usually achieved by magnetic field. In such magnetic field, materials with free carriers exhibit induced anisotropy. We examine the induced anisotropy of III-V semiconductors (GaAs, InP, InSb) by studying the magneto-optical Kerr effect with the terahertz time domain spectroscopy and FTIR spectroscopy - the spectral range from 2 to 680 cm^{-1}. Notably for pure InSb we report a strong effect using a small magnetic field (˜0.3 T). The calculation of the semiconductor permittivity is based on the Drude-Lorentz model[1] and the concentration and mobility of carriers is verified using Hall measurements.

[1] Palik, E. D., and J. K. Furdyna. *Infrared and Microwave Magnetoplasma Effects in Semiconductors.* Reports on Progress in Physics 33, no. 3 (1970): 1193.

HL 60.8 Wed 17:00 H13

Suppression of rotational twin domains in GaP epilayers on Si(111) for improved III-V nanowire growth — •Christian Koppka, Agnieszka Paszuk, Matthias Steidl, Peter Kleinschmidt, and Thomas Hannappel — TU Ilmenau, Institute of Physics, D-98693 Ilmenau, Germany

The growth of a high-quality GaP epilayer on Si(111) could lead to promising hetero-substrates for optoelectronic devices such as high efficiency NW-based multi-junction solar cells, LEDs and fast photodetectors [1]. Low defect densities in the buffer layer are required for further III/V integration and superior optoelectronic properties of the GaP itself. However, epitaxially grown III-V layers on (111) oriented substrates tend to form rotational twin domains (RTDs), which results in multicrystalline layers with poor surface quality [1-2]. In order to suppress the formation of RTDs the impact of the substrate misorientation as well as nucleation conditions during MOVPE growth were investigated. Combining HRXRD, SEM and AFM, we reveal a significant influence of nucleation temperature and substrate offcut direction on the formation of RTDs. The epilayer quality is drastically increased by a low temperature nucleation step. Using Si(111) substrates with 3° misorientation towards <-1-12> as well as improved nucleation conditions the twinned GaP domains are suppressed below 4%. We demonstrate that these quasi-substrates are highly suitable for vertical GaP nanowire growth. [1]I. Miccoli et al., Cryst. Res.Technol. 46, 795 (2011) [2]H. A. Fonseka et al., Nanotechnol. 24, 465602 (2013)

HL 61: Quantum Dots and Wires: Transport Properties

Time: Wednesday 14:45–17:30 Location: H16

HL 61.1 Wed 14:45 H16

Spin-triplet relaxation times of different shells in self-assembled quantum dots — •Kevin Eltrudis[1], Amran Al-Ashouri[1], Andreas Beckel[1], Arne Ludwig[2], Andreas D. Wieck[2], Axel Lorke[1], and Martin Geller[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany — [2]Chair for Applied Solid State Physics, Ruhr-Universität Bochum, Universitätsstr. 150, 44780 Bochum, Germany

Self-assembled quantum dots (QDs) are among the promising candidates for quantum computation devices, which involve a two level quantum system. A possibility is the two-electron excited spin triplet and its singlet ground state. We demonstrate an all-electrical initialization of the spin triplet state and measure - by electrical means - the spin relaxation time in absence of a magnetic field after the injection of the second electron into the p- and the d-shell. We find a similar spin relaxation time of 25 μs (p-shell) and 23 μs (d-shell). The measurement technique we use is based on the time-resolved transconductance spectroscopy [1]. The InAs QDs are embedded in a GaAs/AlGaAs heterostructure (FET), where an electron reservoir (2DEG) coupled to the QDs serves as charge reservoir as well as sensitive detector for the electron states. By charging the QDs resonantly into the triplet states and observing the electron emission during discharge, we are able to record the relaxation of the triplet states. In future measurements in the presence of a magnetic field even longer spin-relaxation times are expected. [1] B. Marquardt. et al., Nature Commun. 2, 209 (2011)

HL 61.2 Wed 15:00 H16

Topological Blockade of Transport in Quantum Dot Arrays — •Mónica Benito[1], Michael Niklas[2], Gloria Platero[1], and Sigmund Kohler[1] — [1]Instituto de Ciencia de Materiales de Madrid, CSIC, 28049 Madrid, Spain — [2]Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

We discuss a transport blockade mechanism in quantum dot arrays and conducting molecules based on an interplay of Coulomb repulsion and the formation of edge states. As a model we employ a dimer chain that exhibits a topological phase transition. The connection to strongly biased electron source and drain enables transport. The topological transition is manifest in the shot noise properties as it is accompanied by a crossover from bunched electron transport to a Poisson process. We develop for both regions a scenario that can be captured by a rate equation. The resulting analytical expressions for the Fano factor agree well with the numerical solution of a full quantum master equation. [1] M. Benito, M. Niklas, G. Platero and S. kohler, arXiv:1511.01348 (2015)

HL 61.3 Wed 15:15 H16

Noise and Transport through self-assembled InAs Quantum Dot Systems — •Jan K. Kühne and Rolf J. Haug — Institut für Festkörperphysik, Leibniz Universität Hannover, Hannover, Germany

We present transport and shot noise measurements through self-assembled single and double quantum dots of InAs at very low temperatures. Quantum effects like the Fermi-edge singularity (FES) lead to peaks in the current and to enhanced suppression of the shot noise in our systems [1]. Further we observe different behavior in the IV - characteristics and the Fano factor depending on the transport direction, due to the asymmetry of the quantum dot and the corresponding change in tunneling rates of the collector and emitter. Especially we compare the different influence of an applied magnetic field.

[1] N. Ubbelohde, K. Roszak, F. Hohls, N. Maire, R. J. Haug, and T. Novotny, Sci. Rep.2,374(2012)

HL 61.4 Wed 15:30 H16

Logical Stochastic Resonance and its Applications in a Coulomb-Coupled Quantum-Dot Rectifier — •Pierre Pfeffer[1], Fabian Hartmann[1], Igor Neri[2], Anne Schade[1], Monika Emmerling[1], Martin Kamp[1], Luca Gammaitoni[2], Sven Höfling[1,3], and Lukas Worschech[1] — [1]Technische Physik and Wilhelm Conrad Röntgen Research Center for Complex Material Systems, Physikalisches Institut, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]NiPS Laboratory, Dipartimento di Fisica, Universita di Perugia, I-06100 Perugia, Italy — [3]SUPA, School of Physics and Astronomy, University of St Andrews, St Andrews, KY16 9SS, United Kingdom

Although noise is largely considered as an adverse factor in electronics, effects like logical stochastic resonance (LSR) can render electronic fluctuations useful. We observe LSR in a semiconductor system consisting of two Coulomb-coupled quantum dots (QDs) and show that voltage fluctuations applied to one of the QDs lead to a rectified and controllable current in the other QD. The system is able to offer several logic functionalities, among them the two universal logic gates NOR and NAND and the logic XOR, which can be accessed and switched between by applying suited noise and gate voltages. Benefiting from this, we demonstrate two different realizations of a half adder and examine their optimal modes of operation. As the presented devices draw their power solely from electronic fluctuations they can be considered as advancements in the field of energy efficient and autonomous electronics.

30 min. Coffee Break

HL 61.5 Wed 16:15 H16

Strongly interacting quantum wires with spin-orbit coupling — •Chris Pedder and Thomas Schmidt — Universite du Luxembourg, Luxembourg.

We study the effect of Rashba spin-orbit coupling on a quantum wire with strong interactions, which can be experimentally realised by depopulating a gated InSb or GaAs wire. When the wire carries a very low density of electrons, it is convenient to model the system in terms of a "Wigner crystal" of electrons localised on lattice sites. At the lowest densities, the Wigner crystal is a one dimensional entity, whereas at intermediate regimes it is known that a "zigzag" crystal consisting of two parallel rows of electrons can form. We investigate the effect of Rashba spin-orbit coupling, which plays an important role for both the spin and charge degrees of freedom, in both these systems with and without an applied magnetic field. We propose detection of these effects via measurement of spin-spin correlation functions of the quantum wire, e.g. by doing STM with a polarized tip.

HL 61.6 Wed 16:30 H16

Electronic Structure and Transport Properties of Thin Silicon Nanowires — •Florian Fuchs[1,2,3], Sibylle Gemming[1,3], and Jörg Schuster[4] — [1]Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Dresden, Germany — [2]Center for Advancing Electronics Dresden (cfaed), Dresden, Germany — [3]Institute of Physics, Technische Universität Chemnitz, Chemnitz, Germany — [4]Fraunhofer Institute for Electronic Nano Systems, Chemnitz, Germany

Silicon nanowires (SiNWs) are promising candidates as building blocks for electronic devices. For the simulation of SiNWs, numerical device simulations, based on the silicon bulk band structure, are often used. When the diameter of the wires is reduced, however, atomistic quantum simulations become mandatory at some point.

In the present work, thin hydrogen-passivated SiNWs with diameters between 1 and 6 nm are studied by means of density functional theory. It is shown that the band gap approaches the bulk value in the limit of infinitely thick nanowires and increases for thin wires due to quantum confinement. Using a radially resolved density of states it is demonstrated, that the density of states is highest in the nanowire center, where most of the current transport would occur, and decreases near the surface. Comparing the density of states between SiNWs with different diameters, the transition to bulk silicon can be observed. This justifies the use of bulk band structure approximations for thicker SiNWs, but also highlights the need for atomistic quantum simulations in case of thinner ones.

HL 61.7 Wed 16:45 H16

Universal Conductance Fluctuation in Ge-doped GaN Nanowires — •Patrick Uredat[1], Matthias T. Elm[1,2], Jan Binder[2], Lars Ostheim[1], Markus Schäfer[1], Pascal Hille[1], Jan Müssner[1], Jörg Schörmann[1], Martin Eickhoff[1], and Peter J. Klar[1] — [1]I. Physikalisches Institut, Heinrich-Buff-Ring 16, Justus-Liebig-Universität Gießen, 35392 Gießen — [2]Physikalisch-Chemisches Institut, Heinrich-Buff-Ring 17, Justus-Liebig-Universität Gießen, 35392 Gießen

Semiconducting III-V nanowires are not only an auspicious material system for future nanoelectronic devices, such as nanoscaled field-effect transistors, ultra-violet light-emitting diodes or other optoelectronic applications, but also an ideal model system for studying mesoscopic effects. Therefore, the transport properties of single Ge-doped GaN nanowires are investigated. Measurements reveal universal conductance fluctuations as well as a weak localization effect. The phase coherence length l_ϕ was obtained by analyzing the quantum interference effects. For slightly doped nanowires inelastic electron-electron scattering seems to be the dominant phase breaking mechanism at low temperatures, whereas for highly doped nanowires quasi-elastic Nyquist-scattering appear to be more prominent. Temperature dependent analysis of the UCFs for different doping levels reveal a quasi one-dimensional transport behavior due to a surface depletion layer in slightly doped nanowires. In contrast, highly doped nanowires seem to have a less confined transport channel.

HL 61.8 Wed 17:00 H16

Electronic structure and transport properties of III-V core/shell nanowires — •Florinda Viñas and Martin Leijnse — Division of Solid State Physics and NanoLund, Lund University, Box. 118, S-22100, Lund, Sweden

We have modeled electron structure and low-temperature transport in III-V core/shell nanowires to establish a relationship between electron-hole hybridization and signatures in thermoelectrical measurements. Nanowires with a GaSb core and an InAs shell (and inverted) are interesting for studies of hybridization effects due to the bulk broken band gap alignment at the material interface. By varying the core radius and shell thickness of such wires we can modify the size of the band gap and create wires with band structures that exhibit hole-electron hybridization states.

The band structures are obtained using 8-band $k \cdot p$ theory together with the envelope function approximation. The calculated energy dispersions are used as input to the Boltzmann equation to study thermoelectric transport quantities such as the Seebeck coefficient, in the diffusive limit.

HL 61.9 Wed 17:15 H16

Electrical transport characteristics and hysteresis in back-gated InAs nanowire FET devices — •Jonathan Becker, Stefanie Morkötter, Phillip Geselbracht, Julian Treu, Simon Hertenberger, Max Bichler, Jonathan J. Finley, Gerhard Abstreiter, and Gregor Koblmüller — Walter Schottky Institut und Physik Department, TU München, Garching, Germany

In this work we present recent results on the electrical transport of nominally undoped MBE grown InAs nanowires (NWs). In particular we explore the influence of growth parameters, microstructure and aspect ratio on the electrical properties of the NWs. Four-terminal measurements on planar, back-gated NW field effect transistor (NWFET) devices revealed room-temperature mobilities ranging from 500 to 2000 cm^2/Vs and on-off ratios of $>10^3$ at 4.2K. The obtained electron densities are in the order of $10^{17}cm^{-3}$. A strong effect of the diameter and the microstructure, altered by growth parameters, on the mobility was observed. The latter was investigated by HRTEM, simulations and temperature-dependent measurements in high detail. Here, the impact of band discontinuities induced by stacking faults and WZ/ZB crystal phase boundaries on electron scattering is evaluated. Furthermore we evaluate the prevalent hystersis in these devices and present techniques to overcome the opposed limitations, paving the way for novel sensing schemes.

HL 62: Gallium Nitride: Optical and Electronic Properties

Time: Wednesday 14:45–18:30 Location: H17

HL 62.1 Wed 14:45 H17

Charge carrier localization in submonolayer InN/GaN superlattices — •Felix Feix, Timur Flissikowski, Caroline Chèze, Raffaella Calarco, Holger T. Grahn, and Oliver Brandt — Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5–7, 10117 Berlin, Germany

The inevitable compositional fluctuations in the random alloy (In,Ga)N lead to the localization of charge carriers with profound implications for their recombination dynamics. Digital alloys composed of an InN/GaN short-period superlattice (SPSL) are envisioned to eliminate alloy disorder and the resulting localization phenomena. However, a recent microscopic investigation of such structures demonstrated that the nominal InN monolayers (ML) in the SPSL have a coverage well below 100 %. Here, we use molecular beam epitaxy to fabricate sub-ML InN/m-ML-GaN superlattices with $m = 6 \ldots 44$ MLs and investigate these structures by temperature-dependent photoluminescence (PL) spectroscopy under both continuous-wave and pulsed excitation. Both the peak energy and the linewidth of the emission band associated to the sub-ML InN wells exhibit an anomalous dependence on temperature indicative of carrier localization. Delocalization is accompanied by a thermally activated quenching of the emission. PL transients reveal a power law decay at low temperatures reflecting that recombining electrons and holes occupy spatially separate, individual potential

minima reminescent of conventional (In,Ga)N quantum wells. These results suggest that essentially the sub-ML InN wells act electronically as two-dimensional random alloys.

HL 62.2 Wed 15:00 H17

Control of optical polarization properties by anisotropic strain in non- and semipolar GaInN/GaN quantum wells — •F. A. Ketzer[1], P. Horenburg[1], E. R. Buss[1], H. Bremers[1], U. Rossow[1], F. Tendille[2], P. De Mierry[2], P. Vennéguès[2], J. Zuniga-Perez[2], and A. Hangleiter[1] — [1]Institut für Angewandte Physik, Technische Universität Braunschweig — [2]Centre de Recherche sur l'Hétéro-Epitaxie, Valbonne, France

In this contribution we show evidence of successful manipulation of anisotropic strain in non- and semipolar multi quantum well (MQW) GaInN/GaN structures. Using AlInN interlayers with different compositions and thicknesses prior to our QWs we are able to control the strain and therefore modify the properties of the emitted light significantly. The growth conditions for the active zone have been kept unchanged. Our samples are grown via low pressure MOVPE on m-oriented pseudo-bulk and $(11\bar{2}2)$ GaN templates grown on patterned r-sapphire substrates. We determine the composition and strain of our MQWs by high resolution X-ray diffraction. With polarization resolved photoluminescence (PL) spectroscopy at low and room temperature we analyze the influence of the unusual anisotropic strain on optical properties due to changes in the valence band structure. The manipulated QWs show good optical properties compared to regular structures. For m-plane we achieve polarization of more than 90% at 445nm and 25% at 525 nm, while the semipolar samples show polarizations of 7% and 18% at 550 nm and 580 nm, respectively. In order to understand the behaviour $\mathbf{k} \cdot \mathbf{p}$ calculations were compared to our measurements.

HL 62.3 Wed 15:15 H17

Optical properties of two dimensional photonic crystal membranes in cubic AlN — •Sarah Blumenthal[1], Matthias Bürger[1], Andre Hildebrandt[2], Jens Förstner[2], Nils Weber[1], Cedrik Meier[1], Dirk Reuter[1], and Donat J. As[1] — [1]University of Paderborn, Department of Physics, Germany — [2]University of Paderborn, Department of Theoretical Electrical Engineering, Germany

Group III-nitride quantum dots (QDs) attracted much attention for the development of optical and quantum optical devices, operating in the UV spectral range. Microresonators enable to control the spontaneous emission of light and to realize an efficient single photon emitter (SPE). Promising candidates for such devices are 2D photonic crystal (PhC) nanocavities. Recently, SPE employing hexagonal QDs in AlN have been realized. However h-GaN QDs exhibit a strong internal electrical field causing a reduced recombination probability of electrons and holes in confined states. This issue may be overcome by using cubic AlN/GaN. We implemented a process to fabricate freestanding c-AlN/GaN membranes with a 2D hexagonal array of holes. We have investigated the optical properties of the QD ensemble and different PhCs (including H1 and L3 cavities) using micro-photoluminescence measurements at room temperature. For both cavity types, fundamental modes with high quality factors were determined. To validate the experimental results, simulations, using the time domain solver from CST Microwave Studio, were done. The simulations fit very well to the experimental results.

HL 62.4 Wed 15:30 H17

Role of coherency strain for optical properties of $In_xGa_{1-x}N$ active layers grown on GaN substrates — •Christoph Freysoldt[1], Siyuan Zhang[1,2], Ying Cui[1], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — [2]Department of Materials Science and Metallurgy, University of Cambridge, United Kingdom

$In_xGa_{1-x}N$ alloys are the material of choice for the optical recombination layers in GaN-based optoelectronic devices. When going from the violet-blue spectral range ($x \approx 15\%$) towards the green range $x > 30\%$), the growth of coherent $In_xGa_{1-x}N$ layers becomes increasingly difficult due to the lattice mismatch between InN and GaN. Yet, significant progress has been made experimentally to improve the quality of high-In films.

Theoretically, $In_xGa_{1-x}N$ alloys have been studied by a variety of methods ranging from multi-band k·p over tight-binding to density-functional theory. In our work, we explore the role of finite coherency strain on the electronic structure of $In_xGa_{1-x}N$ alloys for polar (c-plane) and non-polar (a-plane and m-plane) growth using state-of-the-art density-functional theory. Our calculations highlight that the high strains introduce non-linear effects in the elastic behavior and in the electronic structure that are missed by perturbative treatments of strain. We demonstrate that non-linear strain relaxation breaks the symmetry between a-plane and m-plane for the strain-induced valence band splitting that is relevant for inducing in-plane polarization of the emitted light.

HL 62.5 Wed 15:45 H17

Photoluminescence excitation measurements of molecular beam epitaxial grown cubic GaN/Al(Ga)N quantum well structures — •Tobias Wecker[1], Gordon Callsen[2], Axel Hoffmann[2], Dirk Reuter[1], and Donat J. As[1] — [1]Department of Physics, University of Paderborn, Warburger Straße 100, 33098 Paderborn, Germany — [2]Institut für Festkörperphysik, TU Berlin, Straße des 17. Juni 135, 10623 Berlin, Germany

In recent years group III-nitrides and their compounds have been in the focus of interest for devices based on intersubband transitions in the 1.55 μm spectral region. For such devices the understanding of the complete energy level structure is crucial to manipulate the allowed transitions. Photoluminescence excitation (PLE) spectroscopy gives access to the excited energy levels. In hexagonal group III nitrides the adjustment of the quantum well (QW) energy levels is complicated by the quantum confined stark effect, resulting from spontaneous polarization fields. Due to the higher crystal symmetry this harmful effect is absent in the cubic phase along the (001) direction. We investigate an uncoupled asymmetric cubic $GaN/Al_{0.25}Ga_{0.75}N$ double quantum well and a single cubic GaN/AlN QW grown on 3C-SiC (001) substrate by radio-frequency plasma-assisted molecular beam epitaxy. PLE and photoluminescence spectra, taken at 7 K, show several emission bands. Comparing these emission bands with simulated transitions calculated by a Schrödinger-Poisson solver based on an effective mass model (nextnano[3]) revealed a good agreement between theory and experiment.

HL 62.6 Wed 16:00 H17

Optical and electronic properties of InGaN/GaN core-shell microrod light emitting diodes — •Marcus Müller[1], Peter Veit[1], Frank Bertram[1], Christian Nenstiel[2], Gordon Callsen[2], Matin Mohajerani[3], Jana Hartmann[3], Hao Zhou[3], Hergo-H. Wehmann[3], Axel Hoffmann[2], Andreas Waag[3], and Jürgen Christen[1] — [1]Institut für Experimentelle Phssik, Otto-von-Guericke-Universität Magdeburg — [2]Institut für Festkörperphysik, Technische Universität Berlin — [3]Institut für Halbleitertechnik, Technische Universität Braunschweig

We present a comprehensive study of structural, optical, and electronic properties of three-dimensional, nitride-based, core-shell microrod LEDs. The InGaN/GaN microrod heterostructures were grown via the selective area growth technique by metal-organic vapor phase epitaxy. Using highly spatially resolved cathodoluminescence (CL) and Raman-spectroscopy directly performed on a thin TEM-lamella, we analyze free carrier concentrations of single Si-doped GaN core. Both, CL and Raman measurements reveal a high free carrier concentration of $6.9 \cdot 10^{19}$ cm^{-3} in the bottom part and a decreasing doping level towards the tip of the microrod. Structural investigations show that initial Si-doping of the core has a strong influence on the formation of extended defects in the overgrown shells. Highly spatially resolved CL mappings of the InGaN single quantum well luminescence exhibit a red shifted emission at these defects which most probably indicates indium clustering.

HL 62.7 Wed 16:15 H17

Charge transfer across the GaN nanowire / electrolyte interface — •Jan Philipps, Sara Lippert, Pascal Hille, Jörg Schörmann, Detlev Hofmann, and Martin Eickhoff — 1. Physikalisches Institut, Justus-Liebig-Universität, Gießen, Deutschland

We have investigated the transfer processes of photogenerated charge carriers from GaN nanowires to an electrolyte environment by the means of photoluminescence, current measurements and electron paramagnetic resonance spin trap technique. We find that photogenerated holes can be transferred to the $OH\cdot/OH^-$ redox couple or can be consumed by photoanodic oxidation of the GaN surface. The efficiencies of the two processes strongly depend on the applied bias between the nanowires and the electrolyte. The presented results will be discussed considering the redox potentials in the electrolyte as well as the electronic structure of the semiconductor material and the occupation of surface states in the frame of the surface band bending model.

30 min. Coffee Break

HL 62.8 Wed 17:00 H17

Defect analysis of $(11\bar{2}2)$ semipolar GaN materials and devices — •Matthias Hocker[1], Ingo Tischer[1], Marian Caliebe[2], Ferdinand Scholz[2], and Klaus Thonke[1] — [1]Institute of Quantum Matter / Semiconductor Physics Group, University of Ulm, D-89081 Ulm, Germany — [2]Institute of Optoelectronics, University of Ulm, D-89081 Ulm, Germany

Semipolar GaN layers grown on foreign substrates typically suffer from a high density of extended defects like threading dislocations and stacking faults. We investigate such $(11\bar{2}2)$-oriented GaN layers grown by MOVPE on patterned sapphire substrates by spatially and spectrally resolved low-temperature cathodoluminescence. The emission below the excitonic bandgap region is mostly dominated by basal plane stacking faults of I_1 type, giving rise to a band at ≈ 3.41 eV, which shifts with the strain and doping level in the layers. We compare experimentally determined transition energies to model calculations based on a wurtzite/cubic/wurtzite GaN quantum well model. Also complete semipolar Ga(In)N based light emitting devices are investigated by spatially correlated cathodoluminescence and electron beam induced current measurements in order to visualize the impact of stacking faults and dislocations on the quality and homogeneity of the quantum wells and on the performance of the pn-junction.

HL 62.9 Wed 17:15 H17

Investigation of confined exciton luminescence of PAMBE-grown AlGaN/GaN nanowires for single photon applications — •Johannes Dühn[1], Pascal Hille[2], Jörg Schörmann[2], Martin Eickhoff[2], Jürgen Gutowski[1], and Kathrin Sebald[1] — [1]Institute of Solid State Physics, University of Bremen, Germany — [2]Institute of Experimental Physics I, Justus-Liebig University, Giessen, Germany

Efficient single photon sources are of pivotal importance for experimental quantum optics and cryptography. Currently available schemes of single photon sources and detectors are subject to low signal to noise ratios, which greatly inhibits their utilisation in quantum optical applications. A promising approach to this problem is the usage of confined excitons in wide band gap materials. Because of their huge oscillator strengths, confined excitons have extraordinarily short lifetimes, thus enabling for emitters with high count rates. Due to confinement, these excitons also possess large binding energies, even exceeding the thermal energy at room temperature, which makes them suitable emitters for high-temperature operation. In this work we investigate the micro-PL properties of individual plasma-assisted (PA)MBE-grown Mg-doped single GaN nanodiscs embedded in AlGaN barriers. We identify emissions centered at 3.55eV from the nanodisc, as well as sharp emission lines at 3.35eV most likely originating from excitons bound to stacking faults in the GaN nanowire base. The emission from single excitons bound to defects are investigated with respect to their single photon emission properties by using an HBT interferometer.

HL 62.10 Wed 17:30 H17

InGaN/GaN nanowire heterostructures for multifunctional optochemical sensor systems — •Sara Lippert[1], Marc Riedel[2], Christian Dern[1], Jens Wallys[1], Ervice Pouokam[3], Pascal Hille[1], Jörg Teubert[1], Fred Lisdat[2], Martin Diener[3], and Martin Eickhoff[1] — [1]I. Physical Institute, Justus-Liebig-University, Gießen, Germany — [2]Biosystems Technology, Institute of Applied Life Sciences, Technical University of Applied Sciences, Wildau, Germany — [3]Institute for Veterinary Physiology and Biochemistry, Justus-Liebig-University, Gießen, Germany

InGaN/GaN nanowire heterostructures as nanophotonic probes are presented for the detection and monitoring of biochemical processes in electrolytes. By incorporation of Indium the excitation wavelength was shifted to the visible part of the spectrum. These structures show a stable photoluminescence at room temperature which is sensitive to variations of the pH value and the applied bias voltage [1]. Biasing allows an adjustment of the working point to maximize the sensitivity. With each nanowire acting as an individual probe, dynamical imaging with biochemical contrast becomes feasible. The photoelectrode characteristics are dominated by radiative and non-radiative recombination of photo-generated electron-hole pairs that in turn are determined by the bias-dependent surface band bending in the nanowire electrodes. The photoelectrochemical properties of the InGaN/GaN nanowire are assessed by pH- and bias-dependent photocurrent and photoluminescence measurements.

[1] Wallys, J. et al., Nano Lett., 12, 6180-6186 (2012)

HL 62.11 Wed 17:45 H17

Analysis of in-situ reflectance measurements during growth of AlInN/GaN Bragg reflectors — •Christoph Berger, Armin Dadgar, Jürgen Bläsing, and André Strittmatter — Otto-von-Guericke-Universität Magdeburg

We present in-situ analysis of lattice-matched AlInN/GaN distributed Bragg reflectors. For a comprehensive analysis of the in-situ reflectance monitored at three different wavelengths (405 nm, 633 nm, 950 nm), we first determined the optical constants of AlInN at high (growth) temperature. Therefore, we have grown single AlInN layers on a thick GaN-on-sapphire buffer structure. Fitting the resulting in-situ transients, allowed us to extract the refractive index and extinction coefficient at growth temperature. In combination with the optical properties of AlInN determined at room temperature, we were able to interpolate a temperature dependent dispersion for lattice-matched AlInN. With these data, the complex reflectance transients were simulated with very good agreement. From these simulations, growth rates and the resulting layer thickness were determined and even small growth rate fluctuations could be detected. In addition, the optical characteristic of the final DBR structure has been predicted already from the in-situ measurement. Simulations from high-resolution X-ray diffraction scans agree very well with the results from in-situ analysis.

HL 62.12 Wed 18:00 H17

Nanoscale (in)homogeneities of a thick $In_{0.2}Ga_{0.8}N$ layer grown on high quality bulk GaN substrate — •Max Trippel[1], Gordon Schmidt[1], Peter Veit[1], Sebastian Metzner[1], Thomas Hempel[1], Silke Petzold[1], Frank Bertram[1], Marlene Glauser[2], Lise Lahourcade[2], Raphaël Butté[2], Jean-François Carlin[2], Nicolas Grandjean[2], and Jürgen Christen[1] — [1]Institute of Experimental Physics, Otto-von-Guericke-University Magdeburg, Germany — [2]Institute of Condensed Matter Physics, École Polytechnique Fédérale de Lausanne, Switzerland

InGaN alloys have received much attention for their successful use as active layers for optoelectronic applications. Despite considerable progress in the understanding of this material system the growth of high quality thick InGaN layers is still a challenge due to relaxation and compositional inhomogeneities.

We report on the inhomogeneities of a thick $In_{0.2}Ga_{0.8}N$ layer on nanometerscale using transmission electron microscopy combined with cathodoluminescence spectroscopy (STEM-CL) at 15 K.

A nominally 100 nm thick InGaN layer on top of a 1 μm GaN buffer was grown by metal-organic chemical vapor phase epitaxy (MOVPE) on a high quality free standing GaN pseudo substrate. (S)TEM images show two different regions on the surface: planar areas as well as regions of three dimensional growth. Highly spatially resolved STEM-CL mappings performed at 15 K reveal dominant luminescence at about 465 nm within planar regions and strong inhomogeneities of the InGaN emission in the regions of three dimensional growth.

HL 62.13 Wed 18:15 H17

AlN growth transition between step flow growth and step bunching — •Konrad Bellmann, Alexander Sabelfeld, Christian Kuhn, Tim Wernicke, and Michael Kneissl — Technische Universität Berlin, Institut für Festkörperphysik, Berlin, Germany

Opto-electronic devices operating in the UV range rely on smooth AlN layers with step flow morphology. This work will present a systematic study by metal organic vapor phase epitaxy of AlN layers grown on sapphire substrates to tailor the surface morphology by changing the V/III ratio and the substrate offcut angle between 0.1° and 0.3°. At a growth temperature of 1200°C the transition between step bunching and step flow growth occurs at a V/III ratio of about 5 to 20. This behavior can be explained by a change of the Ehrlich-Schwöbel(ES) barrier, due to the influence of the V/III ratio on the surface energy. However, the transition additionally depends on the offcut of the sapphire substrates which has no influence on the ES barrier. Therefore, a Monte Carlo simulation is presented which is based on the surface adatom diffusion combined with a variable sticking probability at the edges. The ES barrier is implemented by differentiating between an incorporation probability at the step edge from the top or the bottom terrace.

HL 63: Symposium SYQS: Quantum Signatures in Magnetism (Joint session of HL, MA, O and TT, organized by MA)

Time: Wednesday 15:00–17:45 Location: H1

Invited Talk HL 63.1 Wed 15:00 H1

Magnonic macroscopic quantum states and supercurrents — •Burkard Hillebrands[1], Dmytro A. Bozhko[1,2], and Alexander A. Serga[1] — [1]Fachbereich Physik and Landesforschungszentrum OPTIMAS, TU Kaiserslautern, Germany — [2]Graduate School Materials Science in Mainz, Germany

Magnons, the quanta of spin waves, are bosons and can form a Bose-Einstein condensate (BEC) - a spontaneous coherent ground state - established independently of the magnon excitation mechanism. The magnon BEC has zero group velocity and, thus, cannot be directly used for information transport. However, a collective motion of condensed magnons driven by a phase gradient in the condensate wavefunction - a magnon supercurrent - is a most promising candidate for the utilization of magnon macroscopic quantum phenomena at room temperature for spin information transport and processing. We report experimental evidence for the generation of a magnonic supercurrent obtained using Brillouin light scattering experiments. Here the phase gradient is induced by a thermal gradient. A rate equation model describes the experimental findings very well. Several other means to generate the needed gradient of the phase of the condensate wave function will be discussed. The work is supported by the DFG within the SFB/TR 49.

Invited Talk HL 63.2 Wed 15:30 H1

Elementary excitations of magnetic insulators and its heterostructures with metals — •Gerrit Bauer — Institute for Materials Research, Tohoku University, Sendai, Japan

Magnetic insulators such as yttrium iron garnet (YIG) are prime candidates for the search of quantum signatures in magnetism due to their superiors magnetic quality. Metal contacts to magnetic insulators are a possible route to observe them electrically.

In this talk I will review the knowledge about the elementary excitations of magnetic insulators, i.e., magnons, magnon-polarons and magnon-polaritons, as well as their coupling to metal contacts. While to date most experiments can be explained by semiclassical concepts, these excitations offer a route to observe up to now elusive quantum effects.

Invited Talk HL 63.3 Wed 16:00 H1

Cavity Spintronics — •Can-Ming Hu — Department of Physics and Astronomy, University of Manitoba, Winnipeg, Canada R3T 2N2

Strong coupling between magnons and microwave photons has recently been theoretically proposed [1] and experimentally investigated using both microwave transmission [2-4] and electrical detection methods [5]. These works build the foundation for the emerging field of Cavity Spintronics [6], where the development of spintronics merges with the advancement in cavity quantum electrodynamics and cavity polaritons, thereby creating new theoretical and experimental avenues for studying wave physics, developing quantum technology, and facilitating spintronics applications.

Based on the remarkable achievements of the pioneers of Cavity Spintronics, this talk aims to provide a brief introduction of this exciting new frontier of condensed matter research to colleagues working on magnetism, spintronics, and microwave technologies. Related work recently done by our group at the University of Manitoba will be reported [5-8].

[1] Ö. O. Soykal et al., Phys. Rev. Lett. 104, 077202 (2010). [2] H. Huebl, et al., Phys. Rev. Lett. 111, 127003 (2013). [3] Y. Tabuchi, et al., Phys. Rev. Lett. 113, 083603 (2014). [4] X. Zhang, et al., Phys. Rev. Lett. 113, 156401 (2014). [5] L.H Bai, et al., Phys. Rev. Lett. 114, 227201 (2015). [6] C.-M. Hu, arXiv: 1508.01966. [7] B.M. Yao, et al., Phys. Rev. B, 92, 184407 (2015). [8] For more information, please check: http://www.physics.umanitoba.ca/~hu/

15 min. break

Invited Talk HL 63.4 Wed 16:45 H1

Hybrid Quantum Systems - Coupling Color Centers to Superconducting Cavities — •Johannes Majer — TU Wien / Atominstitut

Hybrid quantum systems based on spin-ensembles coupled to superconducting microwave cavities are promising candidates for robust experiments in cavity quantum electrodynamics (QED) and for future technologies employing quantum mechanical effects. The main source of decoherence in this systems is inhomogeneous dipolar spin broadening and a full understanding of the complex dynamics is essential and has not been addressed in recent studies yet. We investigate the influence of a non-Lorentzian spectral spin distribution in the strong coupling regime of cavity QED. We show for the first time experimentally how the so-called cavity protection effect influences the decay rate of coherent Rabi oscillation by varying the coupling strength in our experiment. We then demonstrate how the Rabi oscillation amplitude can be enhanced by two orders of magnitude by pulsing the strongly coupled system matching a special resonance condition. Giving a way improving the coherent manipulation of the spin polarization helping to improve fidelity and performance in hybrid quantum systems.

Invited Talk HL 63.5 Wed 17:15 H1

Quantum enhanced sensing with single spins in diamond — •Fedor Jelezko — Institute of Quantum Optics, Ulm University

I will discuss recent developments transforming quantum control tools into quantum technologies based on single nitrogen-vacancy (NV) centers in diamond. I will present ultrasensitive MRI at nanoscale and recently developed magnetometry protocols that use quantum error correction as a resource. Experiments with novel colour centers including silicon-vacancy (SiV) will also be presented.

HL 64: Focus Session: Semiconductor Heteroepitaxy on Nanopatterned Substrates

State-of-the-art electronic and optoelectronic devices are widely based on layered heteroepitaxial semiconductor systems. As the crystal quality of planar heteroepitaxial layers is often limited by lattice misfit relieving defects, the selective growth on small areas as well as on non-planar, nanopatterned substrates has attracted increasing interest. In these cases the three-dimensional elastic lattice relaxation largely extends the range of material combinations, for which defect-free heteroepitaxial growth is possible. In tandem with the nanopattern-induced modifications of the surface potential and growth characteristics this sets the fundament for the realization of unique architectures and new classes of self-assembled and site-controlled nanostructures, which are required for high-performance devices. Selective-area grown nanowires for example have been demonstrated to exhibit outstanding luminescence properties, and complex hierarchical heterostructures grown on nanowire templates have paved the way for new types of quantum structures and innovative device architectures. Worldwide, numerous research groups and institutes are involved in exploring the fabrication and properties of such nano-heteroepitaxial systems. Therefore, the proposed symposium focusses on experiments and simulations of the heteroepitaxial growth on nanopatterned substrates, structural and nanomorphological aspects as well as control of optical, electronic and transport properties, and device applications. The symposium aims at bundling

the extensive research activitities in this area and at offering a forum for scientists from fields of epitaxial growth, nanopatterning, theory, surface science, characterization, and device fabrication.

Organizers: Thomas Riedl (U Paderborn), Gregor Koblmüller (WSI München), Martin Eickhoff (JLU Gießen)

Time: Wednesday 15:00–18:30 Location: H11

Topical Talk HL 64.1 Wed 15:00 H11

Single site-controlled InGaAs quantum dots grown on patterned GaAs nanoholes — •S. Höfling, S. Maier, S. Unsleber, M. Kamp, and C. Schneider — Technische Physik, Würzburg University

Single semiconductor quantum dots (QDs) are very attractive candidates to control charge and spin carries at the quantum level. They are therefore very promising for applications in fields ranging from nanoelectronics over nanophotonics to spintronics. One of the major challenges regarding the scalable fabrication of single QD based devices is however the precise control of the QD position within device structures. In this presentation, we summarize our results obtained on the site-controlled growth using pre-patterned nanohole templates for the controlled integration of site-controlled QDs into nanoscale devices. By combining this growth technique with a process capable of accurately aligning QDs relatively to subsequently fabricated quantum device structures, several interesting devices like single photon sources and quantum dot memories have been realized.

Topical Talk HL 64.2 Wed 15:30 H11

Nanometer scale correlation of structural and optical properties of individual GaAs/AlGaAs nanorodsby Scanning Transmission Electron Microscope Cathodoluminescence — •Frank Bertram, Marcus Müller, Peter Veit, and Jürgen Christen — Institut für Experimentelle Physik, Otto-von-Guericke-Universität Magdeburg

We will present a direct correlation of the luminescence with crystallographic realstructure of novel GaAs/AlGaAs coreshell nanowires using cathodoluminescence directly performed in transmission electron microscope at liquid helium temperature. The GaAs/AlGaAs coreshell NWs were produced by a unique twostep process enabling the growth of ultrathin GaAs cores. First, GaAs NWs were obtained by molecular beam epitaxy on a [111]-oriented Si. In a second step the GaAs core diameter was reduced by a reverse-reaction using in-situ thermal decomposition of the {110} side wall surfaces leading typically to a diameter down to 7 nm. Subsequently, the cores were overgrown by an AlGaAs passivation shell and a GaAs cap. TEM investigations reveal wurzite structure in the bottom part of the NW with a high density of extended defects whereas the upper part is dominated by the zincblende phase containing few twindefects. Highly spatially resolved CL measurements exhibit a blue shifted emission up to 1.66 eV as compared to bulk GaAs. In particular, we will present a detailed analysis of the impact of structural properties on the luminescence along the wire. Locally sharp emission lines originating from vicinity of twindefects within the ZB-structure indicate effective localization.

Topical Talk HL 64.3 Wed 16:00 H11

Local Heteroepitaxy for Large-Scale Integration — •Heinz Schmid, Mattias Borg, Davide Cutaia, Kirsten Moselund, Moritz Knoedler, Nicolas Bologna, and Heike Riel — IBM Research - Zurich , 8803 Rueschlikon, Switzerland

The cooperative use of unequal materials like silicon and III-Vs can lead to performance benefits and even enable novel devices and applications. Traditionally this has been achieved by clever joining of the individual Si and III-V components in a common package. Alternatively this could be achieved by building the devices directly from Si wafers with embedded III-V layers. However, such wafers are not readily available yet. Here we review our effort on local epitaxy of III-Vs on Si and introduce the concept of template-assisted selective epitaxy (TASE). Various III-V materials with nanowire or thin-film geometries were successfully grown with high yield on Si using TASE and further processed into field effect transistors (FETs) and tunnel-FETs that exhibited excellent performance.

15 min. break.

Topical Talk HL 64.4 Wed 16:45 H11

Fabrication and study of metal contacts on germanium nanowires using electrical biasing in a transmission electron microscope — •Martien den-Hertog[1], Khalil El-Hajroui[1], Clemens Zeiner[3], Alois Lugstein[3], Eric Robin[2], Miguel Lopez-Haro[2], and Jean-Luc Rouviere[2] — [1]Institut Neel, CNRS/UJF/UGA, Grenoble, France — [2]INAC, CEA-Grenoble/UGA, Grenoble, France — [3]Institute for solid state electronics, Vienna, Autriche

Semiconductor nanowires (NWs) are promising candidates for many device applications ranging from electronics and optoelectronics to energy conversion and spintronics. To allow successful device integration the contact quality between for example a NW and metal is of paramount importance. An interesting approach to create an atomically abrupt contact with low electrical resistance on NWs of group IV (silicon and germanium) is to create a metal-semiconductor phase in the extremities of the NW. To understand and control the metal diffusion into the NW that creates a metallic phase, detailed characterization at atomic length scales is necessary to understand how the metal atoms diffuse and incorporate into the formed phase at the reaction front and how these parameters relate to the electrical properties of the same interface. In this work we study two different kind of semiconducting NW devices fabricated on electron transparent Si3N4 membranes. We show in-situ phase propagation of a metal-semiconductor phase of Cu and Al in Ge NWs in the TEM while measuring the current through the device, and analyze the metal diffusion process.

Topical Talk HL 64.5 Wed 17:15 H11

Cubic GaN on pre-patterned 3C-SiC/Si (001) substrates — •Donat Josef As, Ricarda Maria Kemper, Thomas Riedl, and Jörg K.N. Lindner — Department Physik, Universität Paderborn, Warburgerstrasse 100, 33098 Paderborn, Germany

The influence of growth area reduction towards length scales predicted to be effective for defect reduction by the theory of nano-hetero-epitaxy (NHE) is analyzed. This is studied in detail for the first time in the system of meta-stable cubic GaN (c-GaN) grown by plasma-assisted molecular beam epitaxy on pre-patterned 3C-SiC/Si (001) substrates. It is demonstrated that regardless of the pattern symmetry or size, the cubic phase of GaN nucleates on top of all investigated mesa structures. Electron beam lithography followed by a lift-off and a reactive ion etching process is used for tailoring post-shaped SiC structures. A successful reduction of the {111} stacking fault (SF) density is achieved by reducing the (001) top edge length of the posts from ~500 nm down to ~20 nm. Transmission electron microscopy reveals a nucleation of phase-pure and almost defect free c-GaN on top of the smallest SiC nanostructures as predicted by theoretical calculations.

HL 64.6 Wed 17:45 H11

GaAs-based nanowire integration on silicon via template-assisted selective epitaxy — •Moritz Knoedler, Nicolas Bologna, Mattias Borg, Heinz Schmid, Giorgio Signorello, Davide Cutaia, Kirsten Moselund, Marta Rossell, and Heike Riel — IBM Research Zurich, Säumerstrasse 4, 8803 Rüschlikon, Switzerland

As the scaling-down of conventional Si microelectronics is approaching fundamental physical limits, novel materials are heavily being investigated as alternative channel materials, with III-V semiconductor compounds being particularly promising candidates. Thus far, III-V integration into Si technologies has been limited due to poor epitaxial material quality. Our group has recently demonstrated a novel method to directly integrate III-V nanostructures on silicon called template-assisted selective epitaxy (TASE). Nanowires are grown inside lithographically pre-defined oxide templates, allowing for precise tuning of composition and crystal quality, independent from their shape and substrate orientation.

Here we present a comprehensive investigation of GaAs-based epitaxy directly on Si wafers via TASE, by correlating growth parameters with crystal morphology. To this end, nanowires were grown with metal-organic chemical vapour deposition (MOCVD) under different conditions by varying template width, growth duration, tem-

perature, group III molar flows and V/III precursor ratio. Crystal quality was then analyzed at atomic resolution by state-of-the-art double-aberration-corrected (scanning) transmission electron microscopy (STEM/TEM). Zinc blende/wurtzite polytypism and twin defect formation were investigated in detail.

Low-temperature and temperature-dependent micro photoluminescence (PL) spectroscopy was used to further characterize their optical properties. Significant photoemission of the nanostructures even at room temperature was observed. When the GaAs is surrounded by the oxide template or an AlGaAs shell luminescence is much enhanced, indicating reduced surface recombination velocity.

HL 64.7 Wed 18:00 H11

Theoretical analysis of strain and misfit dislocation stability in axial-heteroepitaxial GaAs/InAs nanopillars — •Thomas Riedl[1,2] and Jörg Lindner[1,2] — [1]University of Paderborn, Department of Physics, Warburger Straße 100, 33098 Paderborn, Germany — [2]Center for Optoelectronics and Photonics Paderborn (CeOPP), Warburger Straße 100, 33098 Paderborn, Germany

Heteroepitaxial nanopillars and -wires represent a promising building block for advanced optoeletronic devices like dot-in-wire LEDs or lasers. Such structures offer a large surface-to-volume ratio and the possibility to accommodate considerable lattice mismatch in a pure elastic manner without formation of misfit relieving defects. As misfit dislocations are reported to occur in heterostructure nanowires in case of larger misfit and diameter, it is important to determine the critical wire dimensions for dislocation stability. In the present contribution we analyze this for the case of [111] orientied axial-heteroepitaxial GaAs/InAs nanopillars with zinc blende structure. Because of its applicability to various dislocation configurations and the availability of suitable parametrizations we use atomistic molecular statics simulation based on the Tersoff potential. We find that the defect-free elastically strained state is stable for small wire diameters (< 10 nm for a single 60° dislocation), whereas the dislocated state becomes favorable for larger diameters. In this presentation the influence of dislocation type, wire morphology and chemical width of the heterointerface on the coherent-semicoherent transition is analyzed and discussed. The results are compared with the literature.

HL 64.8 Wed 18:15 H11

Selective nano-heteroepitaxial growth of GeSn islands on nano-patterned Si(001) — Viktoria Schlykow[1], Noriyuki Taoka[1], Marvin Zöllner[1], Oliver Skibitzki[1], Peter Zaumseil[1], •Giovanni Capellini[1,2], Yuji Yamamoto[1], Thomas Schröder[1,3], and Gang Niu[1] — [1]IHP, Frankfurt (Oder) — [2]Dipartimento di Scienze, Italy — [3]BTU Cottbus-Senftenberg

Ge is a promising candidate for optical devices due to its band gap, resulting in high absorption at the telecommunication wavelength. The introduction of Sn into Ge forming GeSn alloys enables further flexibility to engineer the optical properties like the semiconductor band gap. However, crystalline defects induced by lattice mismatch between GeSn and Si are a crucial challenge to realize high performance optical devices. Recently, we demonstrated fully coherent, dislocation free Ge islands on nano-pillar patterned Si (NPP-Si) substrates using nano heteroepitaxy approach. In this study, we demonstrate the selective MBE growth of GeSn islands on NPP-Si at high temperatures. In order to establish selective MBE growth of GeSn on NPP-Si surrounded by SiO2, the impact of growth temperature (500-750 °C) on the selectivity and the Sn incorporation was investigated. XRD, TEM and micro-PL studies confirmed that the growth at 600 °C results in good selectivity and homogeneous distribution of Sn in Ge nano-islands and good optical properties. Growth below 600 °C results in non-selectivity whereas growth above 600 °C leads to better selectivity but an enhanced Sn migration to {111} facets thus reduced Sn incorporation.

HL 65: Frontiers of Electronic Structure Theory: Focus on Topology and Transport III

Time: Wednesday 15:00–18:30 Location: H24

Topical Talk HL 65.1 Wed 15:00 H24

Topological semimetal phases in strained HgTe-based alloys — Tomáš Rauch[1], Steven Achilles[1], •Jürgen Henk[1], and Ingrid Mertig[1,2] — [1]Martin Luther University Halle-Wittenberg, Halle, Germany — [2]Max Planck Institute of Microstructure Physics, Halle, Germany

Topological insulators (TIs) have matured to a class of materials that is studied worldwide with great effort. Prominent examples are HgTe, the Bi chalcogenides, and SnTe. Recently, the set of "original" TIs has been extended by topological semimetals: the topological Dirac and the Weyl semimetals, both of them showing point-like Fermi surfaces in the bulk. Weyl points appear always in pairs with opposite topological charges of ±1; their projections onto the surface Brillouin zone are connected by a Fermi arc, i. e. a sizably spin-polarized topological surface state with an open Fermi contour.

In this presentation I report on theoretical investigations of strained $HgTe_{1-x}S_x$ alloys [1], with surprising results. (*i*) In the strong TI phase, the spin chirality of the topological nontrivial surface state can be reversed by moderate strain and changing the alloy concentration x. (*ii*) On top of this, we observe a Dirac and a Weyl semimetal phase. These findings call for experimental verification and extend significantly the "topological playground" for spin-dependent transport.

[1] T. Rauch, S. Achilles, JH, I. Mertig, Phys. Rev. Letters **114** (2015) 236805.

Topical Talk HL 65.2 Wed 15:30 H24

Topological surface Fermi arcs and the chiral anomaly in Weyl semimetal materials — •Binghai Yan — Max Planck Institute for Chemical Physics of Solids, Dresden

Topological Weyl semimetals represent a novel state of topological quantum matter, which not only possesses Weyl fermions (massless chiral particles that can be viewed as magnetic monopoles in momentum space) in the bulk and unique Fermi arcs generated by topological surface states, but also exhibits appealing physical properties such as extremely large magnetoresistance and ultra-high carrier mobility. In this talk, I will first present our recent theoretical [1] and ARPES [2,3] study on the topological surface states of transition-metal monopnictides, NbP, NbAs, TaP and TaAs. By visualizing the surface Fermi arcs, we discovered their Fermiology evolution with spin*orbit coupling strength. Further, we found a way to manipulate the Fermi arcs by the Lifshitz transition. I will also introduce our recent progress on the magneto-transport in the search for the chiral anomaly effect[4,5]. References: [1] Y. Sun, S. C. Wu, and B. Yan, Phys. Rev. B 92, 115428 (2015). [2] L. X. Yang, et al. Nature Physics 11, 728 (2015). [3] Z. K. Liu, et al. Nature Materials DOI: 10.1038/NMAT4457 (2015). [4] C. Shekhar, et al. Nature Physics 11, 645 (2015). [5] C. Shekhar, et al. arXiv:1506.06577 (2015).

HL 65.3 Wed 16:00 H24

Type-II Dirac cones as unified topological origin of the exotic electronic properties of WTe_2 — •Lukas Muechler[1], Aris Alexandradinata[2], Titus Neupert[3], and Roberto Car[1] — [1]Dept. of Chemistry, Princeton University — [2]Dept. of Physics, Yale University — [3]Princeton Center for Theoretical Science, Princeton University

WTe_2 is a recently discovered layered material with remarkable electronic properties. Transport measurements show an extremely large non-saturating magnetoresistance (MR) with mobilities as high as 167 000 cm^2/Vs at 2 K. Furthermore, recent photoemission experiments discovered circular dichroism in the bulk band structure. We propose a unified explanation for these exotic observations by relating key properties of the bulk electronic structure to that of to that of the mono- and bi-layer material. In particular, we demonstrate that the monolayer is a novel type-II Dirac semimetal in absence of spin-orbit coupling, with Dirac cones that are sufficiently anisotropic to simultaneously harbor electron and hole pockets. The band structure can be characterized by a new $\mathbb{Z}_2 \times \mathbb{Z}_2$ topological invariant defined through non-Abelian Wilson loops. We develop a tight-binding model for the mono- and bilayer of WTe_2 based on Wannier functions from *ab-inito* calculations and extend our findings to the iso-structural compounds $MoTe_2$ and ZrI_2.

HL 65.4 Wed 16:15 H24

Topological surface Fermi arcs and spin-textures of the Weyl semimetals TaAs, TaP, NbAs, and NbP — •Yan Sun[1], Shu-

Chun Wu[1], Claudia Felser[1], and Binghai Yan[1,2] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany. — [2]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany

Very recently the topological Weyl semimetal (WSM) was predicted in the noncentrosymmetric compounds NbP, NbAs, TaP, and TaAs and soon led to photoemission experiments to verify the presumed topological Fermi arcs (FAs)[1,2]. In this work we have performed fully ab initio calculations of these four WSMs and revealed the FAs with spin-momentum-locked spin texture[3]. On the (001) surface, the anion (P or As) terminated surfaces are found to fit photoemission measurements well. By tracing the spin polarization of the Fermi surface, one can distinguish FAs from trivial Fermi circles. By comparing their surface states, we reveal the evolution of topological Fermi arcs from the spin-degenerate Fermi circle to spin-split arcs when the SOC increases from zero to a finite value. Our work presents a comprehensive understanding of the topological surface states of WSMs, which will be helpful for spin-revolved photoemission and transport experiments.

References

[1] L. X. Yang, Z. K. Liu, Y. Sun, et. al. Nat.Phys.11,728, (2015).

[2] Z. K. Liu, L. X. Yang, Y. Sun, et.al Nat. Mater., doi:10.1038/nmat4457,(2015).

[3] Y. Sun, S. Wu, and B. Yan, Phy. Rev. B, 92, 115428, (2015).

HL 65.5 Wed 16:30 H24

New electron states at the Bi/InAs(111) interface — •L Nicolaï[1,2,3], K Hricovini[2,3], J-M Mariot[4], M C Richter[2,3], O Heckmann[2,3], U Djukic[2], T Balasubramanian[5], M Leandersson[5], J Sadowski[5], J Denlinger[6], I Vobornik[7], J Braun[7], H Ebert[7], and J Minár[7,8] — [1]LMU, Munich — [2]LPMS, UCP, Cergy, France — [3]DSM-IRAMIS, Spec, Cea-Saclay, France — [4]LCP-MR, UPMC Univ. Paris 06/CNRS, France — [5]MAX-lab, Lund Univ., Sweden — [6]ALS, Berkeley, USA — [7]EST, Trieste, Italy — [8]Univ. of West Bohemia, Plzeň, Czech Republic

The Bi(111) surface is a prototype system that shows Rashba-split surface states. Theoretical studies [1] predicted non-trivial topological surface states appearing on a single bi-layer of Bi(111) and a more complex behavior was suggested for a variable film thickness as a function of the layer thickness [2]. This clearly indicates that the electronic properties of thin films of this material are quite complex and far from being fully understood. Here we present combined theoretical and ARPES studies on the electronic structure of Bi(111) films grown on InAs(111). Bi grows epitaxially on this substrate and a monocrystal of very high quality is obtained after depositing several monolayers. ARPES experiments on the samples prepared show several new electronic states not reported before. The one-step model of photoemission as implemented in the SPR-KKR package [3] allows us to identify pristine Bi bulk states coexisting with InBi surface states.[1] M. Wada et al., Phys. Rev. B 83, 121310 (2011). [2] Z. Liu et al., Phys. Rev. Lett. 107, 136805 (2011). [3] J. Braun, Rep. Prog. Phys. 59, 1267-1338 (1996).

HL 65.6 Wed 16:45 H24

Two-dimensional topological phases and electronic spectra of topological insulator thin films from *GW* calculations — •Tobias Förster, Peter Krüger, and Michael Rohlfing — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität, 48149 Münster, Germany

We have investigated topological and electronic properties of thin films of the topological insulators Bi_2Se_3, Bi_2Te_3, and Sb_2Te_3 with thicknesses from one to six quintuple layers employing the *GW* method. The quasiparticle band structures show highly improved agreement with experiments compared to DFT. In addition to a correction of the band gaps, the energetic positions and dispersions of the surface states change significantly around $\bar{\Gamma}$ [1]. The common approach of taking the diagonal elements of the self-energy Σ as quasiparticle energies and leaving the wave functions unchanged yields unphysical results which can be overcome by diagonalizing $\mathcal{H}^{\mathrm{QP}}$. The origin of the respective off-diagonal elements in $(\Sigma - V_{xc})$ will be discussed. As the wave functions are updated, the two-dimensional topological phases (quantum spin Hall or trivial) in *GW* differ from DFT for many systems. On the basis of our results, we further argue that one cannot unambiguously conclude the topological phase from fits to ARPES band structures as performed in recent experimental studies.

[1] T. Förster, P. Krüger, and M. Rohlfing, Phys. Rev. B **92**, 201404(R) (2015)

HL 65.7 Wed 17:00 H24

Steady-State Density Functional Theory for Finite Bias Conductances — •Stefan Kurth[1,2] and Gianluca Stefanucci[3,4] — [1]Dept. of Materials Physics, Univ. of the Basque Country UPV/EHU, San Sebastian, Spain — [2]IKERBASQUE, Basque Foundation for Science, Bilbao, Spain — [3]Dept. of Physics, Univ. of Rome "Tor Vergata", Rome, Italy — [4]INFN, Frascati, Italy

In the framework of density functional theory a formalism to describe electronic transport in the steady state is proposed which uses the density on the junction and the steady current as basic variables. In a finite window around zero bias, a one-to-one map is established between the basic variables and both local potential on as well as bias across the junction. The resulting Kohn-Sham system features two exchange-correlation (xc) potentials, a local xc potential and an xc contribution to the bias. For weakly coupled junctions the xc potentials exhibit steps in the density-current plane which are shown to be crucial to describe the Coulomb blockade diamonds. At small currents these steps emerge as the equilibrium xc discontinuity bifurcates. The formalism is applied to a model benzene junction, finding perfect agreement with the orthodox theory of Coulomb blockade.

HL 65.8 Wed 17:15 H24

Revealing the intra-molecular origin of inelastic electron tunneling signal by means of first-principles calculations — •Giuseppe Foti and Hector Vazquez — Institute of Physics, Academy of Sciences of the Czech Republic, Cukrovarnicka 10, Prague, Czech Republic

We explore the intra-molecular contributions to the peaks in the Inelastic Electron Tunneling Spectrum (IETS) of a benzene-based molecular junction by means of DFT-NEGF simulations [1,2]. These contributions are calculated from the bracket of the left- and right- transmission channels with the e-ph coupling matrix by grouping the products into one- and two-atom terms. This combines the geometrical information of the vibrational modes with the electronic properties of the scattering states. Our calculations show how the partial contributions of each atom and bond in the molecule combine to give the total inelastic signal. We find that, for most of the high intensity peaks, these terms sum up constructively while dark modes result from cancellations. We also investigate the relation between the symmetry of the vibrational modes and the cancellation pattern of the different contributions. This analysis enables a real space representation of the intra-molecular contributions associated to each vibrational mode and allows a complete mapping and characterization of the origin of the IETS peaks.

[1] J. M. Soler et al. J. Phys.: Condens. Matter 14, 2745 (2002)

[2] T. Frederiksen et al. Phys. Rev. B 75, 205413 (2007)

HL 65.9 Wed 17:30 H24

An efficient real-time time-dependent density functional theory method and its applications — •Zhi Wang[1], Shu-Shen Li[2], and Lin-Wang Wang[3] — [1]Institut für Physikalische Chemie, Uni-Hamburg, Hamburg, Germany — [2]Institute of Semiconductors, Chinese Academy of Sciences, Beijing, China — [3]Lawrence Berkeley National Laboratory, Berkeley, United States

We have developed an efficient real-time time-dependent density functional theory (TDDFT) method that can increase the effective time step from <1 as in traditional methods to ~0.1 fs. With this algorithm, the TDDFT simulation can have comparable speed to the Born-Oppenheimer (BO) ab initio molecular dynamics (MD). The application of the method will be illustrated for several non-equilibrium systems, e.g., energetic particle colliding onto a TMDC monolayer, and ultrafast charge seperations in photovoltaic systems.

HL 65.10 Wed 17:45 H24

Nonadiabatic geometric phase of a pseudorotating triatomic molecule — •Ryan Requist and Eberhard K. U. Gross — Max Planck Institute of Microstructure Physics, Halle (Saale), Germany

The geometric phase of a real-valued Born-Oppenheimer electronic wavefunction is a topological quantity depending on the winding number of the path around a conical intersection of the adiabatic potential energy surfaces in nuclear coordinate space. We report the calculation of a nonadiabatic molecular geometric phase that takes the full quantum mechanical motion of the nuclei into account through the exact factorization scheme [1]. Nonadiabatic contributions "smear out" the point-like adiabatic Berry curvature, changing the topological invariant into a genuine path-dependent geometric phase [2].

[1] S. K. Min, A. Abedi, K. S. Kim and E. K. U. Gross, Phys.

Rev. Lett. 113, 263004 (2014). [2] R. Requist and E. K. U. Gross, arxiv:1506.09193.

HL 65.11 Wed 18:00 H24

Theoretical investigations of magnetically doped topological insulators — •Jan Minar[1,2], Jurgen Braun[1], and Hubert Ebert[1] — [1]LMU München, Germany — [2]University of West Bohemia, Plzen, Czech Rep.

Band gap opening of topological surface states due to magnetic doping are the subject of a long standing discussion. However, in spite of the progress made during the last years in this field there are still phenomena that are poorly understood and many open issues to be addressed. In several cases, like for example Mn doped Bi_2Se_3 band gap opening does not seem to be of magnetic origin. Here we will present several examples detailed theoretical studies on various bulk as well as surface doped topological insulators by means of the SPR-KKR band structure method. Our results will be discussed in a direct comparison with the corresponding ARPES [1] as well as XAS and XMCD [2,3] experimental data.

[1] J. Sanchez-Barriga et al., Nat. Communications, submitted (2015) [2] A. Ney et al., in preparation [3] J. Honolka et al., in preparation

HL 65.12 Wed 18:15 H24

Trions in a carbon nanotube from ab-initio many-body perturbation theory — •Thorsten Deilmann, Matthias Drüppel, and Michael Rohlfing — Institut für Festkörpertheorie, Universität Münster, Germany

Trion states of three correlated particles (e.g. two electrons and one hole) show up in the optical spectra of doped or gated nanostructures, like carbon nanotubes or transition-metal dichalcogenides.
We demonstrate that trions can be described within ab-initio many-body perturbation theory, as a natural extension of the widely used *GW* method and Bethe-Salpeter equation. This allows for a direct comparison with excitons on equal footing.
We investigate trion states in a semiconducting $(8, 0)$ carbon nanotube, and discuss their spectra, composition, and wave functions. Luminescence from the trions is red-shifted by $\sim 135\,\mathrm{meV}$ compared to the excitons.

HL 66: Topological Insulators (Joint session of DS, HL, O, and TT, organized by MA)

Time: Wednesday 15:00–17:45 Location: H32

HL 66.1 Wed 15:00 H32

Bulk and surface properties of topological insulators from *GW* calculations. — •Irene Aguilera, Christoph Friedrich, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany.

Many-body calculations within the *GW* approximation are attracting much attention in the study of topological insulators (TIs). They have shown to be critical both in the one-shot approach [1] (e.g. for the Bi_2Se_3 family) and in a quasiparticle self-consistent (QS) *GW* method [2] (e.g. for Bi). In both cases, the spin-orbit coupling has to be incorporated directly into the *GW* self-energy [3]. Within the all-electron FLAPW formalism, we have performed DFT, one-shot *GW*, and QS*GW* calculations for well-known TIs. These calculations are very demanding for low-dimensional systems. Therefore, we construct a tight-binding Hamiltonian for the description of topological surface states in a slab geometry. The corresponding parameters are deduced from *GW* calculations of the bulk. With this approach, we discuss the effects of quasiparticle corrections on the surface states of TIs and on the interaction between bulk and surface states. We show that the *GW* bulk and surface band structure agrees better to results from photoemission experiments than the DFT one. [1] Phys. Rev. B 87, 121111(R) (2013). [2] *Ibid* 91, 125129 (2015). [3] *Ibid* 88, 165136 (2013).

We acknowledge the Virtual Institute for Topological Insulators of the Helmholtz Association.

HL 66.2 Wed 15:15 H32

Magnetic Properties of Mn-doped Bi_2Se_3 and Bi_2Te_3: Ab Initio and Atomistic Simulations — •Pavel Baláž[1], Karel Carva[1], Róbert Tarasenko[1], Vladimír Tkáč[1], Jan Honolka[2], and Josef Kudrnovský[2] — [1]DCMP, Charles University, Ke Karlovu 5, CZ-12116 Prague 2, Czech Republic — [2]Institute of Physics, ASCR, Na Slovance 2, CZ-18221 Prague 8, Czech Republic

Ferromagnetic Curie temperature and other magnetic magnetic properties of bulk Mn-doped Bi_2Se_3 and Bi_2Te_3 3D topological insulators are systematically studied by means of atomistic Monte Carlo simulations. Exchange interactions between the Mn magnetic moments have been calculated using ab initio methods. Tight-binding linear muffin-tin orbital method has been employed, together with the coherent potential approximation to describe the high degree of disorder in the system. Spin-orbit interaction is included in the ground state calculation. In the studied materials Mn atoms might either replace a Bi atom (substitutional position) or fill an empty position in van Der Waals gap between the atomic layers (substitutional position). It has been shown that exchange interaction between Mn magnetic moments might lead to a ferromagnetic phase transition. The Curie temperature is shown to be significantly dependent on the concentration of Mn atoms in substitutional and interstitial positions. Theoretical results were compared to recent experimental studies [1].

[1] R. Tarasenko et al., to be published in Physica B: Phys. Cond. Mat., DOI: 10.1016/j.physb.2015.11.022

HL 66.3 Wed 15:30 H32

Transport measurements on ferromagnet / Half Heusler TI bilayer structures — •Benedikt Ernst[1], Robin Klett[2], Jan Haskenhoff[2], James Taylor[3], Yong Pu[3], Günter Reiss[2], Stuard S. P. Parkin[3], and Claudia Felser[1] — [1]Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden — [2]Fakultät für Physik, Universität Bielefeld, 33615 Bielefeld — [3]Max-Planck-Institut für Mikrostrukturphysik, 06120 Halle

Heusler compounds exhibit a manifold of physical properties and attracted in the recent past a lot of interest in the field of spintronic applications due to their half-metallic properties.

In the present work bilayer systems of ferromagnetic materials and half Heusler topological insulators (TI) are studied. The systems were deposited using DC- and RF magnetron co-sputtering. The samples were characterized by X-ray diffraction and electron microscopy techniques. On fabricated devices, the transport properties and spin properties were studied by different measurement techniques including ST-FMR and spin injection experiments.

Additional measurements of the unidirectional spin Hall magnetoresistance were realized. In this effect, we measure a change in the magnetoresistance depending on the direction of the magnetization, which is proportional to the spin Hall angle. We varied the combination of different ferromagnetic materials with different Tis of the YPtBi, YPdBi, LaPtBi and LaPdBi system, and the thicknesses of the layers, to investigate the effects on the transport properties.

HL 66.4 Wed 15:45 H32

Surface preparation and momentum microscopy of the „topological Kondo insulator“ SmB_6 — •Christian Tusche[1,2], Martin Ellguth[1], Fumitoshi Iga[3], and Shigemasa Suga[2,4] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany — [2]Peter Grünberg Institut PGI-6, Forschungszentrum Jülich, 52425 Jülich, Germany — [3]College of Science, Ibaraki University, Japan — [4]Institute of Scientific and Industrial Research, Osaka University, Osaka, Japan

The strongly correlated rare-earth compound SmB_6 is believed to be a topological Kondo insulator, where a topologically non-trivial surface state lives in the hybridization gap at low temperatures. While most experimental studies rely on cleaved surfaces, high resolution- and spin resolved photoemission experiments [1] usually suffer from the short live time of the reactive surface at low temperatures.

Here we present the reproducible surface preparation of large high quality SmB_6 single crystals by in-situ Ar-ion sputtering and controlled annealing. In particular, Sm-rich or B-rich surface terminations are obtained by low ($\approx$1080°C) or high (>1200°C) temperature annealing. Using a momentum microscope [2], wide wave vector regions are stud-

ied by photoemission with He-I ($h\nu$=21.2 eV) and laser ($h\nu$=6.0 eV) excitations, on the Sm-terminated surface. The results reveal localized f-electron resonances at E_F and strong hybridization, paving the way to measure detailed Fermi surface and valence band spin textures.

[1] Suga et al., J., Phys. Soc. Japan 83, 014705 (2014)
[2] C. Tusche, A. Krasyuk, J. Kirschner, Ultramicroscopy (2015)

HL 66.5 Wed 16:00 H32

Spin control in the topological surface state of SnTe — •Nicolas Klier[1], Sam Shallcross[1], Sangeeta Sharma[2], and Oleg Pankratov[1] — [1]Theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7-B2, 91058 Erlangen — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle

The interface of SnTe with a vacuum results in a topological Dirac surface state [1,2]. Based on an effective Hamiltonian derived from tight-binding we investigate the properties of this surface state both with and without an in-plane electric current. The RKKY interaction is found to be strongly non-collinear due to the spin texture of the Dirac state. In the presence of an in-plane current we find (i) a polarization of the surface state and (ii) that the RKKY interaction is strongly modified by the presence of a current leading to a possible "topological spin torque effect".

[1] B.A. Volkov, and O.A. Pankratov, Zh.Eksp. Theor. Fiz. 75, 1362, 1978.
[2] B.A. Volkov, and O.A. Pankratov, JETP Lett.42, 178, 1985.

15 min. break

HL 66.6 Wed 16:30 H32

Adiabatic Pumping of Chern-Simons Axion Coupling — •Maryam Taherinejad[1] and David Vanderbilt[2] — [1]Materials Theory, ETH Zurich, Wolfgang-Pauli-Strasse 27, 8093 Zurich, Switzerland — [2]Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854-0849, USA

The Chern-Simons axion (CSA) coupling θ makes a contribution of topological origin to the magnetoelectric response of insulating materials. Here we study the adiabatic pumping of the CSA coupling along a parametric loop characterized by a non-zero second Chern number $C^{(2)}$ from the viewpoint of the hybrid Wannier representation. The hybrid Wannier charge centers (WCCs), when plotted over the 2D projected Brillouin zone, were previously shown to give an insightful visualization of the topological character of a 3D insulator. By defining Berry connections and curvatures on these WCC sheets, we derive a new formula for θ, emphasizing that it is naturally decomposed into a topological Berry-curvature dipole term and a nontopological correction term. By explicit calculations on a model tight-binding Hamiltonian, we show how the Berry curvature on the WCC sheets is transported by a lattice vector via a series of Dirac sheet-touching events, resulting in the pumping of e^2/h units of CSA coupling during one closed cycle. The new formulation may provide a particularly efficient means of computing the CSA coupling θ in practice, since there is no need to establish a smooth gauge in the 3D Brillouin zone.

HL 66.7 Wed 16:45 H32

Accessing the transport limits of topological states — •Thomas Bathon[1], Paolo Sessi[1], Konstantin Kokh[2], Oleg Tereshchenko[2], and Matthias Bode[1] — [1]Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Novosibirsk State University, 630090 Novosibirsk, Russia

Topological insulators host on their surface spin-momentum locked Dirac states. Beyond their fundamental interest, these materials raised great expectations to create new functionalities in spintronics and magneto-electrics. Their success depends on our understanding of their response to Coulomb perturbations such as electric fields, which can be effectively used to gate their surface. These phenomena have so far been primarily explored by spatially averaging techniques.

Here, by using scanning tunneling microscopy and spectroscopy, we visualize the response of topological states to local charges and electric fields at the nanoscale. We demonstrate that, contrary to the general believe, local electric fields can not be effectively screened by topological states, but penetrate into the bulk indicating a behavior which is far from being metallic. The analysis of our data allows to detect the existence of a finite conductivity which, because of the local character of our measurements, can be safely quantified without being affected by sample inhomogeinities. Finally, we will show how, by taking advantage of this intrinsic limitation, a new approach to tune both charge and spin transport in this fascinating class of materials can be explored.

HL 66.8 Wed 17:00 H32

Interplay between warping and magnetic effects in Fe monolayer on Sb2Te3 — •Farideh Hajiheidari[1], Wei Zhang[1,2], and Riccardo Mazzarello[1,3] — [1]Institute for Theoretical Solid State Physics, RWTH Aachen University, D-52074 Aachen, Germany — [2]Center for Advancing Materials Performance from the Nanoscale, State Key Laboratory for Mechanical Behavior of Materials, Xi'an Jiaotong University, Xi'an 710049, PR China — [3]JARA-FIT and JARA-HPC, RWTH Aachen University, D-52074 Aachen, Germany

Three-dimensional topological insulators (TIs) realize an unconventional electronic phase originating from time-reversal symmetry and strong spin-orbit interaction (SOI). These materials are bulk insulators but possess conducting surface states in the bulk band gap. The surface states are topologically protected against non-magnetic disorder. However, impurities which break time-reversal symmetry induce a band gap in the system. This is of critical importance for potential device applications involving spin-based transport. In this work, we present a density-functional-theory study of the magnetic properties of a Fe monolayer on the (111) surface of the topological insulator Sb2Te3. We optimize the geometry of the system and determine the band structure and the easy axis of magnetization for the Fe atoms. We show that the easy axis is in-plane. In spite of this, the presence of the monolayer leads due to the opening of a gap of the order of meV, due to the interplay between magnetism and warping effects. Finally, we discuss the relevance of our findings to recent experiments about magnetic adatoms and monolayers deposited on TIs.

HL 66.9 Wed 17:15 H32

Towards topological tunnel devices - A versatile method for processing tunnel junctions from high quality single crystals — •Robin Klett[1,2], Karsten Rott[1,2], Daniel Ebke[3], Chandra Shekhar[3], Joachim Schönle[4], Wolfgang Wernsdorfer[4], Stuart Parkin[5], Claudia Felser[1,2], and Günter Reiss[1,2] — [1]Physics Department, Bielefeld University, Germany — [2]Center for Spinelectronic Materials and Devices, Universitätsstraße 25, 33605 Bielefeld, Germany — [3]Max-Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [4]CNRS, Institut NEEL and Univ. Grenoble Alpes, F-38000 Grenoble, France — [5]Max Planck Institute for Microstructure Physics, 06120 Halle/Saale, Germany

We present a new and versatile concept for devices based on topological materials. To maintain their topological character high quality samples with clean interfaces to adjacent functional device components are mandatory. This requirement forms a bottleneck of current research, because very often the established thin film deposition fails to produce such high quality samples and bare surfaces of single crystals lack the necessary flatness. We demonstrate a novel, all-in-ultrahigh-vacuum process that enables to realize, e.g. tunnel junctions, Andreev contacts or SQUID rings from single crystalline bulk material. The validity of the technique is verified and illustrated with tunnel junctions made from cleaved single crystals of the half-Heusler topological superconductor candidate YPtBi.

HL 66.10 Wed 17:30 H32

Effective geometric phases and topological transitions in SO(3) and SU(2) rotations — •Henri Saarikoski[1], J. Enrique Vázquez-Lozano[2], José Pablo Baltanás[2], Junsaku Nitta[3], and Diego Frustaglia[2] — [1]RIKEN Center for Emergent Matter Science, Japan — [2]Departamento de Física Aplicada II, Universidad de Sevilla, Spain — [3]Department of Materials Science, Tohoku University, Japan

We address the development of geometric phases in classical and quantum magnetic moments (spin-1/2) precessing in an external magnetic field. We show that nonadiabatic dynamics lead to a topological phase transition determined by a change in the driving field topology. The transition is associated with an *effective* geometric phase which is identified from the paths of the magnetic moments in a spherical geometry. The topological transition presents close similarities between SO(3) and SU(2) cases but features differences in e.g. the limiting values of the geometric phases [1]. We discuss possible experiments where the effective geometric phase would be observable [2].

[1] H. Saarikoski, J. E. Vázquez-Lozano, J. P. Baltanás, J. Nitta, and D. Frustaglia, arXiv:1511.08315 (2015). [2] H. Saarikoski, J. E. Vázquez-Lozano, J. P. Baltanás, F. Nagasawa, J. Nitta, and D. Frustaglia, Phys. Rev. B 91, 241406(R) (2015).

HL 67: Frontiers of Electronic Structure Theory: Focus on Topology and Transport

Time: Wednesday 18:15–20:30 Location: Poster A

HL 67.1 Wed 18:15 Poster A

Improving anharmonic vibrational calculations from first principles — •Joseph C.A. Prentice, Bartomeu Monserrat, and Richard J. Needs — TCM Group, Cavendish Laboratory, University of Cambridge, UK

The vibrational self-consistent field (VSCF) method, as described in PRB 87 144302, has had several successes in accurately calculating the anharmonic properties of various materials, such as diamond, ice and solid hydrogen. However, a practical issue with the method is the large number of DFT calculations required to map the Born-Oppenheimer energy surface sufficiently accurately. We look at improvements to the method that reduce this computational load, in particular using data on forces from DFT calculations to improve the accuracy of the mapping. Results using this improved method are presented for competing structures of silicate perovskite under lower mantle conditions. Further improvements, involving the inclusion of n-body coupling between phonons, and their possible implementation are also discussed.

HL 67.2 Wed 18:15 Poster A

Towards a practical implementation of second-order Møller-Plesset perturbation theory for solids — •Xiangyue Liu, Arvid Conrad Ihrig, Sergey Levchenko, Igor Ying Zhang, and Matthias Scheffler — *Fritz-Haber-Institut der MPG, Berlin, DE*

The second-order Møller-Plesset perturbation theory (MP2) method is gaining attention in materials science, because it is free from the one-electron self-interaction error. Such error, as a lasting problem in density-functional theory, can lead to a wrong prediction of electronic band gaps, charge transfers, and reaction barriers, all of which are ubiquitous electronic properties or behaviors in condensed-matter systems. However, the unfavourable computational complexity, especially the cubic scaling with respect to the $\boldsymbol{k}$-point number in reciprocal space, limits the applicability of MP2 for solids. In this project we present a practical MP2 implementation for solids in the all-electron full-potential framework. In our implementation, the MP2 correlation energy is evaluated in the atomic-orbital (AO) representation (AO-MP2), which allows for a lower computational scaling in both real and reciprocal spaces[1]. The localized resolution of identity (RI-LVL) technique[2] is adopted to address the memory bottleneck of the AO-MP2 method, making it feasible to handle systems with several hundred atoms per supercell while avoiding the reliance on the disk storage. We demonstrate the accuracy as well as the efficiency of our new MP2 implementation for a diverse set of materials. [1] Levchenko, S. V. *et al.*, Comput. Phys. Comm. **192**, 60, (2015); [2] Ihrig, A.C. *et al.*, New J. Phys. **17** 093020, (2015).

HL 67.3 Wed 18:15 Poster A

Application of the exact exchange functional to magnetic metals within the FLAPW method — •Max Nusspickel[1], Markus Betzinger[1], Christoph Friedrich[1], Andreas Görling[2], and Stefan Blügel[1] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Germany — [2]Lehrstuhl für Theoretische Chemie, Universität Erlangen-Nürnberg, Germany

Orbital-dependent functionals form a promising class of exchange-correlation (xc) functionals in Kohn-Sham density-functional theory. Already the simplest functional of its kind, the exact exchange functional (EXX), cures the unphysical Coulomb self-interaction error of LDA and GGA functionals. In order to obtain a local xc potential from an orbital-dependent functional, the optimized effective potential (OEP) method is used, resulting in an integral equation for the potential. This equation, however, determines the potential only up to a constant.
In spin-polarized metals, the alignment of the spin-up and spin-down potentials is obtained by the requirement of electron number conservation: variations of the potential can lead to a change of the Fermi energy and, hence, to a variation of the densities of both electron spins. In this way, the OEP equations for the spin-up and spin-down potentials are coupled and the spin-dependent xc potential is obtained from a single OEP equation. We discuss the extension of our EXX-OEP implementation within the linearized augmented plane-wave (FLAPW) method and show results for prototype magnetic metals.

HL 67.4 Wed 18:15 Poster A

Electric switchable giant Rashba-type spin splitting in bulk PbS — •Bin Shao[1], Wenhui Duan[2], and Thomas Frauenheim[1] — [1]BCCMS, University of Bremen, Bremen, Germany — [2]Institute for Advanced Study, Tsinghua University, Beijing, China

Realizing electric controllable spin is one of the major challenges in the field of spintronics. A promising approach is to utilize so-called Rashba effect, which arises from the spin-orbit coupling under broken inversion symmetry, leading to a momentum-dependent spin splitting in k-space. However, the sizes of this splitting are usually rather small, which hinders the application of this effect in spintronics. In this work, based on density functional calculation, we predict a giant Rashba-type spin splitting in bulk PbS with space group $P6_3mc$. The phonon spectrum calculation gives evidence of the thermal stability of this system. The origin of the giant Rashba effect has been demonstrated from the deviation of the S ion from the inversion symmetric position, leading to an ferroelectric polarization along c axis. By switching the direction of the ferroelectric polarization, the spin directions of bulk carriers governed by the Rashba effect are completely rotated, which grants a potential approach to manipulate the spin of electrons by an external electric field. Moreover, under a reasonable hydrostatic pressure, the system could obtain the inversion symmetry due to the movement of the S ion backwards to symmetric positions. As a result, the system turns into a topological phase with the massless Dirac cone state at the (001) surface.

HL 67.5 Wed 18:15 Poster A

GW+fRG: Towards an fRG enhancement of ab initio calculations — Jannis Ehrlich[1,2], Carsten Honerkamp[1], Christoph Friedrich[2], and •Stephan Blügel[2] — [1]Institut für theoretische Festkörperphysik, RWTH Aachen University, D-52056 Aachen, Germany — [2]PGI-1 and IAS-1, FZJ & JARA, D-52425 Jülich, Germany

Spin excitations in solids are of fundamental interest for a wide variety of phenomena. Most materials-specific theoretical studies are based on the adiabatic treatment of the spin-degees of freedom in the context of DFT. Approaches based on the *GW* approximation include screening effects due to charge fluctuations but neglect vertex corrections and other contributions like magnetic fluctuations. The functional renormalization group (fRG) can overcome these limitations as it resums a different class of diagrams, among them charge and magnetic fluctuations and vertex corrections. We discuss how the equations for two-particle vertices in the fRG contain the *GW* approximation, the Bethe-Salpeter equation (BSE) and the parquet approach on certain levels of approximations. Thus, a fRG calculation of materials properties could be a powerful approach to improve the *GW* and BSE methods already applied in first-principles calculations. By using recently suggested channel decomposition schemes [1,2] the method has gained in flexibility and in potential for tackling more complex tasks. Here we propose first steps to develop the fRG approach for the *ab initio* calculation of materials properties.

[1] C. Husemann, M. Salmhofer, Phys. Rev. B **79**, 195125 (2009).
[2] W. Wang *et al.*, Phys. Rev. B **85**, 035414 (2012).

HL 67.6 Wed 18:15 Poster A

The quantum anomalous Hall effect in HgMnTe — •Jan Böttcher, Christoph Kleiner, and Ewelina M. Hankiewicz — Uni Würzburg, Institut für Theoretische Physik und Astrophysik, Germany

Recently, the quantum anomalous Hall (QAH) effect was predicted to exist in Mn doped HgTe. Within the QAH phase only one edge state remains at an edge due to an opposite coupling of spin to the magnetization. The experimental proof is however still outstanding. The paramagnetic nature of the Mn impurities gives rise to the formation of Landau levels which makes it experimentally challenging to distinguish the QAH from a conventional quantum Hall (QH) state. Based on the BHZ model, we present an extended study of the transition from the quantum spin Hall to the QAH state as well as the QAH to the quantum Hall state. For this purpose, we make use of the finite difference method and compare the results with analytical calculations. Hallmarks of the QAH states in the presence of magnetic fields are discussed. The BHZ model has natural limitations in the high magnetic field regime. We therefore compare our results with

band structure calculations based on the 8x8 Kane Hamiltonian. Signatures in the magnetoresistance are discussed which might open the door to distinguish the QAH from the QH state in future transport experiments.

We acknowledge financial support by the DFG within SFB 1170 "ToCoTronics".

HL 67.7 Wed 18:15 Poster A

Nonconventional screening of the Coulomb interaction in low-dimensional semiconductors and insulators — Ersoy Sasioglu, •Christoph Friedrich, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Screening effects play a fundamental role in determining the exciton binding energy, electron dynamics, and the effective electron-electron interaction in low-dimensional semiconductors and insulators. Experimental observation of the large exciton binding energies and nonhydrogenic Rydberg series in low-dimensional semiconductors indicate an unusual non-local screening of the Coulomb interaction. By means of first-principles calculations in conjunction with the random-phase approximation (RPA) within the FLAPW method we study the screening of the Coulomb interaction in low-dimensional semiconductors and insulators. For this purpose a novel tetrahedron method has been implemented. We show that the screening in these systems deviates substantially from the bulk behavior, i.e., the screened interaction W cannot be expressed by a simple static dielectric constant. We compare the numerical RPA results to analytical functions derived from image-charge models for the isolated slab and for a repeated slab model. We find a nonconventional screening in low-dimensions. This nonconventional screening explains the deviations from the usual hydrogenic Rydberg series of energy levels of the excitonic states in one- and two-dimensional semiconductors and opens up possibilities for fundamental studies of correlation effects in low-dimensional materials.

HL 68: Metal-Semiconductor Hybrids

Time: Thursday 9:30–12:30 Location: H10

Invited Talk HL 68.1 Thu 9:30 H10

Modifications of material and chemical properties of organic molecules driven by QED phenomena — •Francisco Garcia-Vidal — Departamento de Fisica Teorica de la Materia Condensada and Condensed Matter Physics Center (IFIMAC), Universidad Autonoma de Madrid, Madrid 28049 (Spain)

In this talk we will show how some material and chemical properties of molecules can be tuned and modified by taking advantage of the phenomenon of collective strong coupling. First we will show how exciton conductance in organic materials can be enhanced by several orders of magnitude when the molecules are strongly coupled to an EM confined mode [1]. We furthermore show that by designing the electric field profile of the EM mode that provides the strong coupling, the transport properties can be tuned to achieve exciton harvesting and funneling, i.e., to guide excitons from a collection area to a specific location [2]. Finally, we analyze under which conditions the molecular properties under strong coupling can be understood by the modification of the potential energy surfaces determining nuclear dynamics under the Born-Oppenheimer approximation. In addition, we demonstrate that the nuclear dynamics of the molecules in electronic dark states, which are only weakly coupled to the EM mode, are nonetheless affected by the formation of collective strong coupling [3].

[1] J. Feist and F. J. Garcia-Vidal, Phys. Rev. Lett. 114, 196402 (2015). [2] C. Gonzalez-Ballestero, J. Feist, Esteban Moreno, and F. J. Garcia-Vidal, Phys. Rev. B 92, 121402(R) (2015). [3] J. Galego, F. J. Garcia-Vidal, and J. Feist, Phys. Rev. X 5, 041022 (2015).

HL 68.2 Thu 10:00 H10

Coherent coupling between excitons and surface plasmon polaritons reduces inhomogeneous broadening in a J-aggregate thin film at room temperature — Xuan Trung Nguyen[1,2], •Antonietta De Sio[1,2], Julia Witt[2,3], Gunther Wittstock[2,3], and Christoph Lienau[1,2] — [1]Institut für Physik, Carl von Ossietzky Universität Oldenburg, Germany — [2]Center of Interface Science, Carl von Ossietzky Universität Oldenburg, Germany — [3]Institut für Chemie, Carl von Ossietzky Universität Oldenburg, Germany

Organic molecular aggregates are of particular interest for the development of novel nanostructures for technological applications spanning from artificial light harvesting to all-optical plasmonic switching. The optical spectra of these molecular aggregates are often dominated by structural disorder effects resulting in inhomogeneously broadened absorptive lineshapes at room temperature. By using broadband spectral interferometry we show that inhomogeneous broadening in a model J-aggregate cyanine dye is significantly reduced in the presence of an ultrathin sub-10-nm gold layer and the resulting optical spectra show almost perfect Lorentzian line shapes at room temperature. This surprising result is accompanied with the reduction of electron-phonon interactions (vibronic resonances) and increased delocalization of the wavefunction due to strong electronic coupling to surface plasmon polaritons.

HL 68.3 Thu 10:15 H10

Strong light-matter interaction between Tamm plasmons and exciton-polaritons in ZnSe-based microcavities — •SK. Shaid-Ur Rahman[1], Thorsten Klein[2], Sebastian Klembt[2], Detlef Hommel[2], Jürgen Gutowski[1], and Kathrin Sebald[1] — [1]Semiconductor Optics — [2]Semiconductor Epitaxy, Institute of Solid State Physics, University of Bremen, Bremen, Germany

Cavity polaritons are half-light-half-matter quasi-particles, resulting from strong coupling between quantum well (QW) excitons and cavity photons. One can modulate the polariton eigenenergies by utilizing Tamm plasmons (TPs) which are formed, e.g., at the interface between a metal and the distributed Bragg reflector (DBR) of a microcavity (MC). We will discuss the influence of TPs on the optical properties of ZnSe-based MCs. The MC consists of a 12-fold top DBR, a λ cavity including 3 ZnSe QWs, and a 18-fold bottom DBR. A layer of 40 nm Ag is deposited on top of the MC sample. Anti-crossing between the TP and the cavity mode has been observed in the micro-reflectivity measurements performed for different top layer thicknesses at RT. This built hybrid state possesses a splitting energy of about 40 meV. Measurements at 4K show four resonances due to the hybrid states of Tamm plasmons, heavy-hole, and light-hole exciton-polaritons. On resonance between the TP and the cavity mode the lowest hybrid eigenenergy is about 9 meV red-shifted from the spectral position of the lower polariton energy in the Ag layer free sample. All experimental observations are in good agreement with calculations based on the transfer-matrix method as well as on the coupled-oscillator model.

HL 68.4 Thu 10:30 H10

Proposal of detecting non secular processes through coherent nanooptical spectroscopy — Markus Krecik, Sven M. Hein, Mario Schoth, and •Marten Richter — Institut für Theoretische Physik, Technische Universität Berlin, Germany

Relaxation or coherence conversion processes are often induced by system-bath interactions. In the theoretical description, it is often sufficient to keep only conversion processes between (excitonic) coherences and populations involving nearly resonant density matrix elements (secular processes). However interesting Non-Markovian signatures potentially involve secular and non secular processes. The dissection of secular and non secular processes is routinely carried out in theory, but the identification of a pure non secular observable in experiment is pending. We propose an experimental signal only with contributions from non secular processes. The signal uses a combination of coherent multidimensional spectroscopy and nanoplasmonic metal structures. For controlling the optical selection rules (required by the protocol) the nanooptical structure provides dynamical switches between spatial constant optical fields and field gradients. The signal is calculated for the example of a colloidal semiconductor quantum dot.

[1] Phys. Rev. A 92, 052113 (2015)

30 min. Coffee Break

HL 68.5 Thu 11:15 H10

Plexciton dynamics studied by Transient Absorption Spec-

troscopy — •Emanuele Minutella[1,2], Florian Schulz[1,2], Christian Strelow[1], Horst Weller[1,2], and Holger Lange[1,2] — [1]Institut für Physikalische Chemie, Universität Hamburg, Germany — [2]The Hamburg Centre for Ultrafast Imaging, Hamburg, Germany

Hybrid nanosystems composed of semiconductor nanoparticles (NPs) and metal NPs have different properties then each component of its own. In case of strong coupling, the exciton-plasmon coupling can lead to a collective state, also called plexciton. It is strongly influenced by the energy difference between the two systems, the size of the NPs and their distance. Although this system gives amazing possibilities, e.g. for defined charge and energy transfer in solar cells, experiments on this system remain rare.

To address the dynamics of this system the method of choice is femtosecond transient absorption spectroscopy. By varying the pump wavelength it is possible to perform resonant excitation, either within the exciton or the plasmon, or to excite both off-resonant simultaneously.

Au NPs and CdSe NPs were synthesized by wet chemical synthesis enabling to adjust their size. To control the interparticle distance the CdSe NPs were embedded in a stiff polymer shell with a variable thickness. We show first results on individual Au and CdSe NPs as well as their aggregates.

HL 68.6 Thu 11:30 H10

Control of optical processes in organometal halide perovskites using plasmonic nanoantennas — •Aurora Manzi, Lakshminarayana Polavarapu, Alexander Urban, and Jochen Feldmann — Chair for Photonics and Optoelectronics Ludwig-Maximilians-Universität (LMU), München, Germany

Fluorescence enhancement through the interaction of an emitting material with plasmonic nanostructures has been widely investigated for fluorophores ranging from dye-molecules to quantum dots for various applications. Plasmonic nanoparticles that are in the proximity of an emitting material change the local field and hence the absorption and photoluminescence characteristics of the material.

Perovskites are new materials that have recently attracted strong interest due to their fluorescence properties and possible applications in light emitting devices1. The interaction of perovskite nanocrystals with plasmonic structures could open new pathways for the application of such perovskite nanocrystals in various fields. However, there have not been many studies towards this direction.

In our studies we investigate the effect of plasmonic nanostructures on the photoluminescence of two-dimensional perovskite nanoplatelets. Bowtie nanoantennas were prepared with e-beam lithography and used as plasmonic resonators to study their influence on the optical properties of $CH_3NH_3PbX_3$ (X=Br, I) platelets.

HL 68.7 Thu 11:45 H10

Helicity sensitive terahertz radiation detection by dual-grating-gate high electron mobility transistors — •Philipp Faltermeier[1], Peter Olbrich[1], Willibald Probst[1], Leonhard Schell[1], Takayuki Watanabe[2], Stephane Albon Boubanga Tombet[2], Taiichi Otsuji[2], and Sergey Ganichev[1] — [1]University of Regensburg, Regensburg, Germany — [2]Tohoku University, Sendai, Japan

We report on the observation of a radiation helicity sensitive photocurrent excited by terahertz (THz) radiation in dual-grating-gate (DGG) InAlAs/InGaAs/InAlAs/InP high electron mobility transistors (HEMT). For a circular polarization the current measured between source and drain contacts changes its sign with the inversion of the radiation helicity. For elliptically polarized radiation the total current is described by superposition of the Stokes parameters with different weights. Moreover, by variation of gate voltages applied to individual gratings the photocurrent can be defined either by the Stokes parameter defining the radiation helicity or those for linear polarization. We show that artificial non-centrosymmetric microperiodic structures with a two-dimensional electron system excited by THz radiation exhibit a *dc* photocurrent caused by the combined action of a spatially periodic in-plane potential and spatially modulated light. The results provide a proof of principle for the application of DGG HEMT for all-electric detection of the radiation's polarization state. [1] P. Faltermeier *et al.*, Journal of Applied Physics **118**, 084301(2015)

HL 68.8 Thu 12:00 H10

Electrochemical approaches for controlling plasmonic nanostructures — •Gilles Bourret[1], Tuncay Ozel[2], Martin Blaber[2], George Schatz[2], and Chad Mirkin[2] — [1]Paris-Lodron University, Salzburg, Austria — [2]Northwestern Universty, USA

The optical and electrical properties of heterogeneous nanowires are profoundly related to their composition and nanoscale architecture. However, the intrinsic constraints of conventional synthetic and lithographic techniques have limited the types of multi-compositional nanowires that can be created and studied in the laboratory. Our recent progress in templated syntheses of one-dimensional nanostructures will be briefly disccussed in the context of plasmonics.[1-3] In particular, we report a high-throughput technique that can be used to prepare coaxial nanowires with sub-10 nm control over the architectural parameters in both axial and radial dimensions. The method, which is termed coaxial lithography (COAL),[3] relies on templated electrochemical synthesis and can create coaxial nanowires composed of combinations of metals and semiconductors. The optoelectronic properties of a plasmonic nanoring embedded hybrid core-shell semiconductor nanowire were studied. This demonstrates the potential of this new synthetic technique to radically change nanowire fabrication.

References. [1] G. R. Bourret, T. Ozel, M. Blaber, C. Shade, G. C. Schatz and C. A. Mirkin Nano Lett. 2013, 13, 2270. [2] T. Ozel, G. R. Bourret, A. Schmucker, K. Brown and C. A. Mirkin Adv. Mater. 2013, 25, 4515. [3] T. Ozel, G. R. Bourret and C. A. Mirkin Nature Nanotech. 2015, 10, 319.

HL 68.9 Thu 12:15 H10

Interaction of Porous Silicon Photonic Crystals and Plasmonic Nanostructures for Applications in Surface-Enhanced Raman Spectroscopy — •Martin Fränzl, Stefan Moras, and Dietrich R.T. Zahn — Semiconductor Physics, Technische Universität Chemnitz, Germany

We fabricated porous silicon photonic crystals by electrochemical etching of p-doped silicon in hydrogen fluoride solution. By applying a periodic etching current we obtain a periodic change of the porosity and thus a periodic variation of the effective refractive index. This represents a photonic crystal in one dimension and results in a very high reflectance in the photonic band gap. The plasmonic structures were fabricated using nanosphere lithography leading to metallic nanostructure arrays. These ordered structures show a collective plasmonic resonance with a high absorbance and a very low transmission. We combined these structures by using the porous silicon photonic crystal as substrate for the nanosphere lithography and designed both structures so that the plasmonic resonance is located in the center of the photonic band gap. The properties of the structures were measured using spectroscopic ellipsometry and simulated using effective medium theories and finite-element methods. The high reflectance of the photonic crystal and the absorbance at the plasmonic resonance results in a strong confinement and enhancement of electric fields at the interface. We performed surface-enhanced Raman spectroscopy (SERS) measurements by depositing a thin layer of CoPc on top of the composite structure and report a giant SERS enhancement factor in the order of 10^5.

HL 69: Focussed Session: Oxide Semiconductors for Device and Energy Applications 1

Semiconducting metal oxides possess a very high potential for electronic devices and energy applications. For example, the n-type semiconductor Ga_2O_3 is currently intensively investigated due to its favorable semiconducor properties for power electronics, whereas the p-type semiconductor NiO can serve as important charge extraction barrier, to increase the efficiency of organic photovoltaics. The scope of this focus session encompasses well defined oxide structures of highest material quality and the understanding of their device-related physical properties as essential prerequisites for the application-relevant technological control of semiconducting metal oxides.

Organizers: Andreas Klein (TU Darmstadt), Oliver Bierwagen (PDI Berlin), Holger von Wenckstern (U Leipzig), and Martin Feneberg (OvGU Magdeburg)

Time: Thursday 9:30–13:15 Location: H11

Topical Talk HL 69.1 Thu 9:30 H11

Oxide semiconductors: materials design and applications — •Hideo Hosono — Tokyo Institute of Technology, Yokohama, Japan,

Oxide semiconductors have a long history comparable to IV group element semiconductors. Although industrial application remains still a few, industrial application of thin film transistors with oxide semiconductor (IGZO) channel has started to drive high resolution, large sized OLED-TVs as well as energy-saving LCDs recently, and Ga2O3 with a band gap of ~5eV is attracting as a semiconductor for power electronic applications.

The chemical bonding of oxides is rather different from that of typical semiconductors, which in turn gives unique band structure and crystal structure. In this talk, I review the progress of oxide semiconductors in last 2 decades focusing on materials design and applications utilizing the unique nature of oxides.

Topical Talk HL 69.2 Thu 10:15 H11

Mixing In and Ga sesquioxides - and their polar phases — •Vincenzo Fiorentini — Dept of Physics, Cagliari University, Italy — CNR-IOM, UOS Cagliari, Italy

This talks will report on recent first-principles theoretical work on the In and Ga sesquioxides and their ternary alloy, an up-and-coming materials system for near to deep-UV large-breakdown and transparent-conducting materials. Firstly, a qualitative phase diagram is proposed over all the full composition range. Three structures –monoclinicβ, layered-hexagonal, and cubic bixbyite– are competing for the ground state, and several regions of miscibility and phase separation interlace as function of composition, more or less independently of temperature. Electronic properties, including absorption anisotropy at low x, and a selection of interface band offsets will also be presented. Secondly, the metastable polar phase ε-Ga_2O_3 is shown to be pyroelectric (i.e. locked in a non-switchable polarized structure) with a large ferroelectric-like polarization 0.23 C/m^2 and a diagonal piezoelectric coefficient (0.77 C/m^2) in line with those of III-V nitrides and II-VI oxides. In view of recent growth successes in that direction, the interface of ε-Ga_2O_3 to GaN is studied, both in terms of geometry, offsets, and polarization difference, suggesting interesting potential for power applications.
Work in collaboration with M. B. Maccioni, F. Ricci, R. Fornari.

Topical Talk HL 69.3 Thu 10:45 H11

Exploring and tailoring conductance phenomena in oxide films: An STM study — •Niklas Nilius — Carl von Ossietzky Universität Oldenburg

Electronic properties of classical semiconductors, e.g. Si, are adjustable with high accuracy and form the basis of todays information technology. Also oxides exhibit fascinating electronic features, e.g. a large spread in gap sizes, a correlated electronic behavior, metal-insulator transitions, anomalous temperature and voltage dependencies and superconductivity. Despite this potential, no satisfactory mechanistic understanding of oxide properties has been achieved so far and preparation of phase-clean materials remains challenging.

My talk demonstrates how thin-film oxides of high structural quality can be prepared and explored at atomic length-scales by STM. The approach yields direct correlation between structural parameters and electronic properties of the materials. Moreover, their conductance behavior becomes tunable, e.g. by stoichiometry and defect engineering, doping and interface control. I will present examples for low-gap oxides, e.g. Cu_2O and V_2O_3, and discuss how their electronic response is affected by intrinsic defects and dopants. For wide-gap materials, such as MgO and CeO_2, the interplay between conductance and low-dimensional edge and surface states as well as uncompensated polarity is addressed. Finally, the transition from binary to ternary oxides is introduced as a route to tune electronic properties. My talk aims at providing mechanistic insights into the structure-conductivity relationship rather than presenting materials of direct technological relevance.

15 min. break.

Topical Talk HL 69.4 Thu 11:30 H11

Miscibility and phase separation in $(In_xGa_{1-x})_2O_3$ — •Martin Albrecht[1], Robert Schewski[1], Toni Markurt[1], Tobias Schulz[1], Michele Baldini[1], Günter Wagner[1], Holger von Wenckstern[2], Marius Grundmann[2], Hartwin Peelaers[3], Joel Varley[3], and Chris Van de Walle[3] — [1]Institute for Crystal Growth, Berlin, Germany — [2]Universität Leipzig — [3]Materials Department, University of California, Santa Barbara, California, USA

Group III sesquioxides are distinguished from other wide band gap semiconductors by the fact, that they can be efficiently n-doped despite a wide band gap that ranges from 2.7 eV for In_2O_3 over 4.8 eV for Ga_2O_3 to 8.9 eV for Al_2O_3. Full exploitation of their properties for electronic applications requires band gap engineering formation of solid solutions. The formation of solid solutions in group III sesquioxides is challenging, since, at thermodynamic equilibrium, the binaries exhibit different thermodynamically stable structures (cubic, rhombohedral, and monoclinic) besides a significant lattice mismatch. The oxygen coordination of the metal atoms in the binary alloys is either octahedral, or mixed tetrahedral and octahedral. In this presentation we report on transmission electron microscopy studies on miscibility and phase separation in the system $(In_xGa_{1-x})_2O_3$ grown by PLD. We identify essentially three different phases as dependent on composition, i.e. the monoclinic β-phase in the compositional range up to $x = 0.5$, an ordered hexagonal phase in the range between $x = 0.5$ and 0.75 and the cubic bixbyite phase at higher In contents. In atoms occupy octahedrally coordinated cation sites in the monoclinic phase.

HL 69.5 Thu 12:00 H11

Infrared response of cubic In_2O_3 — •Martin Feneberg[1], Christian Lidig[1], Jakob Nixdorf[1], Oliver Bierwagen[2,3], James S. Speck[3], Zbigniew Galazka[4], and Rüdiger Goldhahn[1] — [1]Institut für Experimentelle Physik, Otto-von-Guericke Universität Magdeburg — [2]Paul Drude Institut für Festkörperelektronik, Berlin — [3]Materials Department, University of California, Santa Barbara, USA — [4]Leibniz-Institut für Kristallzüchtung, Berlin

The infrared optical response of cubic bixbyite In_2O_3 samples is investigated in detail. Samples with different concentrations of free electrons from 1.5×10^{17} up to 1.6×10^{21} cm^{-3} are measured by spectroscopic ellispometry yielding dielectric functions. Besides transerse optical phonon modes a Drude contribution accounting for the free electron gas is observed and analyzed.

The broadening factor in the Drude contribution can be understood as characteristic relaxation time constant. Its frequency dependency is visible in point-by-point fitted dielectric functions, i.e. without assumptions about the line shape. The broadening factor is found to be a constant within errors of measurement.

By comparison with Hall-effect data, the effective electron mass is found to be a function of energy increasing from $m^* = 0.18m_0$ at the Γ-point of the Brillouin zone. This is direct proof of the non-parabolic nature of the conduction band.

HL 69.6 Thu 12:15 H11

Electrical conductivity and gas-response of the In_2O_3 surface electron accumulation layer — •Julius Rombach[1], Oliver Bierwagen[1], Alexandra Papadogianni[1], Markus Mischo[2], Volker Cimalla[2], Oliver Ambacher[3], Theresa Berthold[4], Marcel Himmerlich[4], and Stefan Krischok[4] — [1]Paul-Drude-Institut für Festkörperelektronik, Berlin — [2]Fraunhofer Institut für Angewandte Festkörperphysik, Freiburg — [3]Institut für Mikrosystemtechnik, Freiburg — [4]Institut für Mikro- und Nanotechnologien, Technische Universität Ilmenau, Germany

Indium oxide is a well-known material for conductometric gas sensors, showing a decrease in conductance when exposed to oxidizing gases. In contrast to typically used polycrystalline films, we study MBE-grown single-crystalline In_2O_3 thin films as a model system with reduced complexity. Electrical conductivity of these films essentially consists of two parallel contributions: the bulk of the film and the surface electron accumulation layer (SEAL) of unknown conductance. Both these contributions are varied to understand their effect on the sensor response. Conductivity changes induced by UV illumination in air, forcing desorption of oxygen adatoms on the surface, and gas-response measurements in ozone atmosphere give a measure of the sensor response and show that the sensor effect is only due to the SEAL conductivity. Therefore, a strong sensitivity increase is achieved by reducing

the bulk (or intra-grain) conductivity. Hall and Seebeck measurements will give further details helping to estimate the SEAL electron concentration and mobility.

HL 69.7 Thu 12:30 H11

Surface structure of β-Ga_2O_3(100) via classical and quantum mechanical rainbow scattering — •Marco Busch[1], Eric Meyer[1], Helmut Winter[1], Zbigniew Galazka[2], Klaus Irmscher[2], and Konrad Gärtner[3] — [1]Humboldt-Universität zu Berlin, Institut für Physik, Newtonstrasse 15, 12489 Berlin, Germany — [2]Leibniz-Institut für Kristallzüchtung, Max-Born-Strasse 2, 12489 Berlin, Germany — [3]Institut für Fest- körperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

Fast light atoms and molecules with energies from 200 eV up to several tens of keV are grazingly scattered from a clean and well-ordered β-Ga_2O_3(100) surface. The angular distributions of projectiles scattered in the regime of axial surface channeling show intensity maxima, which can be described with the concept of the classical rainbow scattering and offer the determination of the interaction surface potential. However, for decreasing projectile energy one can observe Bragg peaks in the angular distributions, which can be interpreted within the framework of quantum mechanics only. Here, we present investigations of the quantum scattering from the ex-situ cleaved and in-situ annealed (100) surface of β-Ga_2O_3 single crystals, grown by the Czochralski method. The splittings of Bragg peaks and their intensity modulations were so far exploited to deduce information on the arrangement of the atoms and thereby the termination and relaxation of the topmost surface layer [1]. Based on these investigations, the adsorption of atoms and molecules on the β-Ga_2O_3(100) surface can be studied in detail. [1] M. Busch et al., Appl. Phys. Lett. **105**, 051603 (2014).

HL 69.8 Thu 12:45 H11

Vibrational spectra, Raman and IR properties of Copper-Oxide Phases from first principles — •Marcel Giar, Markus Heinemann, and Christian Heiliger — I. Physikalisches Institut, Justus-Liebig-University, D-35392 Giessen, Germany

Vibrational properties of the three copper oxide phases Cu_2O, Cu_4O_3, and CuO are derived from DFT calculations. Phonon dispersions including non-analytical contributions to the dynamical matrix in the limit $\mathbf{q} \to \mathbf{0}$ are presented as well as derived quantities such as acoustic phonon group velocities and thermodynamics. We further examine Raman and IR properties and their behavior under uniform external pressure. The frequency dependence of the Raman susceptibility and resulting changes in the Raman scattering intensities are also assessed.

HL 69.9 Thu 13:00 H11

Optical properties of single crystalline $SrMoO_3$ thin films — •Aldin Radetinac, Jörg Zimmermann, Karoline Hoyer, Hongbin Zhang, Philipp Komissinskiy, and Lambert Alff — Institute for Materials Science, TU Darmstadt, Germany

The optical properties of pulsed laser deposited highly crystalline $SrMoO_3$ thin films were investigated.[1] Due to their low resistivity below 30 $\mu\Omega$cm, thin films of $SrMoO_3$ are candidates for transparent conductor applications. The transparency of $SrMoO_3$ extends into the ultraviolet range to about 300 nm. In this range, $SrMoO_3$ has a higher transparency at similar sheet resistance as compared to alternative oxide or metallic materials. Density functional theory shows that electron-electron correlation effects are small in $SrMoO_3$ as compared to other low-resistivity transition metal oxides and predicts the optical properties in good agreement with experiment. This work was supported by the DFG project KO 4093/1-1.

[1] A. Radetinac, J. Zimmermann, K. Hoyer, H. Zhang, P. Komissinskiy and L. Alff submitted to J. Appl. Phys. (2015)

HL 70: Semiconductor Lasers I

Time: Thursday 9:30–13:00 Location: H13

HL 70.1 Thu 9:30 H13

Few quantum emitters – small cavities: exact treatment of the electron-photon coupling in mesoscopic quantum devices — •Michael Gegg, Andreas Knorr, and Marten Richter — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Germany

Open many body quantum systems consisting of N quantum emitters (QEs), e.g. dye molecules or quantum dots, coupled to a lossy cavity/optical mode have been subject to extensive research for decades. These systems can be described by N two- (multi-) level systems interacting with bosonic cavity modes including dissipation and pumping in the Lindblad formalism. This provides access to a manifold of interesting applications, such as lasers, parametric amplifiers for normal cavities and spasers or surface plasmon generators for metallic systems.
We develop an exact and numerically scalable solution to the N multi-level system Lindblad equation [1], which provides a dramatic speedup compared to conventional solutions. Especially in the few ($N \sim 1 - 100$) emitter case the solution is a major advance compared to existing techniques, while retaining the full quantum correlations and entanglement properties. Some applications of the developed method will be shown.

[1] M. Richter, M. Gegg, T.S. Theuerholz, A. Knorr, Phys. Rev. B 91: 035306 (2015)

HL 70.2 Thu 9:45 H13

Collective enhancements in many-emitter phonon lasing. — •Leon Droenner, Nicolas Naumann, Julia Kabuss, and Alexander Carmele — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

The confinement of a single acoustic phonon mode and the acoustic analogue of lasing has been experimentally demonstrated on several platforms [1]. However, to achieve threshold-less lasing and high output intensities the strong coupling regime is necessary but still difficult to engineer. To circumvent this ingredient, we propose an N-emitter phonon laser based on a detuned excitation set-up, where either cooling or vibrational amplification can be realized [2]. We show that by detuning the optical excitation to the anti-Stokes resonance of the N-emitter ensemble, that collective enhancements become important. These enhancements are similiar to the super- and subradiance effects in optics but differ in effective density-density shifts. We pinpoint feasible excitation and coupling regimes and show that these collective shifts lead to a strongly enhanced quantum yield. Thereby, we show that the N-emitter setup is a promising route to realize highly efficient phonon lasing.

[1] K. Vahala, M. Herrmann, S. Knünz, V. Batteiger, G. Saathoff, T. W. Hänsch, Th. Udem, Nature Physics 5, 682 - 686 (2009).
[2] Nicolas L. Naumann, Leon Droenner, Alexander Carmele, Andreas Knorr, Weng W. Chow, Julia Kabuss, arXiv:1509.06910 (2015).

HL 70.3 Thu 10:00 H13

High-β Quantum Dot Micropillar Lasers under Optical Injection — •Elisabeth Schlottmann[1], Steffen Holzinger[1], Sören Kreinberg[1], Christian Schneider[2], Martin Kamp[2], Sven Höfling[2], Janik Wolters[1], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, Germany — [2]Technische Physik, Julius-Maximilians-Universität Würzburg, Germany

Injection locking of standard semiconductor lasers, where the slave adapts to the master laser's frequency is well known and is widely applied e.g. for laser stabilization. Here we go beyond the classical injection locking by exploring the quantum limit of injection locking by using a microscopic quantum dot laser as a slave. This device with a high quality factor of Q $\sim$ 70000 and a low mode volume exhibits high spontaneous emission enhancement due to the Purcell effect, enabling stable lasing at intra-cavity photon numbers as low as a few tens. In these devices, small structural asymmetries lead to bimodal emission and gain competition above threshold, resulting in different intensities for the two orthogonal polarization modes.

Under optical injection we achieve frequency locking, surprisingly accompanied by simultaneous strong emission at the slave's solitary

frequency. When the master laser and the stronger mode of the microscopic laser have the same polarization, the stronger mode is "partial injection locked" in a wide range of master-slave detuning. Simultaneously, the orthogonal polarized weak mode suffers a pronounced suppression of emission via gain coupling.

HL 70.4 Thu 10:15 H13

On the threshold behavior of high-β quantum dot micropillar lasers — •Sören Kreinberg[1], Weng W Chow[2], Christian Schneider[3], Frank Jahnke[4], Sven Höfling[3], Janik Wolters[1], Martin Kamp[3], Christopher Gies[4], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, Germany — [2]Sandia National Laboratories, Albuquerque, NM, USA — [3]Technische Physik, Julius-Maximilians-Universität Würzburg, Germany — [4]Institut für Theoretische Physik, Universität Bremen, Germany

We present a comprehensive study on the transition between spontaneous emission and stimulated emission of quantum dot microcavities in the regime of cavity quantum electrodynamics (cQED). The structures are based on high-quality, high-β semiconductor GaAs/AlAs micropillar cavities containing a single layer of optically pumped InGaAs quantum dots (QD) as active medium. A widely used criterion for lasing is a characteristic non-linearity in the in the input-output curve which gradually vanishes with increasing β values in micro- and nanolasers. To provide a conclusive lasing criterion, we show that QD micropillar cavities with almost identical intensity and spectral properties can be easily categorized into lasing and non-lasing classes by analysis of the equal-time second-order photon autocorrelation by means of a Hanbury-Brown and Twiss setup and the excitation-dependent impulse response of the system using time resolved spectroscopy. For a comprehensive picture, we compare our results to a microscopic theory to clearly identify lasing criteria in high-β microcavities.

HL 70.5 Thu 10:30 H13

Effects of single-quantum-dot lasing in the presence of strong coupling — Fabian Gericke[1], Leon Messner[1], Steffen Holzinger[1], Caspar Hopfmann[1], Tobias Heindel[1], Janik Wolters[1], Matthias Florian[2], Frank Jahnke[2], Christian Schneider[3], Martin Kamp[3], Sven Höfling[3], •Christopher Gies[2], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin — [2]Institut für Theoretische Physik, Universität Bremen — [3]Technische Physik, Universität Würzburg, Germany

Nanolasers with only few self-assembled semiconductor quantum dots (QDs) as active medium push solid-state emitter cavity-QED into new operational regimes, where the definition of 'lasing' needs to be closely reexamined. We present insight and results from a theory/experiment collaboration to explore the possibility of lasing in a system that exhibits strong coupling between a single emitter and a high-Q cavity mode. The coupling of higher multi-exciton states of detuned QD emitters is considered as a cavity feeding mechanism in a microscopic theory that treats the light-matter interaction of the few-emitter system non-pertubatively. We demonstrate that strong coupling and lasing can coexist in the experiment, and that the onset of stimulated emission already causes a transition to a single peak in the emission spectrum before strong coupling is lost due to increasing excitation-induced dephasing.

HL 70.6 Thu 10:45 H13

Two color excitation of a single-QD Laser in the strong coupling regime — •Fabian Gericke[1], Martin von Helversen[1], Maximilian Sommer[1], Tobias Heindel[1], Christian Schneider[2], Frank Jahnke[3], Sven Höfling[2], Janik Wolters[1], Martin Kamp[2], Christopher Gies[3], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, 10623 Berlin, Germany — [2]Technische Physik, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [3]Institut für Theoretische Physik, Universität Bremen, 28334 Bremen, Germany

Single semiconductor quantum dots embedded in microcavities offer the unique opportunity to study different regimes of cavity quantum electrodynamics. The light-matter interaction, especially in the coherent coupling regime, is of particular interest for a variety of applications in quantum information processing and novel effects such as single photon nonlinearities.

In this work, we present comprehensive study on quantum dot (QD) microcavity lasers operating at the intersection of weak and strong light matter interaction. By combined resonant and non-resonant excitation, we distinguish between the gain contribution given by a single resonant QD and small number of nonresonant QDs, where the latter are weakly coupled to the lasing mode via e.g. phonon-induced cavity feeding. This enables us to proof the onset of laser oscillations with a single quantum dot as gain medium. The presented results significantly advance the understanding of single quantum dot lasers and stimulate further experiental as well as theoretical investigations.

30 min. Coffee Break

HL 70.7 Thu 11:30 H13

SESAMs for mode locking of red-emitting VECSELs — •Roman Bek[1], Quynh Duong-Ederer[1], Hermann Kahle[1], Thomas Schwarzbäck[1], Michael Jetter[1], Maria A. Cataluna[2], and Peter Michler[1] — [1]Institut für Halbleiteroptik und Funktionelle Grenzflächen, Research Centers SCoPE and IQST, University of Stuttgart, Allmandring 3, 70569 Stuttgart, Germany — [2]School of Engineering, Physics and Mathematics, University of Dundee, Dundee DD1 4HN, United Kingdom

Passively mode-locked vertical external-cavity surface-emitting lasers (VECSELs) emitting in the infrared spectral range have first been realized in 2000. These compact pulsed laser sources have excellent properties such as high output power, short pulse duration and a near diffraction-limited beam profile. In the visible spectrum, VECSELs have been mode-locked by semiconductor saturable absorber mirrors (SESAMs) since 2013 with emission wavelengths between 650 nm and 675 nm.

We present and compare different SESAM designs for mode locking of AlGaInP VECSELs. Our samples are fabricated by metal-organic vapor-phase epitaxy and include Bragg mirrors consisting of AlGaAs/AlAs on GaAs substrates. The active regions contain either GaInP quantum wells or InP quantum dots embedded in AlGaInP barrier layers. Some of the absorber structures are coated with a fused silica layer to improve the mode locking performance. We use v-shaped cavity configurations with the outcoupling mirror used as folding mirror to strongly focus onto the absorber.

HL 70.8 Thu 11:45 H13

Optimization of the cavity design for passively mode-locked VECSELs in the red spectral range — •Quynh Duong-Ederer[1], Roman Bek[1], Hermann Kahle[1], Thomas Schwarzbäck[2], Michael Jetter[1], and Peter Michler[1] — [1]Institut für Halbleiteroptik und Funktionelle Grenzflächen, Research Center SCoPE and IQST, Universität Stuttgart, Allmandring 3, 70569 Stuttgart — [2]TRUMPF Lasersystems for Semiconductor Manufacturing GmbH, Johann-Maus-Straße 2, 71245 Ditzingen

Since the first demonstration of a passively mode-locked VECSEL in 2002, this type of semiconductor laser has become a fundamental element in present research. Pulsed lasers directly emitting in the red spectral range are promising candidates for many applications ranging from spectroscopy to biomedical fields. We successfully demonstrated a SESAM mode-locked VECSEL emitting at around 660 nm with a pulse duration of 2 ps and a repetition rate of 850 MHz. However, due to the cavity design the maximum peak power was limited.
We present in this contribution major improvements to overcome this circumstance. First the plane diamond heat spreader is replaced by a wedged one with a wedged angle of 2° and an anti-reflection coating for the target wavelength. Furthermore, the gain chip mount is modified to match the wedged heat spreader for an enhanced heat dissipation from the chip. This enables us to increase the optical pump power without a thermal roll-over of the device resulting in higher peak power and a stable performance of our mode-locked laser.

HL 70.9 Thu 12:00 H13

Investigations on pump-power dependences of a self-mode-locked VECSEL — •Max Vaupel, Mahmoud Gaafar, Fan Zhang, Christoph Möller, Wolfgang Stolz, Arash Rahimi-Iman, and Martin Koch — Faculty of Physics and Materials Sciences Center, Philipps-Universität Marburg, 35032 Marburg, Germany

Recently, self-mode-locked vertical-external-cavity surface-emitting lasers (SML-VECSEL) were presented as promising saturable-absorber-free pulsed lasers, although, up to now, the responsible effect is not fully understood. In this work, experimental studies have been performed in order to gain insight into the pump-power-dependent mode-locking behaviour of such a laser device and to foster the assumption of Kerr-lensing being significantly involved, by using a Z-cavity

and a linear cavity configuration, respectively. The results show, that generating losses for the continuous-wave resonator mode with a well-placed hardaperture in the cavity leads to mode-locking and therefore pulsed operation for these resonator geometries. ABCD-matrix calculations for the intra-cavity beam radius as a function of a negative or positive Kerr lens inside the VECSEL-chip are in accordance with the obtained results.

HL 70.10 Thu 12:15 H13

Hybrid VCSEL and DFB Organic Microlasers — •Tim Wagner, Markas Sudzius, Andreas Mischok, Hartmut Fröb, and Karl Leo — Institut für Angewandte Photophysik, Technische Universität Dresden, George-Bähr-Str. 1, 01069 Dresden

Two of the numerous resonator architectures are the vertical-cavity surface-emitting laser (VCSEL), in which the laser mode is vertically confined between two highly reflective DBR mirrors, and the distributed-feedback laser (DFB), incorporating a horizontal waveguide with a periodic diffraction grating. We prepare these microlasers using an identical set of materials with Alq$_3$:DCM as the active medium. Although based on entirely different geometries and mechanisms, the two resonators exhibit similar lasing thresholds.

In this work, we design a continuously tunable hybrid device combining both resonators in a composite system, in which second-order Bragg diffraction serves as a coupling mechanism between vertical and lateral modes. Coherent interaction of the different resonances is observed and described by a coupled oscillator model. The analysis of mode dispersions and lasing characteristics leads to the identification of the different mechanisms on optical feedback and losses. Based on the results obtained, novel structures are designed to balance the performances of the vertical and lateral resonator inside the hybrid device.

HL 70.11 Thu 12:30 H13

Design considerations of oxide-confined red emitting electrically pumped VECSEL — •Zhihua Huang, Michael Zimmer, Roman Bek, Hermann Kahle, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen and Research Centers SCoPE and IQST, University of Stuttgart, Allmandring 3, 70569 Stuttgart, Germany

Electrically pumped vertical external cavity surface-emitting laser (EP-VECSEL) is an attractive laser source for compact, low-cost, high-brightness applications. However, achieving high output power with fundamental mode operation is still a challenging work. Here, we present a detailed numerical analysis of EP-VECSEL structure at a wavelength of 665 nm with the focus on the current confinement and thermal management of AlGaInP based devices. We apply an electro-thermal model to treat effective conductivity and current distribution in multiple quantum wells (MQW) and distributed Bragg reflectors (DBRs). By analyzing the diameters and positions of oxide-aperture, different material composition, doping and thickness of current spreading layer (CSL), an improved structure with homogeneous current distribution and a trade-off between optical loss and device resistance is obtained. This configuration contains one oxide-aperture placed at the bottom and a 10 μm thick Al0.10GaInP CSL with medium n-doped concentration. For this optimized structure, simulation results indicate that the emission area in active region with a near Gaussian current distribution can be increased up to about 60 μm. This work provides a significant guideline for the design and optimization of EP-VECSEL.

HL 70.12 Thu 12:45 H13

Semiconductor quantum membrane external-cavity surface-emitting laser — •Hermann Kahle[1], Cherry M. N. Mateo[2], Roman Bek[1], Uwe Brauch[2], Michael Jetter[1], Thomas Graf[2], and Peter Michler[1] — [1]Universität Stuttgart, Institut für Halbleiteroptik und Funktionelle Grenzflächen IHFG and research centers IQST and SCoPE, Allmandring 3 — [2]Universität Stuttgart, Institut für Strahlwerkzeuge IFSW and research center SCoPE, Pfaffenwaldring 43

Due to their simplicity and the efficient optical pumping, vertical external-cavity surface-emitting lasers (VECSELs) are becoming more and more important systems. Furthermore, the good beam quality as well as the open resonator which enables the use of intra-cavity (ic) frequency selective/multiplying elements make them laser systems with an unique palette of benefits. The use of semiconductors as gain material allows bandgap engineering and provides a broad gain. However, most VECSEL systems suffer from the bad thermal conductivity of the substrate and the DBR. A wet-chemically released active region of a VECSEL, sandwiched between anti-reflection coated diamond ic heatspreaders leads to an improved thermal behavior. The absence of the DBR allows us to use regular laser mirrors in the resonator and therefore completely exploit the gain provided by the active region. We present first characterisation measurements of the optically pumped semiconductor quantum membrane external-cavity surface-emitting laser (OPS-MECSEL or QML).

HL 71: Quantum Dots and Wires: Optical Properties

Time: Thursday 9:30–13:00 Location: H15

HL 71.1 Thu 9:30 H15

Exciton dynamics in colloidal CdSe nanoplatelets — •Sebastian Kickhöfel[1], Riccardo Scott[1], Artisom Antanovich[2], Anatol Prudnikau[2], Mikhail Artemyev[2], Alexander Achtstein[1], and Ulrike Woggon[1] — [1]Institute of Optics and Atomic Physics, Technical University of Berlin, 10623 Berlin, Germany — [2]Institute for Physicochemical Problems, Belarusian State University, 220030 Minsk, Belarus

Colloidal nanoplatelets are an active field of optoelectronic research. They combine advantages of colloidal systems like quantum dots and strongly confined 2D semiconductor quantum wells. Their optical absorption and emission can be tailored in a wide range[1]. As there is an increased number of reports showing unique optoelectronic properties like low lasing thresholds and strong electrooptic effects[2,3], a deeper understanding of the electronic structure and carrier dynamics is necessary for understanding these effects. We report the results of time-integrated and time-resolved photoluminescence investigations and modeling, giving a deeper understanding to the charge carrier dynamics in CdSe nanoplatelets. The influence of phonons to that will be discussed. The reported carrier dynamics is an essential prerequisite to understand the optoelectronic processes in CdSe nanoplateles like lasing or their potential use as optically active modulators media.

Literature:
[1] Ithurria, S., et al., Nature Materials 10(12) (2011): 936-941.
[2] Grim, J. Q., et al., Nature Nanotechnology 9(11) (2014): 891-895.
[3] Achtstein, A. W., et al., ACS Nano 8(8) (2014): 7678-7686.

HL 71.2 Thu 9:45 H15

Efficient numerical method for calculating Coulomb coupling elements and its application to two dimensional spectroscopy — •Anke Zimmermann and Marten Richter — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, EW 7-1, Technische Universität Berlin, Germany

The Coulomb coupling is essential for the understanding of several physical processes and plays an important role in a variety of nanostructures. Typically, to calculate the matrix elements of the two-particle Coulomb interaction, a six dimensional spatial integral appears. If the system requires the calculation of a high number of coupling elements, an efficient method for a fast numerical calculation of the Coulomb interaction is needed.

To reduce the numerical complexity of the calculation of Coulomb coupling elements in real space, a Green's function formulation of a generalized Poisson equation is used. The presented method, which is flexible and works for arbitrary geometries and inhomogeneous media, enables a fast calculation of Coulomb coupling elements, since the number of integrals is decreased.

The Coulomb interaction between two colloidal quantum dots depends on the spatial distance and the relative dipole orientation of the nanostructures. To identify the effects of the spatially dependent Coulomb coupling on single excitons and biexcitons, two dimensional spectroscopy can be used. The characteristic optical signatures of different spatial arrangements of the colloidal quantum dots are calculated and discussed.

HL 71.3 Thu 10:00 H15

Time-resolved, temperature-dependent photoluminescence

of F- and SiO_2-capped silicon nanoparticles — Robert Niemöller, Daniel Braam, •Günther M. Prinz, and Axel Lorke — Experimentalphysik und CENIDE, Universität Duisburg-Essen

Silicon is the most important semiconductor in today's microelectronics. A major disadvantage is its indirect bandgap, hindering the fabrication of efficient optoelectronic devices. Instead, silicon nanoparticles show bright luminescence with high quantum yield.

Here, we present time-resolved and temperature dependent photoluminescence (PL) measurements of silicon nanoparticles, capped with fluorinated silicon oxide or silicon dioxide. Apart from a stretched exponential time decay of the PL, we observe, that the intensity for the silicon dioxide-capped nanoparticles shows a maximum at 75K, while the PL intensity for the fluorinated-shell capped silicon nanocrystals increases up to room temperature.

The measured data is fitted with a combination of two models given by Lüttjohann et al. [1] and Suemoto et al. [2]. With this combined model, we can not only simulate the time dependent recombination but also the temperature dependent PL intensity. This simulation fits the luminescence data for both types of silicon nanocrystals, explaining why the fluorinated-shell capped silicon nanocrystals exhibit better luminescence properties.

[1] S. Lüttjohann, et al., EPL 79, 37002 (2007).
[2] T. Suemoto et al., Phys. Rev. B 49, 11005 (1994).

HL 71.4 Thu 10:15 H15

Consequences of light-hole and heavy-hole mixing on the optical properties of III-V-semiconductor quantum dots — •Fritz Weyhausen-Brinkmann[1], Ranber Singh[1,2], and Gabriel Bester[1,2] — [1]Universität Hamburg, Grindelallee 117, 20146 Hamburg, Germany. — [2]The Hamburg Centre for Ultrafast Imaging, Luruper Chaussee 149, 22761 Hamburg, Germany.

We calculate the spin-resolved light-hole and heavy-hole (LH-HH) band mixing in III-V-semiconductor quantum dots (QDs). The exciton emission spectrum of these QDs show optical anisotropy in their growth plane and the directions of polarization are strongly influenced by the LH-HH mixing. In the field of quantum information and quantum processing QDs are hot candidates, e.g. as single photon sources or quantum repeaters, which requires a good understanding of their optical properties. We are using the atomistic empirical pseudopotential approach including spin-orbit coupling to determine the spin-resolved LH-HH mixing of the single particle wave function as a function of strain for different types of QDs [1]. We find that the parallel spin of the light-hole is not negligible in contradiction to earlier model [2] and highlight the consequences of this finding on the polarization anisotropy.

[1] Y. Huo et al. Nature Physics 10, 46-51 (2014).
[2] C. Tonin, R. Hostein, V. Voliotis, R. Grousson, A. Lemaitre, and A. Martinez, Phys. Rev. B 85, 155303 (2012).

HL 71.5 Thu 10:30 H15

Polarization anisotropy of the emission from type-II quantum dots — •Petr Klenovsky[1,2], Dusan Hemzal[1,2], Petr Steindl[1,2], Marketa Zikova[3], Vlastimil Krapek[4], and Josef Humlicek[1,2] — [1]Central European Institute of Technology, Masaryk University, Kamenice 753/5, 62500 Brno, Czech Republic — [2]Department of Condensed Matter Physics, Faculty of Science, Masaryk University, Kotlářská 2, 61137 Brno, Czech Republic — [3]Institute of Physics CAS, Cukrovarnická 10, Praha 6, 162 00, Czech Republic — [4]Central European Institute of Technology, Brno University of Technology, Technická 10, 61600 Brno, Czech Republic

We study the polarization response of the emission from type-II GaAsSb capped InAs quantum dots. We theoretically predict the polarization anisotropy of the emission from this system, experimentally verify it by polarization resolved photoluminescence measurements on samples with the type-II confinement, and show that the polarization anisotropy might be utilized to find the vertical position of the hole wavefunction, solving thus the long standing problem of this system. A proposition for usage in the information technology as a room temperature photonic gate operating at the communication wavelengths as well as a simple model to estimate the energy of fine-structure splitting for type-II GaAsSb capped InAs QDs are given.

HL 71.6 Thu 10:45 H15

Quenching the PL emission of GaN QDs by local FIB-implantation — •Charlotte Rothfuchs[1], Tristan Koppe[2], Nadezhda Kukharchyk[1], Hans-Werner Becker[3], Fabrice Semond[4], Mathieu Leroux[4], Sarah Blumenthal[5], Donat Josef As[5], Hans Hofsäss[2], Andreas D. Wieck[1], and Arne Ludwig[1] — [1]Angewandte Festkörperphysik, Ruhr-Universität Bochum, D-44780 Bochum — [2]II. Physikalisches Institut, Georg-August-Universität Göttingen, D-37077 Göttingen — [3]RUBION, Ruhr-Universität Bochum, D-44780 Bochum — [4]CNRS-CRHEA, F-06560 Valbonne — [5]Department Physik, Universität Paderborn, D-33098 Paderborn

Nowadays, there is an increasing interest in quantum communication technology. GaN QDs as single semiconductor photon sources could be key components for such applications. One possible pathway towards the realization is the post-selection of molecular beam epitaxy-grown QDs by focused ion beam (FIB) implantation. This approach aims for the disabling of all QDs around an intentional one, based on the creation of non-radiative defects in the irradiated regions. Here, we present an unprecedented study on the lattice disorders in the vicinity of both hexagonal and cubic self-assembled GaN/AlN QDs introduced by FIB implantation of gallium ions amongst others. The impact of the ion implantation is investigated by low-temperature and additional temperature-dependent PL measurements. We extend a simple model for the PL degradation of InAs QDs to describe the quenching of the PL emission in the GaN/AlN material system. In particular, the quantum confined Stark effect in the hexagonal QDs is taken into account.

30 min. Coffee Break

HL 71.7 Thu 11:30 H15

Optical investigation of surface Fermi level-pinning in high-periodicity InGaAs nanowire arrays — •Maximilian Sonner, Maximilian Speckbacher, Julian Treu, Stefanie Mörkötter, Kai Saller, Hubert Riedl, Gerhard Abstreiter, Jonathan Finley, and Gregor Koblmüller — Walter Schottky Institut and Physik Department, Tu München, Garching, Germany

Optical investigations of surface Fermi level pinning related effects in InGaAs nanowires (NWs), site-selectively grown by molecular beam epitaxy (MBE) directly on Si (111) substrates, were performed using micro-photoluminescence spectroscopy (PL). In particular, we show that due to the large surface to volume ratio high densities of surface states can lead to pronounced Fermi level pinning and non-radiative recombination, limiting the radiative efficiency of the as-grown NWs. To study these effects in more detail, we provide systematic studies of (i) the diameter dependency and (ii) the InGaAs composition by correlating the luminescence properties in as-grown NWs with NWs passivated by hydrofluoric acid. Power- and temperature-dependent studies show two dominating recombination mechanisms present for NW PL emission: spatially indirect recombination via surface states for small diameters and bulk-like, excitonic transition from WZ/ZB stacking faults [1]. Correlating these results with structural analysis and a tuned carrier concentration via doping experiments will allow further new insights. [1] M. Speckbacher, et al., in preparation (2015)

HL 71.8 Thu 11:45 H15

Spin-lattice relaxation time of InGaAs quantum dots — •Daniel A. Lübke[1], Evgeny A. Zhukov[1], Alex Greilich[1], Erik Kirstein[1], Fabian Heisterkamp[1], Tomasz Kazimierczuk[1], Vladimir L. Korenev[1,2], Dirk Reuter[3], Andreas D. Wieck[3], Dmitri R. Yakovlev[1,2], and Manfred Bayer[1,2] — [1]Experimentelle Physik 2, Technische Universität Dortmund, 44221 Dortmund, Germany — [2]Ioffe Institute, Russian Academy of Sciences, 194021 St. Petersburg, Russia — [3]Angewandte Festkörperphysik, Ruhr-Universität Bochum, 44780 Bochum, Germany

We demonstrate measurements of the spin relaxation time (T_1) of resident electrons and holes in ensembles of InGaAs quantum dots. These measurements are done using a new method exploiting the spin inertia, based on the pump-probe type of measurements. Here the helicity of the pump laser is switched between both circular polarizations with variable frequency, at fixed pump-probe delay. At low frequencies of modulation, the created spin polarization is able to reach its steady state value, the maximal signal. If the pump helicity changes faster, so that the spin polarization cannot reach its steady state, it results in a decreased signal. We use this technique to evaluate the T_1 time in dependence on the longitudinal magnetic field in the range of $\pm 300\,\mathrm{mT}$.

HL 71.9 Thu 12:00 H15

Decay and persistance of spatial coherence in laterally spaced quantum dots — •Pawel Karwat[1], Tilmann Kuhn[2], and Pawel Machnikowski[1] — [1]Department of Theoretical Physics, Wroclaw University of Technology, Wybrzeze Wyspianskiego 27, 50-

370 Wroclaw, Poland — [2]Institut für Festkörpertheorie, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Strasse 10, 48149 Münster, Germany

Some experiments show that collective emission effects [1] play a role in the optical response of systems consisting two (or more) Quantum Dots (QDs), which suggests that they cannot be treated as ensembles of independent emitters. One of the interesting features observed in the experiment is the difference between the time resolved emission under quasi-resonant (optical transition to higher confined shells) and non-resonant (transition to wetting layer or bulk states) excitation. This suggests that spatial coherence, which is lost during carrier capture to the QDs, must be to some extent conserved during relaxation between confined states. In this contribution, we take into consideration the realistic system consisting of two horizontally placed InGaAs QDs, coupled not only to the acoustic phonon reservoir, but also to optical phonons. Using the method of collective modes, we study theoretically the relaxation of polarons in the system. In particular, we investigate the impact of polaron effects into the evolution of spatial coherence. The model allows us to make simulations beyond the Markov limit (by using correlation expansion method).

[1] P. Karwat, P. Machnikowski, Phys. Rev. B 91, 125428 (2015).

HL 71.10 Thu 12:15 H15

Time-integrated and time-resolved luminescence studies of carbon nanodots — •Angelina Vogt[1], Ksenija Sergeeva[1], Frank Dissinger[2], Sebastian Resch[2], Siegfried Waldvogel[2], and Tobias Voss[1] — [1]Institute of Semiconductor Technology and LENA, TU Braunschweig — [2]Institute of Organic Chemistry, Johannes Gutenberg University Mainz

Strongly luminescent and environmentally friendly carbon nanodots (C-dots) with diameters below 10 nm offer a great potential for optimized color conversion in LED displays and selective gas detection in sensing devices. Low toxicity, biocompatibility, excellent chemical and photo stability, inexpensive large-scale fabrication schemes and tunable photoluminescence (PL) emission are among their outstanding properties. Here, we study the luminescence properties of C-dots dissolved in distilled water for different concentrations of the C-dots, different excitation wavelengths and as a function of the laser power. The C-dots were hydrothermally synthesized and measured in the as-grown or a reduced state. In addition, we performed time-resolved studies of the luminescence dynamics with a femtosecond laser system to obtain a better understanding of the excitation and relaxation pathways of the photo-excited electrons, which is still controversially discussed in literature. The results show a luminescence decay time of several nanoseconds with a slightly faster decay on the high energy side of the PL emission. These results are analyzed with a model which takes into account electronic states of different sp2-hybridized carbon molecules which are believed to form the core of the C-dots.

HL 71.11 Thu 12:30 H15

Optical and electrical characterization of single AlGaN/GaN nanowire heterostructures — •Jan Müssener, Pascal Hille, Marius Günther, Daniel Stock, Markus Schäfer, Jörg Schörmann, Jörg Teubert, and Martin Eickhoff — I. Physikalisches Institut, Justus-Liebig-Universität Gießen, 35392 Gießen, Germany

We report on the photoluminescence (PL) characterization of single GaN nanowires (NWs) with embedded AlGaN/GaN heterostructures under application of an external electric field. Group III-nitrides exhibit strong internal polarization-induced electric fields which influence the optical properties via the quantum confined Stark effect (QCSE). Here we present a controlled modification of the internal fields via externally applied axial voltage on a single NW basis. The NWs were grown by plasma assisted MBE and consist of a single nanodisc (ND) embedded in AlGaN barriers. Single NWs were isolated for μ-PL measurements and electrical contacts for bias application were formed using electron beam lithography. The external electric field leads to a suppression or an enhancement of the QCSE which allows for determining the direction (polarity) and magnitude of the internal field. We also report on analogous measurements on 40-fold AlN/GaN heterostructures embedded in GaN NWs. Their complex bandprofile gives rise to numerous contributions in the PL spectrum originating from direct and indirect ND transition or 2DEG states. As each transition exhibits specific and distinct behavior under external electric field, bias-depended μ-PL allows the assignment of different recombination paths.

HL 71.12 Thu 12:45 H15

Characterization of nanocrystalline Si/SiC layers through optical measurements and simulations — •Johannes Hofmann, Charlotte Weiss, and Stefan Janz — Fraunhofer Institute for Solar Energy Systems, Heidenhofstraße 2, 79110 Freiburg, Germany

Silicon (Si) nanocrystal materials are subject to intense research concerning their application in Si-based tandem solar cells, since exploiting finite size effects in the Si nanostructures allows for modifying band structure properties and thus tailoring absorption characteristics.

Annealing of sub-micrometer amorphous-Si_xC_{1-x}:H layers ($x > 0.5$) deposited by plasma-enhanced chemical vapor deposition yields layers comprising a silicon carbide (SiC) matrix and therein embedded Si nanoclusters with a characteristic size of a few nanometers. For this work we investigate the optical properties of such layers by spectral ellipsometry, spectrophotometry measurements as well as photoluminescence measurements; structural characterization (X-ray diffraction, Fourier transform infrared spectroscopy) is also performed. Thickness variation sample series are analyzed by means of model based spectrum simulation and subsequent regression analysis. Scanning electron microscopy cross section images serve as references for thickness determination. Consequently, an optical thickness measuring method for annealed layers depending on their composition is provided. It is furthermore aimed at detecting the contribution of finite size effects in Si nanocrystals to the optical properties of the layers.

HL 72: Focus Session: Functionalization of Semiconductors I

Kerstin Volz, Sangam Chatterjee (Universtität Marburg), Michael Dürr (Universtität Giessen)

Time: Thursday 9:30–12:45 Location: H16

Invited Talk HL 72.1 Thu 9:30 H16

Group IV alloys: New tricks with Silicon — •Detlev Grützmacher — Peter Grünberg Institute - 9 and JARA-FIT, Forschungszentrum Jülich, 52425 Jülich, Germany

Group IV alloys, namely semiconductor alloys composed from C, Si, Ge and Sn offer new routes for band engineering on Si. In particular GeSn alloys have been predicted to have a fundamental direct band gap more than 30 years ago. Using reactive gas source epitaxy (RGSE) finally the limitations due to Sn precipitation and low solubility of Sn in Ge have been overcome and prestine crystal quality is achieved. Optically pumped lasers using various geometries have been fabricated from GeSn alloys with Sn concentrations up to 14.5%. Light emitting diodes (LED)working at room temperature have been realised using p- and n-type doped GeSn layers. Additionally, hetero- and multiple quantum well structures including SiGeSn, GeSn and strained Ge layers have been deposited and employed for LEDs. Moreover, the low effective mass of electron and holes in GeSn alloys and accordingly their predicted high mobility and carrier injection velocity makes these alloys interesting candidates for ultra low power devices. The potential of group IV alloys as a platform for electronic-photonic integrated circuitry is discussed.

HL 72.2 Thu 10:00 H16

MOVPE growth studies of Ga(PBi) on GaP and on GaP/Si — •Lukas Nattermann, Nikolai Knaub, Andreas Beyer, Wolfgang Stolz, and Kerstin Volz — Materials Sciences Center and Faculty of Physics, Philipps-Universität Marburg, Germany

Dilute bismide containing materials can play an important role in addressing the issue of finding new highly efficient lasers. In the last few years a growing body of literature has emerged, especially on the growth and characterization of Ga(AsBi) on GaAs. The growth on GaP makes achieving a direct band gap on Si possible by alloying Bi and N. In this work we will present the first Ga(PBi) structures grown with metal organic vapour phase epitaxy on GaP and on GaP on Si. By careful characterization with high resolution X-ray diffraction, atomic force microscopy, secondary ion mass spectrometry, photoluminescence

spectroscopy and scanning transmission electron microscopy, we will show that we have achieved high quality Ga(PBi) with Bi fractions up to 8%. Carbon incorporation due to low temperature growth as well as results from optical measurements will be discussed.

Acknowledgements: We gratefully acknowledge support from German Science Foundation (DFG) in the framework of the RTG1782 "Functionalization of Semiconductors".

HL 72.3 Thu 10:15 H16

X-ray Fluorescence of individual GaAs/InGaAs/GaAs core-shell nanowires grown by molecular beam epitaxy on silicon (111) — •Ali Al Hassan[1], Hanno Küpers[2], Ryan B. Lewis[2], Danial Bahrami[1], Abbes Tahraoui[2], Lutz Geelhaar[2], and Ullrich Pietsch[1] — [1]Naturwissenschaftlich-Technische Fakultät der Universität Siegen, 57068 Siegen, Germany — [2]Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5-7, 10117 Berlin, Germany

The growth of GaAs/In(x)Ga(1-x)As/GaAs core-shell nanowires (NWs) on silicon is a challenging route to combine optoelectronics with the silicon technology. Due to the different lattice parameters, growth of the InGaAs shell onto the NW core side plane is affected by epitaxial strain. X-ray diffraction (XRD) measurements taken on NW ensembles with momentum transfer perpendicular to the NW axis show separated Bragg peaks for core and shell materials. We probed the spatial homogeneity of the Indium distribution in the shell layers of individual core-shell NWs by means of X-ray fluorescence (XRF) analysis using a 50nm x 50nm sized white x-ray beam. For low indium contents within the InGaAs layer (nominal values of 15% and 25%), the Indium distribution within the six side facets is almost homogeneous. On the other hand, NWs with 60% of indium show randomly distributed indium-rich aggregates at the core circumference. The result are compared with XRD and SEM measurements.

Invited Talk HL 72.4 Thu 10:30 H16

SiGe heterostructures for photonics interconnects — •Giovanni Isella[1], Jacopo Frigerio[1], Andrea Ballabio[1], Daniel Chrastina[1], Vladyslav Vakarin[2], Papichaya Chaisakul[2], Laurent Vivien[2], and Delphine Marris-Morini[2] — [1]L-NESS, Dipartimento di Fisica, Politecnico di Milano, Polo di Como, Via Anzani 42, I 22100 Como, Italy — [2]IEF, Univ. Paris-Sud, CNRS, Univ. Paris-Saclay, UMR 8622, Bât. 220, 91405 Orsay Cedex, France

Over the last years Ge/SiGe multiple quantum wells (MQW) have received a great attention in the context of silicon photonics for the realization of efficient electro-absorption modulators based on the quantum confined Stark effect. At present day, one of the main challenges toward the integration of Ge/SiGe MQW modulators is their coupling with Si-compatible passive optical components such as waveguides. In particular, the integration with silicon waveguides is very difficult due to the presence of a thick SiGe layer which act as a virtual substrate (VS) for the MQW stack. We demonstrate that the VS can be used as a low loss optical waveguide by choosing a suitable compositional mismatch with respect to the MQW stack. A photonic interconnection made by a Ge/SiGe MQW modulator connected to a Ge/SiGe MQW photodetector through a SiGe waveguide has been fabricated and tested in order to demonstrate the great potential of this approach. More complex SiGe heterostructures, such as coupled QWs can be employed to attain efficient phase modulation. Moreover the building blokcs required for the fabrication of passive waveguide devices such as ring-resonators and optical filters can also be implemented in a SiGe material platform.

30 min. Coffee Break

HL 72.5 Thu 11:30 H16

III/V on Si by selective area growth for optoelectronics — •Bernardette Kunert, Weiming Guo, Yves Mols, Robert Langer, and Kathy Barla — Imec, Kapeldreef 75, B-3001 Leuven, Belgium

III/V compound materials and hetero-structures are well established in conventional optoelectronic applications due to their direct band gap structure. However, in the field of Silicon Photonics the successful integration of a laser diode with sufficient life time is still unsolved. The monolithic growth of high quality III/V materials on Si substrate would open up a huge field of applications, combining the mature functionalities of Si microelectronics with the excellent optoelectronic properties of III/V hetero-structures. But the lattice mismatch between most interesting III/V candidates and Si initiates the formation of misfit and threading dislocation defects. The selective area growth of III/V materials on patterned Si wafer is a novel integration approach to achieve a low defect density in the active III/V layers. A high aspect ratio in patterned trenches leads to an efficient trapping of defects in the bottom of the trench whereas the top region has a high crystal quality (aspect ratio trapping (ART)). This presentation is an introduction to selective growth of III/V materials on patterned 300mm Si wafers by metal organic vapour phase epitaxy (MOVPE). A new approach to realize a III/V laser diode on patterned Si substrates will be discussed based on first achieved results.

HL 72.6 Thu 12:00 H16

Quantitative investigation of high resolution HAADF STEM images of Ga(NAsP) laser structures — •Lennart Duschek, Tatjana Wegele, Andreas Beyer, Wolfgang Stolz, and Kerstin Volz — Material Sciences Center and Faculty of Physics, Philipps-Universität Marburg, Germany

Growing suitable III/V laser structures for optical data transmission on silicon substrate is a highly focused goal to achieve the integration of optics on electronic devices. The quaternary material system Ga(NAsP) is a promising candidate because it can be grown lattice-matched on silicon substrate and is a direct bandgap semiconductor. Due to its metastability, Ga(NAsP) has to be grown at rather low temperatures, i.e. 575°C. Post- growth thermal annealing allows the reduction of certain types of structural defects and thus improves the optical properties. Annealing at high temperatures e.g. 975°C can cause changes in the structure of the material [1]. This contribution will show high resolution scanning transmission electron microscopy images (STEM) of Ga(NAsP) with different Nitrogen and Phosphorous concentration, recorded at varied detector regions, collecting electrons scattered in different angles. Furthermore simulation results of these given structures will be shown and discussed in comparison to the experimental images. Acknowledgements: We gratefully acknowledge support from German Science Foundation (DFG) in the framework of the RTG1782 "Functionalization of Semiconductors".

[1]*S. Gies et al., J. Cryst. Growth, vol. 402, pp. 169*174, Sep. 2014.

HL 72.7 Thu 12:15 H16

Identification of anti-phase boundaries on a GaP/Si(001) cross-sectional surface — Christopher Prohl[1], Henning Döscher[2], Peter Kleinschmidt[2], Thomas Hannappel[2], and •Andrea Lenz[1] — [1]Technische Universität Berlin, Institut für Festkörperphysik, 10623 Berlin, Germany — [2]Helmholtz Center Berlin for Materials and Energy, 14109 Berlin, Germany

GaP-based materials are of high interest for realization of epitaxial integration of III-V layers for optoelectronics on Si(001) substrates due to the small lattice mismatch of GaP compared to Si. However, the growth of polar GaP on non-polar Si substrates leads to anti-phase domains accompanied with anti-phase boundaries (APBs), which are charged structural defects, reducing the device performance. Here, we present a cross-sectional scanning tunneling microscopy (XSTM) investigation of APBs at an epitaxially grown GaP/Si(001) interface. The APB can be identified by a brighter contrast and by surface step edges starting/ending at the position of an APB. The specific image contrast mechanisms of APBs oriented along different directions are discussed in detail. On the atomic scale the change of the atomic position of P and Ga atoms along growth direction is directly observed, in agreement with the structure model of APBs in the GaP lattice.
This work was supported by the DFG, project LE 3317/1-1.

HL 72.8 Thu 12:30 H16

Gain Spectroscopy on Ga(N,As,P)/(B,Ga)(As,P) Heterostructures — •Florian Dobener[1], Peter Ludewig[2], Kerstin Volz[1], Wolfgang Stolz[1,2], and Sangam Chatterjee[1] — [1]Faculty of Physics and Materials Science Center, Philipps-Universität Marburg, D-35032 Marburg, Germany — [2]$NAsP_{III/V}$ GmbH, Am Knechtsacker 19, D-35041 Marburg, Germany

The realization of monolithically integrated on-chip laser sources for optical data transmission remains one of the major goals of optoelectronic integration nowadays. The quaternary III-V material system Ga(N,As,P) promises to fulfil this task as composition variations allow both, bandgap engineering and tuning of the lattice constant through the control of nitrogen and phosphorous incorporation, potentially covering the near-infrared regime as well as the datacom wavelength.

Here, we investigate two series of Ga(N,As,P) multiple quantum well samples grown by metal-organic vapour-phase epitaxy. Either the substrate temperature or the chemical composition was systematically varied. Room temperature optical gain measurements by the variable stripe-length method show a maximum modal gain of about 100 cm^{-1} for the best samples, helping to identify the optimum growth conditions according to the amplification performance.

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

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

HL 73.1 Thu 9:30 H17

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

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

HL 73.2 Thu 9:45 H17

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

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

HL 73.3 Thu 10:00 H17

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

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

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

HL 73.4 Thu 10:15 H17

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

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

HL 73.5 Thu 10:30 H17

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

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

30 min. Coffee Break

HL 73.6 Thu 11:15 H17

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

Long regarded as a model system for studying insulator-to-metal transitions, vanadium dioxide features a rich phase diagram including at least three insulating states and one metallic state. Recently, the effects of strain on the transition temperature and nanoscale domain structure have been brought into focus. In this regard scattering-type near-field microscopy in the multi-terahertz regime [10-100 THz] has been proven to be a valuable tool for imaging the spatial heterogeneity of the transition. However, so far no time-resolved near-field studies have been undertaken. Here, we show the local pump-probe behavior of a single-crystalline vanadium dioxide nanobeam upon near-infrared photoexcitation. We probe with an ultrafast multi-terahertz pulse and see a modulation of the photoconductivity along the c_R-axis of the wire. This modulation qualitatively matches the different switching susceptibilities inside the wire upon thermal heating. We therefore propose that the switching susceptiblity is built into the wire already at room-temperature, most likely by strain.

HL 73.7 Thu 11:30 H17

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

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

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

HL 73.8 Thu 11:45 H17

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

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

HL 73.9 Thu 12:00 H17

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

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

HL 73.10 Thu 12:15 H17

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

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

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

HL 73.11 Thu 12:30 H17

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

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

HL 73.12 Thu 12:45 H17

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

The Anderson metal-insulator transition (MIT) has long been studied, but there is still no agreement on its critical exponent when comparing

experiments and theory. In this work, we employ *ab initio* methods to study the MIT that occurs in phosphorus-doped silicon (Si:P) when the density of the dopants is increased. Our strategy consists in using ONETEP, an implementation of linear scaling DFT, to model an effective potential between the P atoms, which is used in a Monte Carlo simulation to randomly distribute the impurities in the host material. We then combine these spatial configurations with the DFT data into an effective tight-binding Hamiltonian for a system of Si:P close to the critical concentration of the MIT. In this way we characterise the MIT in Si:P including the *ab initio* determined possible spatial correlations in P and the electronic interactions between the donated electrons. The extent of the resulting electronic states is characterised by the participation numbers and their scaling.

HL 73.13 Thu 13:00 H17

General DFT+NEGF approach for modeling metal-semiconductor interfaces — •Daniele Stradi[1], Umberto Martinez Pozzoni[2], Anders Blom[2], Mads Brandbyge[1], and Kurt Stokbro[2] — [1]DTU Nanotech, Technical University of Denmark, DK-2800 Kgs. Lyngby, Denmark — [2]QuantumWise A/S, Freubjergvej 3, Postbox 4, DK-2100 Copenhagen, Denmark

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

HL 74: Transport: Molecular Electronics and Photonics 1 (Joint session of CPP, DS, HL, MA, O and TT, organized by TT)

Time: Thursday 9:30–13:00 Location: H23

HL 74.1 Thu 9:30 H23

Pulling and Stretching a Molecular Wire to Tune its Conductance — •Gaël Reecht[1,4], Hervé Bulou[1], Fabrice Scheurer[1], Virginie Speisser[1], Fabrice Mathevet[2], César González[3], Yannick J. Dappe[3], and Guillaume Schull[1] — [1]IPCMS, Strasbourg, France — [2]Laboratoire de Chimie des Polymères, Paris, France — [3]CEA IRAMIS, Saclay, France — [4]Freie Universität Berlin, Berlin, Germany

Molecular junctions are perceived as the ultimate step toward the miniaturization of electronic components based on organic materials. Here, a low temperature scanning tunnelling microscope is used to lift a polythiophene wire from a Au(111) surface while measuring the current traversing the molecular junction. Conductance traces recorded during the lifting procedures reveal abrupt increases of the current intensity, which we associate to detachments of the wire subunits from the surface, in apparent contradiction with the expected exponential decrease of the conductance with wire length. With, ab initio simulations we reproduce the experimental data and demonstrate that this unexpected behavior is due to release of mechanical stress in the wire. Therefore, with the high control ability of the STM, by stretching the suspended molecular wire, we are able to tune its conductance properties.

HL 74.2 Thu 9:45 H23

STM-induced luminescence of single molecule junction — •Michael Chong[1], Gael Reecht[1], Hervé Bulou[1], Alex Boeglin[1], Fabrice Mathevet[2], Fabrice Scheurer[1], and Guillaume Schull[1] — [1]Institut de Physique et Chimie des Matériaux de Strasbourg - CNRS - France — [2]Laboratoire de Chimie des Polymères - CNRS - Université Pierre et Marie Curie, Paris, France

Electroluminescence of a single molecule can be induced by means of scanning tunneling microscopy. When a molecule is placed between two metallic electrodes it is necessary to decouple it using thin insulating layers in order to measure its intrinsic luminescence. A direct contact with the electrodes (tip and substrate), necessary if we envision to build single molecule electronic devices, results in quenching or broadening of the fluorescence of the molecule. We use on-surface polymerization to embed a cromphore molecule in a molecular chain. The STM tip is then used to lift the chain in order to decouple the cromophore from the surface yet mantaining a circuit like configuration trough the molecular chain. The current generated by applying a bias to the electrodes excites the cromophore that then exhibits narrow line luminescence and vibronic peaks allowing chemical identification the emitting unit.

Moreover we demonstrate that this configuration allows to control the lifetime of the excited state of the emitting molecule by two orders of magnitude by changing the coupling of the single molecle with the substrate adjusting the tip-sample separation. This system might open the way to electro-plasmonic devices at the single molecule level.

HL 74.3 Thu 10:00 H23

Effects of spin-orbit coupling and many-body correlations in STM transport through copper phthalocyanine — Benjamin Siegert, •Andrea Donarini, and Milena Grifoni — Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

The interplay of exchange correlations and spin-orbit interaction (SOI) on the many-body spectrum of a copper phtalocyanine (CuPc) molecule and their signatures in transport are investigated. We first derive a minimal model Hamiltonian in a basis of frontier orbitals which is able to reproduce experimentally observed singlet-triplet splittings; in a second step SOI effects are included perturbatively. Major consequences of the SOI are the splitting of former degenerate levels and a sizable magnetic anisotropy, which can be captured by an effective low-energy spin Hamiltonian. We show that STM-based magnetoconductance measurements can yield clear signatures of both these SOI induced effects.

HL 74.4 Thu 10:15 H23

Conductance trend in linear oligoacenes controlled by quantum size-effects — •Richard Korytar[1], Tamar Yelin[2], Nirit Sukenik[2], Ran Vardimon[2], Bharat Kumar[3], Colin Nuckolls[3], Oren Tal[2], and Ferdinand Evers[1] — [1]Institute of Theoretical Physics, University of Regensburg, Germany — [2]Chemical Physics Department, Weizmann Institute of Science, Rehovot, Israel — [3]Department of Chemistry, Columbia University, New York, United States

In conventional electronics, the conductance of a wire decreases with length according to Ohm's law. In molecular electronics, quantum effects lead to a richer phenomenology. Oligoacenes are organic molecules which consist of (linearly) fused benzene rings. Recently, Yelin et al. [submitted] studied conductance of oligoacenes directly coupled to Ag leads and found increase of conductance with molecular length.

I will show that transport through oligoacenes is governed by a quantum size effect which controls the alignment and width of the lowest unoccupied molecular orbital. These ideas will be supported by first-principles transport calculations using density-functional theory.

Linear oligoacenes are one of the simplest realizations of zig-zag terminated graphene nano-ribbons. In the long-wire limit, I will demonstrate that the conductance as a function of the molecular length shows surprising oscillations with period of approx. 11 rings [1].

[1] R. Korytár, D. Xenioti, P. Schmitteckert, M. Alouani, and F. Evers, Nature Communications **5**, 5000 (2014).

HL 74.5 Thu 10:30 H23

Investigation of charge transfer processes in single crystals based on π-conjugated molecules — •Antonia Morherr[1], Alisa Chernenkaya[2], Sebastian Witt[1], Katerina Medjanik[3], Michael Bolte[1], Martin Baumgarten[4], Harald O. Jeschke[1], Roser Valentí[1], and Cornelius Krellner[1] — [1]Goethe-Universität Frankfurt, 60438 Frankfurt a. M., Germany — [2]Johannes Gutenberg-Universität, 55099 Mainz, Germany — [3]Lund University, MAX-lab, 22100 Lund, Sweden — [4]MPI für Polymerforschung, 55021 Mainz, Germany

Designing new charge transfer (CT) materials for tuning the physical properties ranging from metallicity over superconductivity to Mott insulators and the understanding of mechanisms of CT is of great interest [1]. New CT crystals of π-conjugated molecules as donors can be obtained by physical vapor transport (PVT) [2]. (Fluorinated) tetracyanoquinodimethane (TCNQ-F_x, x=0, 2, 4) was used as acceptor material to grow different CT salts. The crystal structure was detected by X-ray diffraction. Further spectroscopic measurements as infrared and NEXAFS measurements were applied on these single crystals to investigate the CT process. The analysis of N1s and F1s K-edge spectra shows changes for different acceptor strengths. Ab initio calculations for all compounds underline these results. This systematic investigation of CT materials helps to understand the CT process in more detail.

[1] N. Toyota, M. Lang, J. Müller, Low-Dimensional Molecular Metals, Springer-Verlag, Berlin, 2007
[2] B. Mahns et al., Cryst. Growth Des. **14**, 1338 (2014)

HL 74.6 Thu 10:45 H23

Single Molecule Junctions with Epitaxial Monolayer Graphene Electrodes — •Konrad Ullmann[1], Pedro B. Coto[2], Susanne Leitherer[2], Michael Thoss[2], and Heiko B. Weber[1] — [1]Lehrstuhl für Angewandte Physik und Interdisziplinäres Zentrum für Molekulare Materialien, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU) — [2]Institut für Theoretische Physik und Interdisziplinäres Zentrum für Molekulare Materialien, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)

To study transport through single molecules, a two dimensional, open-access testbed for individual molecules is desirable. Therefore we use epitaxial monolayer graphene to fabricate electrodes for single molecule junctions. With the help of a feedback-controlled electro-burning process nanometer sized gaps can be formed reproducibly. Using these electrodes, we studied transport through molecules with different anchor groups at low temperatures. Strong similarities in results obtained with the MCBJ-technique underline the high quality of our experimental data. For a fullerene-endcapped molecule we are able to assign features from the I-V characteristics to internal molecular degrees of freedom [1].

[1] K. Ullmann et al., Nano Lett. **15**, 3512 (2015)

HL 74.7 Thu 11:00 H23

Simulation of Electron Transport through Graphene-Molecule Junctions — •Susanne Leitherer[1], Uwe Frank[1], Konrad Ullmann[2], Pedro B. Coto[1], Heiko Weber[2], and Michael Thoss[1] — [1]Institute for Theoretical Physics and Interdisciplinary Center for Molecular Materials, University Erlangen-Nürnberg — [2]Chair of Applied Physics and Interdisciplinary Center for Molecular Materials, University Erlangen-Nürnberg

Charge transport in single-molecule junctions with graphene electrodes is investigated using a combination of density functional theory (DFT) electronic structure calculations and Landauer transport theory. In particular, we study covalently bonded molecule-graphene junctions as well as junctions, where the molecule is weakly bonded to graphene by van der Waals interaction [1]. Considering different examples for molecular bridges between graphene electrodes, we analyze the transmission probability and current-voltage characteristics. In junctions with zigzag terminated graphene electrodes, we find edge states, which can induce additional transport channels [2]. Furthermore, local conductance properties are investigated in the nanojunctions.

[1] K. Ullmann et al., Nano Lett. **15**, 3512 (2015)
[2] I. Pshenichnyuk et al., J. Phys. Chem. Lett. **5**, 809 (2013)

15 min. break

HL 74.8 Thu 11:30 H23

Electron transport through C_{20} molecular junction — •Shigeru Tsukamoto and Stefan Blügel — PGI-1/IAS-1, Forschungszentrum Jülich and JARA, Jülich, Germany

We present electron transport properties of C_{20} molecular junctions, which are evaluated within the framework of the density functional theory. The C_{20} molecular junctions employed in this work are composed of a pair of Al bulk electrodes and a single C_{20} molecule, which is known as the smallest fullerene molecule. The scattering wave functions of the molecular junctions are calculated by solving the Kohn-Sham equation by means of the over-bridging boundary matching method, which is based on the real-space finite-difference formalism. The transmission properties are extracted from the scattering wave functions and the electron transmissions are evaluated by the Landauer-Büttiker formula. The electron transmissions and the scattering wave functions are further analyzed by using the eigenchannel decomposition technique. As the result of the eigenchannel analysis, although the total transmission value is $\sim 3.0G_0$ at around the Fermi level, more than five transmission channels are found to contribute to the electron transport, and none of the eigenchannels are opened to 100%. From the spatial distributions of the eigenchannels, we can see that the HOMO states of C_{20} molecule, which are three-fold degenerated and occupied to one-third, mainly contribute to the transport. In addition, the LUMO state is also found to contribute as one of the eigenchannels at around the Fermi level. In the talk, we will present electron transport calculations with different molecular orientations.

HL 74.9 Thu 11:45 H23

Quantum interference effect transistor via "Kondo Blockade" in single molecule junctions — •Andrew Mitchell[1] and Jens Paaske[2] — [1]Institute for Theoretical Physics, Utrecht University, 3584 CE Utrecht, The Netherlands — [2]Niels Bohr Institute, University of Copenhagen, DK-2100 Copenhagen, Denmark

Single molecule junctions are basic building blocks of molecular electronics devices. The full power of these devices will be realized by exploiting inherent quantum mechanical effects. Two of the most striking quantum phenomena, with no classical analogue, are quantum interference (QI) due to competing electron transport pathways, and the Kondo effect (KE) due to entanglement and strong electronic interactions. Both QI and KE are widely observed in experiments. The description of QI accounts for the complexities of molecular structure, but is typically non-interacting. By contrast, the Anderson impurity model is usually used to describe interactions and the Kondo effect, but totally neglects molecular structure. In this talk I discuss the subtle interplay between QI and KE in a unified theory, showing that a novel gate-tunable "Kondo Blockade" regime can be exploited to realize an efficient quantum interference effect transistor.

HL 74.10 Thu 12:00 H23

Quantitative *ab initio* simulations of nanocarbon-metal extended contacts — •Artem Fediai[1,2], Dmitry Ryndyk[1,2], and Gianaurelio Cuniberti[1,2,3] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden — [2]Center for Advancing Electronics Dresden, TU Dresden — [3]Dresden Center for Computational Materials Science, TU Dresden, 01062 Dresden, Germany

Recently developed approach presented in [1] allows to get quantitative information about the resistance R_c, effective contact length L_c, and contacts resistance scaling $R_c(L_c)$ in different extended side contacts depending on the electrode material. We apply this approach to find a contact resistance of side CNT-metal contacts, transfer length in graphene-metal contacts and electronic properties of the diodes with CNT channel and asymmetric contacts (with the electrodes made of different metals). These kinds of *ab initio* simulations were previously impossible due to numerical intractability of the side contacts longer then several nanometers. Our approach explicitly uses extended contact model concept, enforced by modular approach. This allows us to overcome numerical problems and understand physical processes in extended contacts.

[1] A. Fediai, D.A. Ryndyk, G. Cuniberti, PRB **91**, 165404 (2015)

HL 74.11 Thu 12:15 H23

Molecular switches for dangling bond circuits — •Thomas Lehmann[1,2], Dmitry A. Ryndyk[1,2], and Gianaurelio Cuniberti[1,2] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, Germany — [2]Dresden Center for Computational Materials Science (DCMS), TU Dresden, Germany

On the road to atomic-scale electronic circuits, dangling bond wires are promising candidates. Dangling bonds are formed by selectively

removing hydrogen from a passivated silicon surface [1,2] and multiple dangling bonds in a row feature extended electronic states. Those quasi 1D surface structures can be used as atomic scale interconnects. In such circuits, molecules, which can controllably passivate or depassivate a dangling bond can provide logical inputs for constructing simple logic elements. In this talk, we present recent studies combining density-functional based approaches with Green function methods of a molecular switch for dangling bond wires on silicon.

[1] T. Hitosugi, T. Hashizume, S. Heike, S. Watanabe, Y.Wada, T. Hasegawa, K. Kitazawa, Jpn. J. Appl. Phys. **36**, L361 (1997)
[2] H. Kawai, F. Ample, Q. Wang, Y. K. Yeo, M. Saeys, C. Joachim, J. Phys. Condens. Matter **24**, 095011 (2012)

HL 74.12 Thu 12:30 H23

Switchable negative differential resistance induced by quantum interference effects in porphyrin-based molecular junctions — •Daijiro Nozaki[1], Lokamani Lokamani[2], Alejandro Santana-Bonilla[2], Arezoo Dianat[2], Rafael Gutierrez[2], Gianaurelio Cuniberti[2], and Wolf Gero Schmidt[1] — [1]Lehrstuhl für Theoretische Physik, Universität Paderborn, Paderborn, Germany — [2]Institute for Materials Science, TU Dresden, Dresden, Germany

Charge transport through a carbon-based molecular switch consisting of different tautomers of metal-free porphyrin embedded between graphene nanoribbons is studied by combining electronic structure calculations and nonequilibrium Green's function formalism. Different low-energy and low-bias features are revealed, including negative differential resistance (NDR) and antiresonances, both mediated by subtle quantum interference effects. Moreover, the molecular junctions can display moderate rectifying or nonlinear behavior depending on the position of the hydrogen atoms within the porphyrin core. We rationalize the mechanism leading to NDR and antiresonances by providing a detailed analysis of transmission pathways and frontier molecular orbital distribution.

[1] D. Nozaki, J. Phys. Chem. Lett. **6**, 3950 (2015).

HL 74.13 Thu 12:45 H23

Base alignment dependence on Seebeck coefficient of DNA: A diagrammatic non-equilibrium transport theory approach — •Yoshihiro Asai[1], Yueqi Li[2], Limin Xiang[2], Julio L. Palma[2], and Nongjian Tao[2] — [1]Research Center for Computational Design of Advanced Functional Materials, AIST, Central 2, Umezono 1-1-1, Tsukuba, Ibaraki 305-8568, Japan — [2]Center for Bioelectronics and Biosensors, Biodesign Institute, Arizona State University, Tempe, Arizona 85287-5801, USA

Theoretical calculation of temperature dependence of transport properties at finite bias voltage and/or at finite temperature gradient requires careful description of low energy excitations. Incorporation of phonon transport and its coupling to electron transport by no means should play a crucial role to describe the low energy physics. One of the authors succeeded to describe theoretically the temperature cross over behavior of the electric conductance found in the experiment of a long oligothiophene single molecular wires. The diagrammatic nonequilibrium transport theory is useful to describe the problem qualitatively. While the necessity of the non-perturbative approach to the problem is clear, it would be interesting to know how far we could go within the perturbative framework given that any reliable non-perturbative approach for the problem is not available at present. Here, we apply the theory to discuss the base alignment dependence of the Seebeck coefficient of DNA in the hopping temperature region. We will make comparative discussions on our theoretical results with our experimental ones.

HL 75: Organic Electronics and Photovoltaics II (Joint session of CPP, DS, HL and O, organized by CPP)

Time: Thursday 9:30–12:45 Location: H40

Invited Talk HL 75.1 Thu 9:30 H40

Patterned organic ferroelectric memory diodes by solution micromolding — •Paul Blom, Thomas Lenz, Simon Benneckendorf, Kamal Asadi, and Dago de Leeuw — Max Planck Institute for Polymer Research, Ackermannweg 10, Mainz, Germany, D-55128

Ferroelectric polymers are promising candidates for memory technology, since they provide two bistable non-volatile polarization states corresponding to a Boolean 1 and 0, which can repeatedly be switched by an external field. The most widely investigated organic ferroelectric is the copolymer of poly(vinylidene fluoride) and trifluoroethylene (P(VDF-TrFE)). However, implementation of ferroelectric capacitors into integrated circuits is hampered by the read-out of the information being destructive. This problem can be overcome by using phase separated blends of P(VDF-TrFE) with a semiconducting polymer. The bistable polarization state of the P(VDF-TrFE) yields the binary information that can be read-out non-destructively by the current through the semiconducting columns. Phase separation however is a random process that yields a spatially undefined microstructure. Here we use solution micromolding to obtain a linear grating of P(VDF-TrFE). he space in between the lines is backfilled with a semiconducting polymer, resulting in a binary array between two electrodes. The resulting ferroelectric diode can be programmed reversibly in a low resistive on-state and high resistive off-state. When the bias is turned off, the information is retained. The performance can be optimized by down scaling the lateral dimensions of the binary array.

HL 75.2 Thu 10:00 H40

A new Figure of Merit for Organic Solar Cells with Transport-limited Photocurrents — •Dieter Neher[1], Juliane Kniepert[1], Arik Elimelech[1], and L. Jan Anton Koster[2] — [1]University of Potsdam, Potsdam, Germany — [2]Zernike Institute for Advanced Materials, Groningen, The Netherlands

Organic semiconductors exhibit superior absorption properties but suffer from low mobilities. Organic solar cells, therefore, display non-ideal JV-curves. Here, we present a closed-form analytical expression for the JV-curves of organic solar cells, based on the model in reference [1]. The expression is able to reproduce simulated JV-curves for a wide range of mobilities, generation rates and recombination parameters. Most importantly, the model delivers a novel figure of merit α to express the balance between free charge recombination and extraction in low mobility photoactive materials. This figure of merit is shown to determine critical device parameters such as the apparent series resistance and the fill factor. We also find α to be related to the parameter θ as defined in reference [2], showing that the approaches published in [1] and [2] are closely related. With that, we can accurately reproduce the gradual decrease of the fill factor with increasing recombination coefficient, decreasing mobility and increasing thickness.

[1] U. Würfel, D. Neher, A. Spies, S. Albrecht, Nat Commun 2015, 6, 6951 [2] D. Bartesaghi et al., Nat Commun 2015, 6, 7083

HL 75.3 Thu 10:15 H40

Design Rules for Organic Donor-Acceptor Heterojunctions: Pathway for Charge Splitting and Detrapping — •Carl Poelking and Denis Andrienko — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Organic solar cells rely on the conversion of a Frenkel exciton into free charges via a charge-transfer state formed on a molecular donor-acceptor pair. These charge-transfer states are strongly bound by Coulomb interactions and yet efficiently converted into charge-separated states. A microscopic understanding of this process, though crucial to the functionality of any solar cell, has not yet been achieved. Here we show how long-range molecular order and interfacial mixing generate homogeneous electrostatic forces that can drive charge separation and prevent minority carrier trapping across a donor-acceptor interphase. Comparing a variety of small-molecule donor-fullerene combinations, we illustrate how tuning of molecular orientation and interfacial mixing leads to a trade-off between photovoltaic gap and charge-splitting and detrapping forces, with consequences for the design of efficient photovoltaic devices.

[1] J. Am. Chem. Soc., 2015, **137**, 6320-6326
[2] Nature Materials, 2015, **14**, 434-439

HL 75.4 Thu 10:30 H40

Investigation of the hybrid charge transfer state at ZnO/organic interfaces — •Fortunato Piersimoni[1], Stefan Zeiske[1], Johannes Benduhn[2], Raphael Schlesinger[3], Norbert Koch[3], Koen Vandewal[2], and Dieter Neher[1] — [1]Institute of Physics and Astronomy, University of Potsdam, Potsdam, Germany — [2]Institut für Angewandte Photophysik, Technische Universität Dresden, Dresden, Germany — [3]Institut für Physik & IRIS, Adlershof Humboldt-Universität zu Berlin, Berlin, Germany

This contribution aims to study the Charge Transfer States (CTS) in hybrid systems based upon organic small molecules and ZnO. Those systems were investigated by means of spectrally resolved electroluminescence (EL) and external quantum efficiency (EQE). The presence of Hybrid CTSs is proven by the appearance of a distinct peak in the EL and EQE spectra located below the energy gap of the molecules or ZnO. The energy gap (Egap) between the ZnO conduction band and the donor HOMO was tuned either by varying the ZnO work function through self-assembled monolayers of polar molecules, or by employing organic donors with different HOMO energy. The correspondence between the EL peak position and the Egap attributes this emission to radiative recombination between an electron on the ZnO and a hole on the organic material. Notably all samples displayed a linear relation between the maximum of the EL spectrum and the 2/3 power of the electric field F, in accordance to the confinement of the HCTS in a rectangular electrostatic potential well, implying a certain degree of delocalization perpendicularly to the donor/acceptor interface.

HL 75.5 Thu 10:45 H40

PBDT[2F]T: Insight into the Secrets of a Wide Band-Gap Polymer with 7% Power Conversion Efficiency — •Julien Gorenflot[1,2], Andreas Paulke[3], Fortunato Piersimoni[3], Federico Cruciani[2], Dieter Neher[3], Pierre M Beaujuge[2], and Frédéric Laquai[2] — [1]Max Planck Institut für Polymerforschung, Mainz, Germany — [2]Universität Potsdam, Potsdam, Germany — [3]King Abdullah University of Science and Technology (KAUST), Thuwal, Saudi Arabia

PBDT[2F]BT:fullerene blends exhibit performance up to 75% higher than the reference P3HT:PCBM solar cells [1]. Using femto- to microsecond transient absorption, we investigate the origin of those outstanding properties. We find that geminate recombination losses of photogenerated charge carriers are nearly absent in PBDT[2F]BT:fullerene blends. Field-dependent measurement as well as morphological and energy levels characterization reveal efficient and field-independent charge generation, enabling excellent short-circuit current and fill factor. Strikingly, this outstanding generation is achieved in spite of a rather low offset between the polymer's excitons and the blend's charge transfer state energy levels, which allows for an open circuit voltage as high as 0.9 V. Replacing the fluorine substituents by hydrogen in those polymers results in only moderate performances, thus highlighting the importance of molecular design. This is discussed in terms of energy levels and blends morphology.

[1] J. Wolf et al., Chem. Mater. 27, 2015

15 min. break

HL 75.6 Thu 11:15 H40

The Meaning of Charge Carrier Density in Charge Extraction Experiments — •Juliane Kniepert, Edgar Nandayapa, and Dieter Neher — University of Potsdam, Potsdam, Germany

Charge extraction experiments are a powerful tool to extract important information on the charge carrier dynamics, such as the effective charge carrier mobility and the order and coefficient of nongeminate recombination, from charge carrier densities under steady state conditions. However, it is often neglected that the extracted carrier density in these experiments is highly sensitive to the actual carrier distribution in the device, which can be very inhomogeneous due to high carrier injection at the contacts, imbalanced mobilities or fast recombination. This is particularly true for organic solar cells, which usually have thin active layers and low intrinsic carrier densities. These conditions may lead to an erroneous interpretation of the results. We show with numerical simulations and experiments how the extracted carrier density is influenced by intrinsic (mobility, recombination coefficient, injection barriers) and extrinsic (layer thickness, illumination, bias) parameters. From these results we deduce experimental conditions for which reliable values for the carrier density, mobility and recombination coefficient can be obtained.

HL 75.7 Thu 11:30 H40

Rapid non-geminate recombination in organic solar cells — •Jona Kurpiers[1], John Love[1], Christopher Proctor[2], Thuc-Quyen Nguyen[2], and Dieter Neher[1] — [1]Institute of Physics and Astronomy, Soft Matter Physics, University of Potsdam, Germany — [2]Department of Chemistry & Biochemistry, University of California, Santa Barbara, USA

In the last years a dramatic increases in the efficiency of solution processed bulk heterojunction (BHJ) solar cells have been reported. However, the fundamental processes involved in the conversion of absorbed photons to free charges are still not fully understood. In this work, we use time delayed collection field (TDCF) experiments with exceptionally high time resolution to investigate the charge carrier dynamics in polymer-fullerene and small molecule-fullerene systems. TDCF experiments reveal rapid non-geminate recombination on the 20 ns time-scale, even for charge carrier densities comparable to one sun illumination. This loss becomes significantly accelerated at higher pulse fluences for the polymer-fullerene device. To identify the reason for this rapid loss, the recombination dynamics were further investigated on devices with different thicknesses. It is concluded that the primary reason for the nongeminate loss observed at the short time scale in the polymer blend is recombination of charges close to the contacts. In the small-molecule system however, the loss mechanism differs completely. Specifically, we find a rapid filling of traps on short time scales. Our work shows evidence that these rapid loss channels are essential to understand and can dramatically affect device operation.

HL 75.8 Thu 11:45 H40

Temperature dependent competition between different recombination channels in organic heterojunction solar cells — •Theresa Linderl, Ulrich Hörmann, Sergej Beratz, Mark Gruber, Stefan Grob, Alexander Hofmann, and Wolfgang Brütting — Institute of Physics, University of Augsburg, 86135 Augsburg

A modification of the Shockley-Queisser theory is presented with a special focus on constellations, where a linear extrapolation of the temperature dependence of the open circuit voltage V_{OC} results in the optical gap of the absorber rather than in the intermolecular charge transfer (CT) gap. Depending on the electronic coupling strength between donor and acceptor molecules, either singlet or CT recombination is dominant in different temperature regimes. These regimes are separated by a transition temperature T_{tr} that is, in the case of small energy level offset and weak electronic coupling, around 300 K or even below. For α-sexithiophene (6T)/diindenoperylene (DIP) solar cells with elevated substrate temperature during 6T deposition the linear extrapolation of the temperature dependent V_{OC} yields a value of 2.07 eV, whereas the extrapolation for the device evaporated at room temperature results in a value of 1.90 eV. Heating the substrate during 6T deposition leads to a molecular configuration at the interface where the coupling between donor and acceptor molecules is strongly reduced compared to the device evaporated at room temperature. This results in a transition temperature well below room temperature which is confirmed by temperature dependent electroluminescence measurements.

HL 75.9 Thu 12:00 H40

Ambipolar Charge Transfer In Single-Wall Carbon Nanotube Based Bulk-Heterojunctions — •Michael Auth[1], Andreas Sperlich[1], Florian Späth[2], Tobias Hertel[2], and Vladimir Dyakonov[1,3] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg — [2]Institute of Physical and Theoretical Chemistry, Julius Maximilian University of Würzburg, — [3]Bayerisches Zentrum für Angewandte Energieforschung (ZAE Bayern), 97074 Würzburg

The exceptional electrical conductivity of Single-Wall Carbon Nanotubes (SWNT) makes them potentially interesting to improve charge transport in organic photovoltaics (OPV). Additionally, their near infrared absorption bands can improve the spectral response of conventional polymer-fullerene bulk-heterojunctions. Until now, only few OPV devices containing purified semiconducting SWNTs were reported regarding the charge transfer properties of solar cell absorbers. For this study we prepared highly purified semiconducting (6,5)-SWNT samples, which we investigated in combination with known OPV donors and acceptors, namely the fullerene acceptor $PC_{60}BM$ and the conjugated polymer P3HT. Using Electron Paramagnetic Resonance, we found specific signatures for charge carriers localized on either SWNTs, P3HT or $PC_{60}BM$ and revealed the potential ambipolarity of SWNTs, leading to either hole transfer from $PC_{60}BM$ or elec-

tron transfer from P3HT. Furthermore our measurements confirmed exceptional SWNT purity, with respect to doping, dangling bonds or catalyst residue. In conclusion, we see a high application potential of (6,5)-SWNTs in OPV and, generally, in optoelectronic devices.

HL 75.10 Thu 12:15 H40

Influence of the Heterojunction's Interface on the Dynamics of Separated Charges Recombination in Organic Photoactive Materials — •Julien Gorenflot[1,2], Niva Alina Ran[3], Mike Heiber[3], Guillermo Bazan[3,4], Thuc-Quyen Nguyen[3,4], and Frédéric Laquai[1,2] — [1]Max Planck Institut für Polymerforschung, Mainz, Germany — [2]King Abdullah University of Science and Technology (KAUST), Thuwal, Saudi Arabia — [3]University of California Santa Barbara, Santa Barbara, California, United States — [4]Faculty of Science King Abdulaziz University, Jeddah, Saudi Arabia

A recent study has indicated that the energetic density of shallow trap states, specifically at the interface between the electron donor and the electron acceptor, could be responsible for the apparent high recombination order observed in organic photoactive blends [1]. In order to elucidate this issue, we carried out investigations on a material system that allows for well-controlled donor/acceptor interactions. Films of the small-molecule donor, H1, can be processed such that H1 molecules are either stacking with their pi-face perpendicular or parallel to the substrate. By evaporating a layer of the acceptor molecule C60 on the films, we study the effect of molecular orientation at the donor/acceptor interface on charge recombination using transient absorption spectroscopy. We compare the two bilayer systems to a bulk heterojunction also using H1, which is expected to have a mixture of face-on and edge-on donor/acceptor interactions as well as a much larger interface area. [1] J. Gorenflot et al., J. Appl. Phys.115, 144502 (2014)

HL 75.11 Thu 12:30 H40

Resonant GISAXS on ternary thin film systems — •Mihael Coric[1], Nitin Saxena[2], Jan Wernecke[3], Stefanie Langner[3], Peter Müller-Buschbaum[2], Michael Krumrey[3], and Eva M. Herzig[1] — [1]Technische Universität München, Munich School of Engineering, 85748 Garching, Germany — [2]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — [3]Physikalisch-Technische Bundesanstalt (PTB), Abbestraße 2-12, 10587 Berlin, Germany

Using additives to influence the properties of a material is an extensively used method in material science. It is also an approach to achieve morphological control in binary thin film systems like in organic photovoltaic systems. If the third component is also a polymer the morphological characterization poses a challenge since the sophisticated thin film characterization methods like grazing incidence small angle x-ray scattering (GISAXS) carried out a high x-ray energies can only distinguish between different electron densities. Using x-ray energies near the absorption edges of certain elements contained in the polymers enables a much higher contrast between the different materials, increasing the distinguishability of the different components within the active film of the organic solar cell. However, it is also challenging to interpret the scattering data correctly since some approximations routinely carried out in the theory used for interpretation of hard x-rays are no longer valid. We show our systematic measurements at the sulphur and chlorine edge and explain the advantages we can take out of the measurements to analyze the morphology of this ternary thin film.

HL 76: Frontiers of Electronic Structure Theory: Focus on Topology and Transport IV

Time: Thursday 10:30–13:15 Location: H24

Topical Talk HL 76.1 Thu 10:30 H24

Transport phenomena in broken-symmetry metals: Geometry, topology, and beyond — •Ivo Souza — Universidad del País Vasco, San Sebastián, Spain

While topological quantization is usually associated with gapped systems – Chern insulators and topological insulators – it can also occur in broken-symmetry metals, where the Fermi surface (FS) consists of disjoint sheets: the Berry-curvature flux through each sheet is quantized, defining an integer Chern index. Using ferromagnetic bcc Fe as an example, I will describe how the FS Chern numbers are related to the chiral degeneracies ("Weyl points") in the bandstructure. When placed in a static magnetic field, a Weyl (semi)metal will display the chiral magnetic effect (CME), where an electric field pulse $\mathbf{E} \parallel \mathbf{B}$ drives a transient current $\mathbf{j} \parallel \mathbf{B}$. Weyl semimetals with broken inversion and mirror symmetries can also display a "gyrotropic magnetic effect" (GME), where an oscillating magnetic field drives a current and, conversely, an electric field induces a magnetization. The GME is the low-frequency limit of natural optical activity. It is governed by the intrinsic magnetic moment (orbital plus spin) of the Bloch electron on the FS, in much the same way that the anomalous Hall effect and CME are governed by the FS Berry curvature. Like the Berry curvature, the intrinsic magnetic moment should be regarded as a basic ingredient in the Fermi-liquid description of transport in broken symmetry metals.

Topical Talk HL 76.2 Thu 11:00 H24

Dirac Fermions in Antiferromagnetic Semimetal — •Peizhe Tang, Quan Zhou, Gang Xu, and Shou-Cheng Zhang — Department of Physics, McCullough Building, Stanford University, Stanford, California 94305-4045, USA

The analogues of elementary particles in condensed matter systems have been extensively searched for because of both scientific interests and technological applications. Recently massless Dirac fermions are found to emerge as low energy excitations in the materials named Dirac semimetals. The currently known Dirac semimetals are all nonmagnetic with both time-reversal symmetry T and inversion symmetry P. Here we show that Dirac fermions can exist in one type of antiferromagnetic systems, where T and P are broken but their combination PT is respected. We propose orthorhombic antiferromagnet CuMnAs as a candidate, analyze the robustness of the Dirac points with symmetry protections, and demonstrate its distinctive bulk dispersions as well as the corresponding surface states by ab initio calculations. Our results give a new routine towards the realization of Dirac materials, and provide a possible platform to study the interplay of Dirac-related physics and magnetism.

HL 76.3 Thu 11:30 H24

Spin Hall effect in non-collinear antiferromagnets Mn3X (X=Sn, Ge, Ga) — •Yang Zhang[1,3], Yan Sun[1], Claudia Felser[1], and Binghai Yan[1,2] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [2]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany — [3]Leibniz Institute for Solid State and Materials Research, 01069 Dresden, Germany

Recently, large anomalous Hall effect (AHE) was realized in non-collinear antiferromagnetic (AFM) compounds Mn3X (X=Sn, Ge, Ga). We have found that the nonzero Berry curvature – origin of the AHE observed – will lead to another topological effect, the spin Hall effect (SHE) in the titled compounds. We have systematically investigated the intrinsic SHE and revealed large spin Hall conductivity [~1000 ((*/e)*(S/cm)], which is comparable to that of the well-know SHE material Pt. Our work present a new family of AFM compounds for the room-temperature spintronic applications.

HL 76.4 Thu 11:45 H24

Electronic reconstruction and anomalous Hall conductivity in 3*d*-oxide honeycomb lattices within the corundum structure — •santu baidya and rossitza pentcheva — Fakultät für Physik and Center of Nanointegration (CENIDE), Universität Duisburg-Essen, 47057 Duisburg

The electronic structure of 3*d* transition metal oxide honeycomb layers confined in the corundum structure (α-Al_2O_3) along the [0001] direction is investigated using density functional theory including an on-site Coulomb term (GGA+U). While in some cases (e.g. $(M_2O_3)/(Al_2O_3)_5$, M=Fe, Co, V, Cr, Ni) the confined geometry preserves the magnetic and electronic ground state properties of the corresponding bulk corundum compound M_2O_3, strong deviations from the bulk behavior are observed in the case of Ti_2O_3 and Mn_2O_3 bilayers. Our results indicate a formation of a quasi two-dimensional electron gas with a vertical confinement of ∼5 Å for Ti_2O_3 and ∼8.5 Å for Mn_2O_3. As a function of lateral strain $(Ti_2O_3)/(Al_2O_3)_5$ undergoes a metal-to-insulator transition associated with a switching of orbital

polarization. In the metallic state the Dirac point can be tuned to the Fermi level by variation of the c/a ratio. Including spin-orbit coupling a finite anomalous Hall conductivity is observed in $(M_2O_3)/(Al_2O_3)_5$ (M=Ti, Mn).

HL 76.5 Thu 12:00 H24

Anomalous hall effect in triangular antiferromagnetic ordered structure — •Hao Yang[1], Sun Yan[2], Felser Claudia[2], Parkin Stuart[1], and Binghai Yan[2] — [1]Max Planck Institute of Microstructure Physics, 06120 Halle(Saale), Germany — [2]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany

The anomalous Hall effect (AHE), a fundamental transport phenomenon of electrons in solids, has been believed to appear in ferromagnetic materials. Very recently AHE is revealed in noncollinear antiferromagnetic compounds. In this work, we have systematically investigated the AHE in antiferromagnetic materials Mn3X (X=Ir, Ge, Sn, Ga), where noncollinear 120-degree type antiferromagnetic spin order exists in the quasi-layered lattice. Assisted by the symmetry analysis, we demonstrate the strong anisotropy of the intrinsic anomalous Hall conductivity that is determined by the Berry curvature in the band structure. Our work well interprets recent experiment observations and predicts novel antiferromagnetic material candidates for the spintronic application.

HL 76.6 Thu 12:15 H24

Anomalous Hall conductivity and orbital magnetization as local quantities — •Antimo Marrazzo[1] and Raffaele Resta[2] — [1]THEOS, EPF Lausanne, Switzerland — [2]Dipartimento di Fisica, Univ. Trieste, Italy

Anomalous Hall conductivity (AHC) and orbital magnetization (OM) are—from a theorist's viewpoint—closely related: both have an expression as **k**-space integrals of the appropriate geometrical quantity. The **k** space is an artificial construct: all bulk properties are embedded in the ground state density matrix in **r** space, independently of the boundary conditions. Is it possible to address AHC and OM as local properties, directly in **r** space? For insulators, two recent papers have proved that the answer is affirmative: both AHC (quantized in insulators) and OM can be evaluated from a local formula over bounded samples. A rationale can be found in the "nearsightedness" of the density matrix: but since this is *qualitatively* different in insulators and metals (exponential vs. power law) it is not obvious that the same successful approach can be extended to metals. Using model Hamiltonians, we have performed simulations over 2D bounded metallic flakes, where the T-invariance is broken in two alternative ways: either à la Haldane, or by a macroscopic **B** field. In both cases, our simulations show that the relevant quantity can be extracted from a knowledge of the electron distribution in the bulk region of the sample only. This looks counterintuitive because the OM of a magnetized sample owes to currents localized near its surface; but the key reason for the success of the local approach to AHC and OM is that the formulas are *not* based on currents.

HL 76.7 Thu 12:30 H24

Laser induced DC photocurrents in a Topological Insulator thin film — •Thomas Schumann[1], Nina Meyer[1], Gregor Mussler[4], Eva Schmoranzerová[2], Dagmar Butkovicova[2], Helena Reichlová[3], Lukas Braun[5], Christian Franz[6], Michael Czerner[6], Pertr Němec[2], Detlev Grützmacher[4], Tobias Kampfrath[5], Christian Heiliger[6], and Markus Münzenberg[1] — [1]IfP, EMA University Greifswald, Germany — [2]MFF, Charles University, Prague, Czech Republic — [3]FZU, Prague, Czech Republic — [4]PGI-9, Jülich, Germany — [5]FHI Berlin, Germany — [6]University of Gießen, Germany

Topological Insulators (TI) open up a new route to influence the transport of charge and spin in a surface film via spin-momentum locking [1,2]. It has been demonstrated experimentally [2] that illumination by circularly polarized light can result in excitation of a helicity-dependent photocurrent.We report our recent results on laser induced photocurrents in a terniary 3D TI thin film. The resulting photocurrents are classified after [1,2] and we show that there are at least two signals visible, for example in time dynamics, which behave different in the suggested parameters.

We acknowledge the funding of the DFG via the SPP 1666 Topological Insulators and the joint DAAD PPP Czech Republic project FemtomagTopo. [1]S.D.Ganichev,W.Prettl,J.Phys.: Condens. Matter 15 (2003) R935-R983

[2]J.W.McIver,D.Hsieh,H.Steinberg,P.Jarillo-Herrero and N.Gedik, Nature Nanotechnology 7, 96-100 (2012)

HL 76.8 Thu 12:45 H24

Robustness of exchange protocols of Majorana fermions in quantum wire networks — •Christian Tutschku[1], Rolf W. Reinthaler[1], Chao Lei[2], Allan H. MacDonald[2], and Ewelina M. Hankiewicz[1] — [1]Faculty of Physics and Astrophysics, University of Würzburg, Würzburg, Germany — [2]Department of Physics, University of Texas at Austin, USA

The interface between topological non-trivial, one-dimensional, spinless p-wave superconductors and the vacuum is connected to the appearance of Majorana edge-modes [1], whose non-trivial exchange statistics makes them promising candidates for topological quantum computation [2]. Via T-Bar structures build of 1D-nanowires we can manipulate and exchange the Majorana fermions by purely electrical means [3]. By applying a tight binding approach we solve the time dependent Bogoliubov-de Gennes equations for the Kitaev chain model [1] and also cure the problem of an appearing additional Majorana-boundstate located at the T-Bar crossing point for small lattice constants. Furthermore we analyze how the robustness of the exchange protocols is affected by non-adiabatic effects or by a finite overlap of the Majorana bound states.

We acknowledge financial support by the DFG within SFB 1170 ToCoTronics.

[1] A. Y. Kitaev, Physics-Uspekhi **44**, 131 (2001)
[2] D. A. Ivanov, PRL **86**, 268 (2001)
[3] J. Alicea et al., Nature Physics **7**, 412 (2011)

HL 76.9 Thu 13:00 H24

Unpaired Majorana modes in Josephson junctions arrays with gapless bulk excitations — •Manuel Pino Garcia — Department of Physics and Astronomy, Rutgers The State University of New Jersey, 136 Frelinghuysen rd, Piscataway, 08854 New Jersey, USA

The search for Majorana bound states in solid-state physics has been limited to materials which display a gap in their bulk spectrum. We will show that such unpaired states appear in certain quasi-one-dimensional Josephson junctions arrays with gapless bulk excitations. The bulk modes mediate a coupling between Majorana bound states via the Ruderman-Kittel-Yosida-Kasuya mechanism. As a consequence, the lowest energy doublet acquires a finite energy difference. For realistic set of parameters this energy splitting remains much smaller than the energy of the bulk eigenstates even for short chains of length L ~ 10. In this talk, we first explain the JJA system and how to model it with an Ising-like Hamiltonian. Then, a qualitative argument is employed to obtain the low-energy effective theory using unpaired Majorana modes. We will show numerical results which confirm the validity of this effective theory and discuss problems that may arise in the experimental realization of our proposal.

HL 77: Graphene III: Electronic Properties

Time: Thursday 10:30–12:45 Location: S053

HL 77.1 Thu 10:30 S053

PEEM of epitaxial graphene on silicon carbide — •Richard Hönig, Christoph Keutner, Cornelis Hilscher, Ulf Berges, and Carsten Westphal — Experimentelle Physik I, TU Dortmund, Otto-Hahn-Straße 4, 44227 Dortmund, Germany

Graphene is a promising candidate for two-dimensional electronic structures. Especially epitaxial graphene on silicon carbide (SiC) is in the focus of current studies, due to the well-established infrastructure for SiC in the semiconductor-industry.

We present photoemission electron microscopy (PEEM) studies of epitaxial graphene, grown by confinement controlled sublimation (CCS). This technique is a suitable tool for producing large areas of homogeneous graphene. The resulting flake-sizes of graphene ex-

ceed the resolution of scanning tunneling microscopy. However, the PEEM-technique provides a better suited resolution up to the mesoscopic scale. Hence, PEEM was chosen to study and characterize these graphene/SiC-samples.

Here, we will demonstrate the first characterization procedures and results. In the future, samples with an adequate amount of graphene will be used for further studies, including the real-time imaging of intercalation-processes.

HL 77.2 Thu 10:45 S053

Graphene growth on structured SiC — •Alexander Stöhr[1], Jens Baringhaus[2], Aleixei Zakharov[3], Christoph Tegenkamp[2], and Ulrich Starke[1] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart, Deutschland — [2]Leibniz-Universität Hannover, Hannover, Deutschland — [3]MAX IV Laboratory, Lund University, Lund, Schweden

Despite its missing band gap, graphene is reviewd as a potential successor of silicon for applications in logical devices. Nowadays, few techniques are available to introduce a band gap into the band structure of graphene. One of the most promising methods is the confinement of its charge carriers into quasi one-dimensional stripes, so called graphene nanoribbons. Unfortunately, the usual approach to structure graphene by lithography techniques leads to disorder and defects at the edges of the nanoribbons, which then dominat the electronic states of the ribbon. To circumvent this problem, we structure our SiC-crystal prior to the graphene growth. After the growth process a faceting of the sidewalls by 23-28° was observed by AFM. On those areas which are inclined towards the non-structured surface, diffraction spots and a π-band were observed in microscopic LEED and ARPES, respectively. Those experimental findings confirm the growth of ordered graphene on the facets.

HL 77.3 Thu 11:00 S053

A new candidate for silicon carbide (3x3) surface reconstruction — •Jan Kloppenburg[1,3], Lydia Nemec[2,3], Björn Lange[4], Matthias Scheffler[3], and Volker Blum[4] — [1]Université catholique de Louvain — [2]Technische Universität München — [3]FHI Berlin — [4]Duke University

Silicon carbide (SiC) is a primary substrate for high quality epitaxial graphene growth. Graphene growth on SiC(000-1) surface is significantly different from the well controlled monolayer graphene growth on the silicon face. On the carbon face, a (3x3) surface as a precursor phase precedes graphene growth changing the thermodynamics compared to the Si-face[1]. Despite more than a decade of research the precise atomic structure of the (3x3) surface reconstruction of SiC(000-1) is still not clear. Here, we employ an *ab initio* random structure search (AIRSS) based on van-der-Waals corrected PBE density functional theory (DFT) to identify the reconstruction in the C-rich range. Our search reveals a new lowest energy surface reconstruction model for the C-rich SiC(000-1) face that was not previously reported[2] and that would explain the very different graphitization behaviour compared to the Si-face. Simulated STM images are in excellent agreement with previously reported experimental findings[3,4].

[1] Nemec et al, *Phys. Rev. Lett.* **111**, 065502, 2013
[2] Nemec et al, *Phys. Rev. B* **91**, 161408, 2015
[3] Hiebel et al, *Phys. Rev. B* **80**, 235429, 2009
[4] Hiebel et al, *Phys. Rev. B* **45**, 154003, 2011

HL 77.4 Thu 11:15 S053

Characterisation of Graphene Electrodes — •Markus Manz[1], Martin Lottner[1], Martin Stutzmann[1], and Jose Garrido[1,2] — [1]Walter Schottky Institut, Technische Universität München, Garching, Germany — [2]Catalan Institute of Nanoscience and Nanotechnology, Barcelona, Spain

The biocompatibility and flexibility of graphene devices allow for long-term in vivo detection of action potentials [1]. Thus, graphene has a serious advantage over former approaches [2] using other materials, which are rigid or brittle. Furthermore, the transparency of graphene micro electrodes allows for simultaneous optical stimulation/imaging and electrical recording [1]. While graphene has a high in plane conductivity, the out of plane conductivity of undoped single layer graphene (SLG) is rather low. This is a major drawback for the detection of neurotransmitters through their respective redox reactions. Therefore, various methods have been developed to increase the out of plane conductivity and 'activate' [3] the SLG electrodes. We investigated two methods of graphene 'activation', namely ozonization and doping with nitric acid. We characterized the modified electrodes using cyclic voltammetry, impedance spectroscopy, and Raman spectroscopy. We then compared the sensitivity of the untreated and 'activated' electrodes towards the neurotransmitters norepinephrine and dopamine.

[1] Kuzum, D. et al., Nat. Commun. 5:5259doi: 10.1038/ncomms6259 (2014). [2] Kwon, K. Y. et al. in Biomedical Circuits and Systems Conference (BioCAS), 2012 IEEE 164-167 (2012). [3] Kasry, A. et al., ACS Nano 4, 3839-3844 (2010).

HL 77.5 Thu 11:30 S053

Ultraclean Freestanding Graphene by Pt-metal catalysis — •Jean-Nicolas Longchamp, Conrad Escher, and Hans-Werner Fink — Physics Department of the University of Zurich, Winterthurerstrasse 190, CH-8057 Zürich, Switzerland

When using graphene as a substrate in electron microscopy, the presence of residues is obstructive because the latter are often of the same size as the object under study. While the growth of defect-free single-layer graphene by means of chemical vapor deposition (CVD) is nowadays a routine procedure, easily accessible and reliable techniques to transfer graphene to different substrates in a clean manner are still lacking. We have discovered a method for preparing ultraclean freestanding graphene using the catalytic properties of platinum metals. Complete catalytic removal of a sacrificial PMMA layer only requires annealing in air at a temperature between 175°C and 350°C. Here, we will describe in detail the preparation process for obtaining ultraclean freestanding graphene by Pt-metal catalysis. The presentation of low-energy electron holography and TEM investigations will demonstrate that areas of ultraclean freestanding graphene as large as 2 microns square can now routinely be prepared.

HL 77.6 Thu 11:45 S053

Nano-scaled graphene solution-gated field-effect transistors — •Peter Knecht[1], Benno Martin Blaschke[1], Karolina Stoiber[1], Martin Letter[1], Simon Drieschner[1], and Jose Antonio Garrido[2] — [1]Walter Schottky Institut, TU München, Garching, Germany — [2]Catalan Institute of Nanoscience and Nanotechnology, Barcelona, Spain

Graphene solution-gated field-effect transistors (SGFETs) are a promising biosensing platform, due to their unique properties such as high charge carrier mobility, low electronic noise, good electrochemical performance and an excellent biocompatibility. The recording of cell action potentials using graphene SGFETs has already been demonstrated. However, the sensing area of several hundred square micrometer is not small enough to resolve potential changes on a subcellular level. In this work, we present the fabrication of nano-scaled graphene SGFETs where the transistor area is reduced to 0.01 square micrometer. The dependence of the transistor's transconductance and the electronic low frequency noise on size and shape of the sensing area is studied. In addition, we investigate if the reduced device size leads to a more pronounced dependence of the device's performance on the graphene quality. Finally, the recording of cell action potentials using the nano-scaled devices is demonstrated and compared to micro-scaled graphene SGFETs.

HL 77.7 Thu 12:00 S053

Graphene wrinkles: their conductivity, crystallinity, and reactivity — •Raul D. Rodriguez[1,2], Tao Zhang[3], Jana Kalbacova[1,2], Devang Parmar[1], Akhil Nair[1], Zoheb Khan[1], Mahfujur Rahaman[1], Ihsan Amin[2], Jacek Gasiorowski[1], Evgeniya Sheremet[1], Rainer Jordan[2], Michael Hietschold[1], and Dietrich R.T. Zahn[1,2] — [1]Institut für Physik, Technische Universität Chemnitz, Chemnitz 09107, Germany — [2]Center for Advancing Electronics Dresden (cfaed), Germany — [3]Professur für Makromolekulare Chemie, Department Chemie, Technische Universität Dresden, Mommsenstrasse 4, 01062 Dresden, Germany

Wrinkles appear to be unavoidable in graphene produced by chemical vapor deposition (CVD) on copper. Despite its generality, isolating the role of wrinkles on overall electrical conductivity, crystallinity, and chemical reactivity of CVD-grown graphene remains an open issue. We investigate the reactivity of basal planes and wrinkles in graphene with polystyrene bromide (PSBr) and correlate it with electrical conductivity, defect concentration, and doping with a special resolution from the micro- to the nano-scale. We show that wrinkles dominate the chemical reactivity of CVD graphene, and moreover, that doping with the same functionality can yield opposite electronic type to the basal plane regions (n- vs. p-type). These results expand our understanding of wrinkles in CVD graphene towards engineering for novel applications.

HL 77.8 Thu 12:15 S053

Conversion of pyrrolyl-thiophenol self-assembled monolayers (SAMs) into carbon nanomembranes (CNMs) and graphene — •Christof Neumann[1], Matthias Füser[2], Michael Mohn[3], Ute Kaiser[3], Andreas Terfort[2], and Andrey Turchanin[1] — [1]Institute of Physical Chemistry, Friedrich Schiller University Jena, 07743 Jena — [2]Institute of Inorganic and Analytical Chemistry, Goethe University Frankfurt, 60348 Frankfurt — [3]Electron Microscopy Group of Materials Science, Ulm University, 89081 Ulm

The conversion of aromatic self-assembled monolayers (SAMs) into carbon nanomembranes (CNMs) and graphene presents a promising pathway to the production of a broad variety of functional 2D materials [1]. The properties of these materials can be flexibly tuned via an appropriate choice of the molecular building units for SAMs. Here we investigate the conversion of 4-(1H-pyrrol-1-yl)thiophenol and 4-(2,5-dimethyl-1H-pyrrol-1-yl)thiophenol SAMs on polycrystalline copper foils into CNMs via the electron induced crosslinking. Furthermore, we study the pyrolytic transformation of these CNMs into graphene at temperatures up to 800 °C. We characterize these different conversion steps and the resulting physical and chemical properties of CNMs and graphene by a number of complementary experimental techniques including X-ray photoelectron and Raman spectroscopy, high-resolution transmission electron and helium ion microscopy as well as by electric transport measurements. [1] P. Angelova et al.,: A Universal Scheme to Convert Aromatic Molecular Monolayers into Functional Carbon Nanomembranes, ACS Nano 7, 6489 (2013)

HL 77.9 Thu 12:30 S053

Extracellular stimulation of electrogenic cells using graphene devices — •Karolina Stoiber[1], Martin Lottner[1], Markus Manz[1], Simon Drieschner[1], Benno Blaschke[1], Martin Stutzmann[1], and José A. Garrido[1,2] — [1]Walter Schottky Institut, Technische Universität München, Garching, Germany — [2]Catalan Institute of Nanoscience and Nanotechnology, Barcelona, Spain

Graphene is a highly conductive, chemically stable, flexible and biocompatible material. Therefore, Graphene microelectrode arrays (GMEAs) are a promising bio-sensing and cell stimulation platform in neural implants. In this work, the electrical stimulation of HEK293 and HL1 cells through extracellular voltage trains by GMEAs is presented. Further, the investigation of the biocompatibility of graphene foam and its capability for extracellular stimulation is discussed.

GMEAs with circular electrodes were fabricated using standard photo-lithography techniques. For the characterization of the devices Raman-spectroscopy and cyclic voltammetry were used. The cell membrane potential of HEK293 cells was monitored during extracellular stimulation via patch-clamping. HL1 cells, a cardiomyocyte-like cell line, were dyed with a calcium-sensitive fluorophore and the modulation of their firing frequency upon stimulation was recorded.

Graphene foam devices were fabricated as previously described. The devices were characterized electrochemically and their capability for extracellular stimulation of HL1 cells tested.

HL 78: 2D Materials beyond Graphene: Dynamics and Excitation

Time: Thursday 10:30–13:30 Location: S054

Invited Talk HL 78.1 Thu 10:30 S054

Spin- and Pseudospin-Polarized Excited States in bulk WSe_2 — Roman Bertoni[1], Christopher Nicholson[1], Lutz Waldecker[1], Michele Puppin[1], Claude Monney[2], Cephise Cacho[3], Hannes Huebener[4], Umberto De Giovannini[4], Angel Rubio[4], Martin Wolf[1], and •Ralph Ernstorfer[1] — [1]Fritz-Haber-Institut der MPG, Berlin, DE — [2]University of Zurich, Zurich, CH — [3]Rutherford Appleton Laboratory, Didcot, UK — [4]University of the Basque Country, San Sebastian, ES

The peculiar electronic structure of layered semiconducting transition metal dichalgogenides (TMDC) like WSe_2 gives rise to internal quantum degrees of freedom of the electrons in addition to the spin, namely valley and layer pseudospins. Employing XUV-based time- and angle-resolved photoemission spectroscopy (trARPES) with resonant excitation of excitonic transitions, we observe circular dichroism in the excited state population in the K valleys of the topmost trilayer of bulk WSe_2. Such spin-, valley and layer-polarized excitations are a manifestation of broken site symmetry in an inversion-symmetric crystal. The valley- and layer-resolved view on excited state dynamics provided by trARPES is complemented by the investigation of electron-lattice coupling in multilayer WSe_2 with femtosecond electron diffraction. Latter studies reveal the dynamics of global energy transfer from electronic to vibrational degrees of freedom in TMDCs subsequent to excitonic as well as interband excitation.

HL 78.2 Thu 11:00 S054

Exciton dynamics in two-dimensional materials with strong spin-orbit interaction: $MoSe_2$ versus WSe_2 — •Daniel Schmidt[1], Tillmann Godde[2], Johannes Schmutzler[1], Marc Assmann[1], Jörg Debus[1], Freddie Withers[3], Osvaldo Del Pozo-Zamudio[2], Konstantin S. Novoselov[3], Andre Geim[3], Manfred Bayer[1], and Alexander Tartakovskii[2] — [1]Experimentelle Physik 2, Technische Universität Dortmund, D-44221 Dortmund, Germany — [2]Department of Physics and Astronomy, University of Sheffield, Sheffield S3 7RH, UK — [3]School of Physics and Astronomy, University of Manchester, Oxford Road, Manchester M13 9PL, UK

Monolayers of semiconducting transition metal dichalcogenides such as MoS_2, WS_2, $MoSe_2$ and WSe_2 have attracted considerable attention following the discovery of the indirect-to-direct bandgap transition from bulk to monolayer material and the coupling of spin and valley degrees of freedom in atomically thin layers. An important characteristic of these compounds is the strong spin-orbit interaction, which leads to a splitting between dark and bright exciton sub-bands. A detailed understanding of dark and bright exciton dynamics and non-radiative processes is important for light emitting applications as has been demonstrated in other systems such as phosphorescent organic light emitting diodes. We measure time-integrated and -resolved PL in monolayers of $MoSe_2$ and WSe_2 in a wide range of temperatures from 10 to 300K and gain insights into the exciton and trion dynamics. Our study reveals similar carrier dynamics for both materials, whereas pronounced differences have been observed for the overall PL intensities.

HL 78.3 Thu 11:15 S054

Electron dynamics in eiptaxial single layer MoS_2 — •Antonija Grubisic-Cabo[1], Jill A. Miwa[1], Signe S. Gronborg[1], Jonathon M. Riley[2], Jens C. Johannsen[3], Cephise Cacho[4], Oliver Alexander[4], Richard T. Chapman[4], Emma Springate[4], Marco Grioni[3], Jeppe V. Lauritsen[1], Phil D. C. King[2], Philip Hofmann[1], and Soren Ulstrup[1] — [1]Aarhus University, DK — [2]University of St. Andrews, UK — [3]Ecole Polytechnique Federale de Lausanne, CH — [4]CLF, STFC Rutherford Appleton Laboratory, UK

The current understanding of the optical properties and excited carrier dynamics in single-layer and few-layer transition metal dichalcogenides relies largely on a series of photoluminescence and differential absorption measurements. Since excitons dominate the optical response, the dynamics of free carriers cannot be studied directly. Here, we use time- and angle-resolved photoemission spectroscopy to directly measure free carriers in epitaxial single layer MoS_2 grown on either Au(111) or on graphene. For MoS_2/Au(111) we determine an ultrafast (50 fs) extraction of excited free carriers via the metal and ascertain a direct quasiparticle band gap of 1.95 eV. The observed quasiparticle gap is significantly smaller than the theoretically estimated value for free-standing MoS_2. This can be explained by a strong renormalisation of the band gap. For MoS_2 on graphene, we find indications of induced band shifts that lead to a time-dependence of the electronic structure.

HL 78.4 Thu 11:30 S054

Understanding optical properties of atomically thin semiconductors from a many-body perspective — •Matthias Drüppel, Thorsten Deilmann, Peter Krüger, and Michael Rohlfing — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität, 48149 Münster, Germany

Transition metal dichalcogenides (TMDCs) open the door to a fascinating, fast growing field of two dimensional atomically thin semicon-

ductors. This increases the demand for novel theoretical techniques, which allow to reliably calculate the optical properties in large systems, the inclusion of substrates or even correlation between more than two particles.

We take the state of the art approach of DFT → GW → Bethe-Salpeter equation (BSE) and apply the efficient LDA+GdW [1] method. This enables us to describe many-body electronic excitations at moderate numerical cost, being able to treat systems of up to 100 atoms. In the LDA+GdW approximation the quasiparticle self-energy corrections result from the difference between the correct semiconducting screening and hypothetical metallic screening.

Our results show how the optical properties of TMDCs are modified in different situations, e.g. when the screening of the substrate is taken into account, in the presence of vacancies, or when three excited particles form a correlated trion state.

[1] M. Rohlfing, Phys. Rev. B. **82**, 205127 (2010)

HL 78.5 Thu 11:45 S054

Scanning tunneling light emission from single layer MoS_2 — •Christian Lotze, Nils Krane, Julia Läger, Gaël Reecht, and Katharina J. Franke — FU Berlin, FB Physik, Arnimallee 14, 14195 Berlin

Transition-metal dichalcogenides form a group of interesting 2d materials. Among them, the semiconductor MoS_2 has attracted great interest, because it has been shown that it turns from an indirect-gap into a direct-gap semiconductor when reduced to a single layer [1]. As such, potential applications involve its usage for instance as light emitting device.

Here, we present a combined low temperature scanning tunneling (STM) and light emission (LE) study on MoS_2/Au(111). The STM geometry allows to locally inject electrons or holes with the tip into the single layer MoS_2. Inelastically tunneling electrons and holes can give rise to emission of photons [2,3]. Here, we detect and analyze spectrally resolved the electroluminescence from the MoS_2 monolayer on Au(111). We correlate these LE spectra with the electronic structure, that we obtained from scanning tunneling spectroscopy. Moreover we will look into the spatial variation of the LE signals and the role of defect sites.

[1] Mak *et al.*, PRL 105, 136805 (2010)
[2] Berndt *et al.*, PRL 67, 3796 (1991)
[3] Hoffmann *et al.*, Phys. Rev. Lett. 93, 076102 (2004)

HL 78.6 Thu 12:00 S054

Ultrafast photocurrent dynamics in monolayer MoS2 — Eric Parzinger, Anna Vernickel, Alexander Holleitner, and •Ursula Wurstbauer — Walter Schotty Institut and Physik Department, Technical University of Munich, Germany

Atomically thin semiconducting transition metal dichalcogenides such as MoS_2 are emergent materials for optical and electronic circuits. For possible high-frequency applications, we investigate the ultrafast photocurrents in monolayer MoS_2 on a picosecond time scale utilizing a recently developed pump-probe spectroscopy [1-3]. The observed photocurrent contains three major contributions [4]. An initial ultrafast response of $\leq$ 5ps is followed by an exponential decay within a few hundreds of picoseconds. The third very slow contribution peaks at around 1.5 ns. This slow part dominates the overall time-integrated photocurrent intensity. We discuss the impact of laser-induced heating, the one of built-in fields at metal contacts, and the role of trap states. We acknowledge the financial support by the ERC-grant NanoREAL, the DFG excellence cluster Nanosystems Initiative Munich (NIM), and BaCaTec. [1] L. Prechtel, et al. Nature Communications 3, 646 (2012). [2] A. Brenneis, et al. Nature Nanotechnology 10, 135 (2015). [3] C. Kastl, et al. Nature Communications 6, 6617 (2015). [4] E. Parzinger et al. (2016).

HL 78.7 Thu 12:15 S054

Electronic excitations in transition metal dichalcogenides under the influence of dielectric environments — •Malte Rösner[1], Alexander Steinhoff[2], Roelof Groenewald[3], Frank Jahnke[2], Stephan Haas[3], Christopher Gies[2], and Tim O. Wehling[1] — [1]Institut für Theoretische Physik and Bremen Center for Computational Materials Science, Universität Bremen, Bremen, Germany — [2]Institut für Theoretische Physik, Universität Bremen, Bremen, Germany — [3]Department of Physics and Astronomy, University of Southern California, Los Angeles, CA, USA

We present a material-realistic approach to describe electronic interaction effects in transition metal dichalcogenides. On the basis of the Wannier function continuum electrostatics (WFCE) method [1], we are able to include the effects of the dielectric environment, which could serve as a promising tuning knob to control 2D material's properties. We study the doping dependence and the influence of different types of dielectric environments to electronic and plasmonic properties. We find electronic band structure and plasmon dispersion changes on the eV scale.

[1] M. Rösner et al., Phys. Rev. B 92, 085102 (2015)

HL 78.8 Thu 12:30 S054

Optoelectronic properties of sub-nanometer WS2 and TiS3 investigated by scanning near-field optical microscopy and nano-FTIR spectroscopy by using synchrotron radiation — •P. Patoka[1], G. Ulrich[1], A. Nguyen[2], A. Lipatov[3], A. Sinitskii[3], P. Hermann[4], B. Kästner[4], A. Hoehl[4], L. Bartels[2], P. Dowben[5], G. Ulm[4], and E. Rühl[1] — [1]Physikalische Chemie, Freie Universität Berlin, Germany — [2]Dept. of Chemistry, Univ. of California Riverside, U.S.A. — [3]Dept. of Chemistry, Univ. of Nebraska-Lincoln, U.S.A. — [4]Physikalisch-Technische Bundesanstalt (PTB), Germany — [5]Dept. of Physics and Astronomy, Univ. of Nebraska-Lincoln, U.S.A.

Among the 2D electronic materials that have received increased attention recently are the transition metal dichalcogenides (TMD). These materials, especially below nanometer thickness, exhibit promising optoelectronic properties for applications in low-dimension electronic circuits. The combined use of scattering-type near-field optical microscopy and the broadband synchrotron radiation source MLS (PTB, Berlin) allows for the highly sensitive spectromicroscopic characterization of such 2D semiconductors with a spatial resolution below 30 nm. We will present recent results on near-field imaging and nano-FTIR spectroscopy in mid-infrared regime down to monolayer thick TMD structures. Investigated are optical responses of WS2, such as its interaction with the optical phonon mode of the SiO2 substrate. We will also show evidence for high charge accumulation at the edges of the TiS3 structures revealed by optical mapping using tunable CO2 laser.

HL 78.9 Thu 12:45 S054

Investigations on the Phonon Spectrum of $TiSe_2$ in the CDW Phase — •Roland Hott, Rolf Heid, and Frank Weber — Karlsruhe Institute of Technology, Institute of Solid State Physics, P.O.B. 3640, D-76021 Karlsruhe, Germany

We report recent results of our investigations on the Charge Density Wave (CDW) phase transition in $TiSe_2$, performed both experimentally by means of high resolution Inelastic X-ray Scattering (IXS) as well as theoretically by Density Functional Theory (DFT) based ab-initio phonon calculations [1].

We extended our calculations to the case of Cu-doping where we found a huge hardening of the CDW-related soft phonon due to strong chemical bonding of the Cu atoms to the $TiSe_2$ host lattice. Moreover, we investigated the phonon spectrum of $TiSe_2$ in the CDW phase where we find the expected stabilisation of the lattice. Nevertheless, we still obtain here a sizeable electron-phonon coupling for the phonons which derive from the soft phonons of the normal (CDW-undistorted) phase.

[1] F. Weber, S. Rosenkranz, J.-P. Castellan, R. Osborn, G. Karapetrov, R. Hott, R. Heid, K.-P. Bohnen, A. Alatas, PRL **107**, 266401 (2011)

HL 78.10 Thu 13:00 S054

Ultrafast carrier multiplication in 1T-$TiSe_2$ — •Stephan Michael[1], Steffen Eich[1], Henry C. Kapteyn[2], Margaret M. Murnane[2], Michael Bauer[3], Kai Rossnagel[3], Hans Christian Schneider[1], Martin Aeschlimann[1], and Stefan Mathias[4] — [1]University of Kaiserslautern — [2]JILA, University of Colorado and NIST — [3]University of Kiel — [4]University of Göttingen

1T-$TiSe_2$ is a transition metal dichalcogenide, which has a charge density wave (CDW) state below a temperature of around 200 K, which may be due to an excitonic insulator mechanism and/or an Jahn-Teller effect. We studied optically excited carrier dynamics on ultrashort timescales in the CDW phase using time-resolved ARPES measurements and an effective two-band model including carrier-carrier Coulomb scattering. In the framework of this model we analyze the ultrafast response of this material to optical excitation, which is seen in the experiment. We show that carrier multiplication in the form of impact ionization is the most satisfactory explanation for the ultrafast redistribution of spectral weight observed in the ARPES measure-

ments.

HL 78.11 Thu 13:15 S054

Charge density wave kinetics in 1T-TaS_2 monitored by ultrafast LEED — •Simon Schweda[1], Gero Storeck[1], Sebastian Schramm[1], Max Gulde[1], Kai Rossnagel[2], Sascha Schäfer[1], and Claus Ropers[1] — [1]IV. Physikalisches Institut, Universität Göttingen, D-37077 Göttingen — [2]Institut für Experimentelle und Angewandte Physik, Universität Kiel, D-24098 Kiel

We developed an ultrafast low-energy electron diffraction (ULEED) setup for the study of time-resolved structural dynamics at surfaces, extending our previous approach operating on ultrathin films in transmission [1]. A laser-driven nanometric needle emitter provides well-collimated electron pulses with durations of few tens of ps at the sample for electron energies in the range of 50-200 eV.

In a first application of this technique, we investigate optically induced transitions between charge density wave (CDW) phases [2] at a single-crystalline 1T-TaS_2 surface. In particular, the recovery of the nearly commensurate (NC) room-temperature phase after laser-excitation to the incommensurate (IC) phase is resolved in the time-domain. We find a strong dependence of the formation time on the energy density deposited. Furthermore, at higher optical fluences, the appearance of metastable NC antiphase domains is observed, caused by a rapid quench after optical excitation. Our results demonstrate the potential of ULEED for the study of complex ultrafast structural and electronic processes at surfaces.

[1] M. Gulde et al., Science 345, 200 (2014)
[2] M. Eichberger et al., Nature 468, 799 (2010)

HL 79: Focus Session: Physics and Application of Emergent 2D-semiconductors and their Heterostructures 1

Time: Thursday 11:15–13:15 Location: H8

HL 79.1 Thu 11:15 H8

Defects in two-dimensional materials: their production under irradiation, evolution and properties from first-principles calculations — •Arkady Krasheninnikov — Helmholtz Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Germany — Department of Applied Physics, Aalto University, Finland

Following isolation of a single sheet of graphene, many other 2D systems such as hexagonal BN and transition metal dichalcogenides (TMDs) were manufactured. Among them, TMD sheets have received particular attention, as these materials exhibit intriguing. Moreover, the properties can further be tuned by introduction of defects and impurities. In my talk, I will present the results [1] of our first-principles theoretical studies of defects (native and irradiation-induced) in inorganic 2D systems obtained in collaboration with several experimental groups. I will further discuss defect- and impurity-mediated engineering of the electronic structure of 2D materials.

[1] Nature Comm. 6 (2015) 6736; ACS Nano 9 (2015) 3274; ACS Nano (2015) DOI: 10.1021/acsnano.5b04851; Phys. Rev. B 91 (2015) 125304; Adv. Mater. 26 (2014) 2857; Phys. Rev. X 4 (2014) 031044; see http://physics.aalto.fi/~ark/publist.html for complete list of publications.

HL 79.2 Thu 11:30 H8

Phonon induced line broadening and population of the dark exciton in a deeply trapped localized emitter in monolayer WSe2 — •Yu-Ming He[1,3], Chao-Yang Lu[3], Jian-Wei Pan[3], Sven Höfling[1,2,3], and Chrisitian Schneider[1] — [1]Technische Physik and Wilhelm Conrad Röntgen Research Center for Complex Material Systems, Physikalisches Institut, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]SUPA, School of Physics and Astronomy, University of St Andrews, St Andrews, KY16 9SS,United Kingdom — [3]Hefei National Laboratory for Physical Sciences at the Microscale and Department of Modern Physics, & CAS Center for Excellence and Synergetic Innovation Center in Quantum Information and Quantum Physics, University of Science and Technology of China, Hefei, Anhui 230026, China

We study locally trapped single excitons in a mechanically exfoliated WSe2 monolayer semiconductor with respect to their temperature stability, spectral diffusion and decay dynamics. We identify strong signatures of phonon induced spectral broadening in these emitters for elevated temperatures accompanied by temperature induced luminescence quenching. A direct correlation between the drop in intensity at higher temperatures with the phonon induced population of dark states in WSe2 is established.

HL 79.3 Thu 11:45 H8

Gate voltage dependence of the electron mobility in monolayer $MoS_2 - LiNbO_3$ field effect transistors — •Wladislaw Michailow[1], Edwin Preciado[2], Florian Schülein[1], Benjamin Möller[1], Ariana Nguyen[2], David Barroso[2], Miguel Isarraraz[2], Gretel von Son[2], I-Hsi Lu[2], Velveth Klee[2], John Mann[2], Andreas Hörner[1], Achim Wixforth[1], Ludwig Bartels[2], and Hubert Krenner[1] — [1]Insitut für Physik, Universität Augsburg, Germany — [2]University of California, Riverside, USA

In field effect transistors (FETs) based on novel two-dimensional semiconductor materials, detailed knowledge of the density and the mobility of charge carriers in the conducting channel is of paramount importance. In the most common approach the field effect mobility and charge carrier density are determined by a simple parallel-plate capacitor model. In this model the carrier mobility is assumed to be independent of the gate potential. Here we report on investigations of monolayer $MoS_2 - LiNbO_3$ FETs [1] in which we determined the source-drain current and the capacitance as function of gate voltage. We analyze both using a theoretical model of a two-dimensional free electron gas. This analysis allows us to derive both the charge carrier density and the mobility over the full $\pm 40\,V$ range of gate voltage. Using our advanced analysis we show that for our structure the established parallel-plate capacitor model is oversimplified and overestimates the carrier mobility by a factor of $\gtrsim 4$.

[1] E. Preciado et al., Nat. Commun. **6**, 8593 (2015).

HL 79.4 Thu 12:00 H8

Resistivity switching in chalcogenide based interfacial phase change materials — •Nicki F. Hinsche and Kristian S. Thygesen — Center for Atomic-scale Materials Design, Technical University of Denmark, 2830 Kgs. Lyngby, Denmark

Chalcogenide based phase change materials (PCM) are emerging candidates for next generation non-volatile, ultra-fast memories. In contrast to conventional amorphous-crystal phase transition driven PCM, e.g. $Ge_2Sb_2Te_5$, recently a new type of PCM device named *interfacial phase change memory* (iPCM) was proposed [1]. Here the electrical pulse induced movement of the atoms is limited to the interface, therefore substantially reducing the switching energies and allowing for shorter switching times.

By means of DFT electronic-structure [2] and Boltzmann transport calculations [3], we discuss for an iPCM GeTe-Sb_2Te_3 heterostructure the electrical resistivity change caused by the structural switching at the interface. With a close relation of the material system to the family of topological insulators, ferroelectrics [4] and thermoelectrics, the possibility of a ferroelectric controllable topological phase transition and the ultra-fast modification of the thermoelectric properties, applicable for fast thermal switches, will be analysed additionally.

[1] R. E. Simpson *et al.*, Nature Nanotechnology **6** 8501(2011); [2] J. Enkovaara *et al.*, J. Phys.: Condens. Matter **22** 253202 (2010); [3] N. F. Hinsche *et al.*, ACS Nano **9** 4406 (2015) [4] A. V. Kolobov *et al.*, APL Mater. **2** 066101 (2014)

HL 79.5 Thu 12:15 H8

Electrical properties of CVD Molybdenum disulfide — •Wajid Awan[1], Tommy Schönherr[1], Artur Erbe[1], Stefan Facsko[1], and Xinliang Feng[2] — [1]Helmholtz-Zentrum Dresden-Rossendorf — [2]Technische Universität Dresden

Two dimensional materials are attractive for the use in next-generation nanoelectronic devices as compared to one dimensional material because it is relatively easy to fabricate complex structures from them. Recently the layered 2D semiconducting Transition metal dichalcogenides came into the picture and got a place in a wide range of novel

applications as well as in basic research. Strikingly, MoS_2 receives significant attention since it undergoes transition from indirect bandgap (bulk form) to a direct bandgap (1.2eV) semiconductor if thinned out to a single atomic layer. The bandgap is an essential property for tunable 2-D nanodevices. We performed electrical transport measurements at room temperature for CVD grown MoS_2 on SiO_2/Si substrate. Standard Electron beam lithography (EBL) was used to pattern Gold (Au) metal contacts on MoS_2 flakes. For the purpose of sample characterization, we performed the Atomic Force Microscopy (AFM) and Raman Spectroscopy techniques, respectively, which confirm that the thickness of the CVD grown MoS_2 triangular flakes corresponds to single layers. Low temperature characterization of the electrical properties of the layers elucidates the exact mechanisms of charge transport in the 2d-layers. This knowledge will be used to modify the electrical properties in a controlled way, for example by ion irradiation.

HL 79.6 Thu 12:30 H8

Nonlinear Optics in a Rydberg-Excited Semiconductor Cavity — •Valentin Walther, Robert Johne, and Thomas Pohl — Max Planck Institute for the Physics of Complex Systems, Dresden

Recent experiments have demonstrated excitons with extraordinarily large binding energies in some two-dimensional semiconductors (TMDCs), whose Rydberg states give rise to giant interactions and, therefore, hold great promise for optical utility.

We evaluate the optical response under conditions of electromagnetically induced transparency (EIT), accounting for the full excited level structure and numerous decoherence mechanisms in a semiconductor. Strong exciton-exciton interactions result in enormous effective photon-photon potentials. Using experimental parameters, we show that the photonic nonlinearity exceeds that of traditional semiconductors by several orders of magnitude and we assess the material properties required for coherent optical applications.

Further, we investigate interesting optical effects in the transverse mode structure of a driven-dissipative cavity arising from the unusually large nonlinearity.

HL 79.7 Thu 12:45 H8

Thermal expansion and transport in van-der-Waals solids from first-principles — •Daniel Lindroth, Per Hyldgaard, and Paul Erhart — Chalmers University of Technology, Gothenburg, Sweden

We have performed first-principles calculations for lattice thermal expansion and transport in the bulk of the transition metal dichalcogenides (TMDCs) MoS2, MoSe2, MoTe2, WS2, WSe2 and WTe2 using density functional theory (DFT) and the semi-classical phonon Boltzmann transport equation (BTE) within the relaxation time approximation (RTA).

Proper modeling of the lattice thermal conductivity is important for an accurate prediction of the thermoelectric figure of merit and better understanding of potentially high performing novel materials such as van der Waals heterostructures based on TMDCs. To this end, we have conducted a thorough investigation of the mentioned TMDCs based on DFT calculations using a recently published van der Waals density functional (vdW-DF-cx) in conjunction with anharmonic modeling of phonon lifetimes using third order interatomic force constants that allows for solutions to the BTE within the RTA as implemented in the phono3py code. We found that our calculations agrees with theoretical expectations as well as with experimental data where available. The methods used thus provide a promising framework for further investigation of more complex systems with potentially novel thermal properties.

HL 79.8 Thu 13:00 H8

Enabling a new class of electronic devices using self-aligned nanodomain boundaries to open a charge transport gap in trilayer graphene — •Victor Aristov[1,2,3], Olga Molodtsova[1,4], Sergey Babenkov[1], Tsung-Wei Huang[5], Askar Syrlybekov[6], Mourad Abid[7], Dmitry Marchenko[8], Jaime Sánchez-Barriga[8], Partha Sarathi Mandal[8], Andrei Varykhalov[8], Yuran Niu[9], Barry Murphy[6], Sergey Krasnikov[6], Olaf Lübben[6], Alexander Chaika[2,6], and Han-Chun Wu[6] — [1]DESY, Hamburg, Germany — [2]ISSP RAS, Chernogolovka, Russia — [3]TU Bergakademie, Freiberg, Germany — [4]ITMO, Saint Petersburg, Russia — [5]National Taiwan University, Taipei, Taiwan — [6]Trinity College, Dublin, Ireland — [7]King Saud University, Riyadh, Saudi Arabia — [8]BESSY, Berlin, Germany — [9]Max-lab, Lund, Sweden

Trilayer graphene reveals unique electronic properties interesting for fundamental science and technological applications. The ability to achieve a high on-off current ratio is the central question in this field. We propose a simple method to achieve a current with high on-off ratio by opening a transport gap in trilayer graphene with self-aligned periodic nanodomain boundaries (NBs). Our low temperature transport measurements clearly demonstrate that the self-aligned periodic NBs induce a huge charge transport gap, more than 1.3 eV at 10 K. As a result of our study the feasibility of creating new electronic nanostructures with high on-off current ratios using graphene on cubic-SiC/Si wafers was shown. This work was supported by the RAS, RFBR grants No 140200949 and 140201234, by SPP 1459 of DFG.

HL 80: Hybrid and Perovskite Photovoltaics IV (Joint session of CPP, DF, DS and HL, organized by HL)

Time: Thursday 14:45–18:30 Location: H2

HL 80.1 Thu 14:45 H2

Synthesis of perfectly oriented and micrometer-sized MAPbBr3 perovskite crystals for thin film photovoltaic applications — •Nadja Giesbrecht[1], Johannes Schlipf[2], Andreas Binek[1], and Pablo Docampo[1] — [1]Department of Chemistry and Center for NanoScience (CeNS), University of Munich (LMU), Butenandtstr. 5-13, 81377 Muenchen,Germany — [2]Lehrstuhl fuer Funktionelle Materialien, Physik-Department, Technische Universitaet Muenchen, James-Franck-Str. 1, 85748 Garching, Germany

Wide band-gap perovskites such as methylammonium lead bromide (MAPbBr3) are interesting materials for photovoltaic applications due to their potentially high open-circuit voltage. However, the fabrication of high quality planar films has not been investigated in detail for this material. We report a new synthesis approach for the fabrication of bromide based perovskite planar films based on the control of the deposition environment. The correlation of photocurrent and perovskite crystal properties in photovoltaic devices is studied. We achieve dense layers with large and perfectly oriented crystallites, as confirmed with grazing incidence wide angle X-ray scattering (GIWAXS). This represents the first solution-processed MAPbBr3 perovskite film with such a high degree of order. The current output was found to depend on crystal order in the perovskite film with internal quantum efficiencies approaching unity. Hence, our work not only gives a new pathway to tune morphology and crystal orientation, but demonstrates its importance for planar perovskite solar cells.

HL 80.2 Thu 15:00 H2

Structural properties of hybrid perovskites from first principles — •Jingrui Li[1], Jari Järvi[1,2], Hugo Levard[1], and Patrick Rinke[1] — [1]Aalto University, Helsinki, Finland — [2]University of Helsinki, Finland

Hybrid perovskites have received rapidly growing interest in recent years as promising photoactive materials in emergent photovoltaic technologies. We present a first-principles analysis of the atomistic structure of the methylammonium lead triiodide ($CH_3NH_3PbI_3$) perovskite in this work, with a particular focus on the orientation of $CH_3NH_3^+$ cations and its interplay with the inorganic matrix. Relativistic density functional theory calculations were performed using the all-electron local-atomic-orbital code `FHI-aims`. Our results indicate that (i) the lattice constants obtained by incorporating the long-range van der Waals interactions (using the Tkatchenko-Scheffler method) in the PBE exchange-correlation functional agree well with experiments; (ii) hydrogen bonding between the ammonium group and the I^- anions plays the decisive role in the position of the $CH_3NH_3^+$ cation and the shape of the PbI_3^{2-} framework; (iii) the reorientation of $CH_3NH_3^+$ is limited due to the high barriers ($\sim$ 80 meV). Based on these findings we establish a self-consistent multiscale model, in which the energetically favorable alignment of $CH_3NH_3^+$ dipoles in the ma-

terial is determined by combining classical electrostatics and statistics with structure relaxation in DFT. Our procedure produces representative "pseudo random" methylammonium lead triiodide supercells that will form the basis of further first-principles work.

HL 80.3 Thu 15:15 H2

Micrometer size grains of hybrid perovskite through rapid melting procedure — •Oleksandra Shargaieva, Felix Lang, Jörg Rappich, Carola Klimm, Manuela Klaus, Bernd Rech, and Norbert Nickel — Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Kekuléstr. 5, 12489 Berlin (Germany)

Interest in hybrid perovskites as an absorber has flared since the first successful attempts in dye solar cells (DSCs) and continues to grow as a promising material for solar cells application. The usage of such compounds is often associated with the opportunity to substitute existing materials due to the remarkable simplicity of the production process and its low costs. On the other hand, solution based processing of solid perovskite layers often includes difficulties with crystallization, which could result in the formation of grain boundaries. This type of crystalline defect has a strong impact on the performance of devices and tends to lower the power conversion efficiency.

In our work, we propose a new solvent-free approach to produce perovskite type compounds based on its melting process. This simple technic allows to obtain bulk material with grain sizes of several micrometers. Melting process enables the control of the crystallization of hybrid perovskite and by that suppresses grain boundaries formation. Furthermore, the procedure was optimized and successfully introduced into thin-film fabrication. Consequently, melting of perovskites gives a possibility to decrease non-radiative recombination and therefore, can improve the performance of the device.

HL 80.4 Thu 15:30 H2

J-V Hysteresis Observed in Methylammonium Lead Halide Perovskite Films at Different Voltage Scales — •Martina Stumpp, Raffael Ruess, Jonas Horn, Jan Tinz, Christoph Richter, and Derck Schlettwein — Justus-Liebig-Universität Gießen, Institut für Angewandte Physik, Heinrich-Buff-Ring 16, D-35392 Gießen, GERMANY

Hysteresis in the current-voltage curves of methylammonium lead halide films deserves detailed investigation because it can affect their applicability in perovskite solar cells. In the current study, J-V hysteresis of $CH_3NH_3PbI_3$ and $CH_3NH_3Pb(I_{0.95}Br_{0.05})_3$ prepared via different established deposition techniques was studied in a symmetric contact geometry of microstructured gold electrode arrays on SiO_2/Si wafers. The measured J-V characteristics showed a different behavior of hysteresis depending on the applied voltage range. Residual currents at zero applied bias were observed following positive or negative poling showing persistent polarization of the perovskite films. At higher bias voltages, additional inverted hysteresis loops were measured pointing at a decrease in barrier height and width at blocking perovskite/metal contacts, presumably caused by migrating iodide ions. The net J-V characteristics in this voltage range can be simulated by two diodes operated back-to-back. Time-dependent studies were performed to analyze the decay of the different observed polarization phenomena in the films during either short-circuit or continuous sweeping of the bias.

HL 80.5 Thu 15:45 H2

Water infiltration in methylammonium lead iodide: fast and inconspicuous — •Christian Mueller[1,2,3], Bernd Epding[2,3], Tim Helder[2,3], Michael Sendner[2,3], Annemarie Pucci[2,3], Wolfgang Kowalsky[1,2,3], and Robert Lovrincic[1,3] — [1]IHF, TU Braunschweig, Germany — [2]KIP, Universität Heidelberg, Germany — [3]InnovationLab, Heidelberg, Germany

Extensive research efforts over the last few years led to a significant increase in power conversion efficiency of organometal-halide perovskite (such as $CH_3NH_3PbI_3$) solar cells up to over 20%. However, our understanding of physical/chemical processes in the material lags behind device progress. For instance, the impact of water on $CH_3NH_3PbI_3$-based devices, despite being well documented, is still not well understood and as such remains controversial.

Herein we use IR spectroscopy in controlled atmosphere to demonstrate that water infiltration into $CH_3NH_3PbI_3$ occurs much faster and at much lower humidity than previously thought. We show that the exposure of $CH_3NH_3PbI_3$ to ambient environment leads to an increase of the photocurrent by more than one order of magnitude in lateral devices. Based on transient photocurrent measurements we speculate that the effect is associated with enhanced proton conduction when light is combined with water and oxygen exposure. Our results suggest that water infiltration plays an important role in the optoelectronic properties of $CH_3NH_3PbI_3$ based devices, well beyond the known water triggered degradation processes[1].

[1] C. Mueller et al., Chem. Mater., 27 (22), p. 7835-7841, 2015

HL 80.6 Thu 16:00 H2

Graphene on Hybrid Solar Cells: from Silicon and Perovskite towards Tandem Solar Cells — •Felix Lang, Matthias Zellmeier, Marc A. Gluba, Steve Albrecht, Jörg Rappich, Lars Korte, Bernd Rech, and Norbert H. Nickel — Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Institut für Silizium Photovoltaik, Kekuléstr. 5, 12489 Berlin, Germany

A variety of hybrid solar-cell architectures require the deposition of a highly transparent and conductive contact. However, deposition techniques for conventional transparent conductive oxides typically degrade the topmost organic layers. A non-destructive wet transfer process of large area graphene from the growth substrate onto the desired sample is the clear choice to tackle this challenging problem.

Here, we present for the first time the implementation of graphene on hybrid crystalline silicon/P3HT solar cells. Despite identical V_{OC} and superior external quantum efficiency, device performance is limited by graphene sheet resistance. To overcome this limitation we combined in-situ graphene doping with an absorber with a higher band gap. Both measures reduce the impact on the device performance.

Implementation of graphene on the perovskite $CH_3NH_3PbI_3$ therefore enabled a semi-transparent device concept showing superior internal quantum efficiency compared to conventional Au-contacted solar cells. The graphene contact enabled an optical sub-band gap transmission of around 60 % for the complete device. This paved the way for the development of a four terminal crystalline silicon/perovskite tandem solar cell with a power conversion efficiency of 13.2 %.

HL 80.7 Thu 16:15 H2

GW for transition metal perovskites — •Zeynep Ergonenc, Bongjae Kim, Peitao Liu, Georg Kresse, and Cesare Franchini — University of Vienna, Faculty of Physics and Center for Computational Materials Science

The ab initio calculation of quasiparticle (QP) energies beyond density functional theory is a technically and computationally challenging problem. In condensed matter physics the most widely used approach to determine QP energies is the GW approximation. The GW method has been widely applied to many elemental and binary semiconductors, but its application to more complex compound such as perovskites is less abundant. In this work we apply the GW technique to transition metal perovskites with different occupancies of d orbitals. We show that much care must be taken to obtain converge QP band structure in terms of number of unoccupied orbitals and k-points sampling. Accurate extrapolation procedures to the infinite-basis-set limit and infinite-k-point limit are necessary.

30 min. Coffee Break

HL 80.8 Thu 17:00 H2

Controlling the optical properties of organic/inorganic halide perovskites by means of size and composition — •Verena A. Hintermayr, Lakshminarayana Polavarapu, Alexander S. Urban, and Jochen Feldmann — Chair for Photonics and Optoelectronics, Department of Physics, Ludwig-Maximilians-Universität (LMU), Amalienstaße 54, 80799 Munich, Germany

Organic/Inorganic halide perovskites display a huge potential for not only photovoltaic, but also light emitting applications. In order to improve the efficiency and functionality of applications based on this material a better control of their optical properties is desirable. Here, we present a general colloidal synthesis method for the preparation of hybrid organic/inorganic halide perovskite nanocrystals (NCs) with different size and composition. We have prepared highly stable perovskite NCs that show strong quantum confinement and NCs that exhibit bulk like optical properties. We additionally investigate the tunability of the optical properties of the NCs by systematically modifying their halide content (I, Br and Cl). This work opens up a simple synthetic route for the preparation of perovskite NCs with controllable dimensionality and composition.

HL 80.9 Thu 17:15 H2

Dynamics and nature of photo-excited carriers in

$(CH_3NH_3)PbI_3$ organic-inorganic perovskite — •Daniel Niesner[1,2], Haiming Zhu[1], Tyler J. S. Evans[1], Bryan J. Kudisch[1], Prakriti P. Joshi[1], Kiyoshi Miyata[1], M. Tuan Trinh[1], Manuel Marks[1], and X.-Y. Zhu[1] — [1]Department of Chemistry, Columbia University, New York, NY 10027, USA — [2]Festkörperphysik, FAU Erlangen-Nürnberg, D-91058 Erlangen, Germany

Thin film solar cells based on organic-inorganic perovskites are the rising star in photovoltaics. The photophysics and transport mechanism behind the outstanding device performance remain a matter of debate. I will present the results of a study on carrier dynamics in vapor-deposited thin films of $(CH_3NH_3)PbI_3$, combining time-resolved two-photon photoemission, transient absorption, and photoluminescence.

After optical excitation with sufficient photon energy ($\geq$ 2.15 eV), highly excited electrons relax quickly ($\leq$ 0.3 ps) to a region of the conduction band with a low density of states, located 0.3 eV above the band minimum. In parallel, polaron formation takes place on a time scale of 0.28 ± 0.04 ps, matching the time scale of cation motion. Polaronic screening suppresses further energy relaxation and thermalization. The polaron maintains a significant excess energy for more than 60 ps.

The excess energy can be utilized to overcome energy barriers at grain boundaries and contacts. Harvesting it directly would result in a solar cell with an efficiency exceeding the Shockley-Queisser limit.

HL 80.10 Thu 17:30 H2

Infrared spectroscopic study of vibrational modes and water infiltration in methylammonium lead halide perovskites — •Michael Sendner[1,2], Christian Mueller[1,2,3], Tobias Glaser[1,2], Annemarie Pucci[1,2], Wolfgang Kowalsky[1,2,3], and Robert Lovrincic[2,3] — [1]Kirchhoff-Institut für Physik, Universität Heidelberg — [2]InnovationLab GmbH, Heidelberg — [3]Institut für Hochfrequenztechnik, TU Braunschweig

The interactions of the organic cation with the inorganic lattice in organo-metallic halide perovskites influence the vibrational properties of the cation which can be measured in the mid infrared (IR) spectral region. We determined the infrared optical properties of different methylammonium lead halide perovskite films ($CH_3NH_3Pb(I/Br/Cl)_3$) and derived the full dielectric function [1]. The peaks of the vibrational modes are assigned by means of the comparison with MP2 calculated modes of the free methylammonium cation. The influence of the inorganic cage and the processing is discussed. Furthermore, we utilize IR spectroscopy to investigate the influence of water onto perovskite thin films. We show that the infiltration of water into $CH_3NH_3PbI_3$ appears much faster and at much lower humidity than previously known [2]. We suggest a molecular picture of this infiltration where water molecules have a strong impact on the hydrogen bonding between the methylammonium cations and the surrounding Pb-I cage. [1] T. Glaser et al. J. Phys. Chem. Lett. 2015, 6 (15), 2913-2918 [2] C. Müller et al. Chem. Mater., 2015, 27 (22), 7835-7841

HL 80.11 Thu 17:45 H2

Temperature and excitation density dependence of two-photon photoluminescence of perovskite CH3NH3PbBr3 — •Heiko Linnenbank[1], Michael Saliba[2], Lili Gui[1], Bernd Metzger[1], Giuseppe Nasti[2], Jeanette Kadro[2], Anders Hagfeldt[2], Michael Graetzel[2], and Harald Giessen[1] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany — [2]Laboratory of Photonics and Interfaces, École polytechnique fédérale de Lausanne, Station 6, 1015 Lausanne, Switzerland

Recently solution processed organometallic halide perovskites have attracted much attention due to their simple processability, strong light absorption and favorable emission properties, which promises the realization of efficient on chip lasers. While several studies have been focused on one-photon excited luminescence processes like amplified spontaneous emission or lasing, only less attention has been paid to two-photon excited processes. In contrast to the usually expected quadratic dependence upon the excitation density in the case of two-photon photoluminescence, we rather measure a 4th power dependence at room temperature in the case of CH3NH3PbBr3. Such an excitation density dependence is a strong hint for a biexcitonic or exciton collision processes, which are rather unlikely at room temperature. To clarify the origin of the 4th power dependence, we investigate the form as well as the excitation density dependence of the photoluminescence spectra with respect to the sample temperature, revealing a suppression of the 4th power dependence with decreasing temperature.

HL 80.12 Thu 18:00 H2

Dark field photoluminescence and scanning electron beam measurements on single organic/inorganic halide perovskites of varying geometry and composition — •Alexander Richter, Verena Hintermayr, Lakshminarayana Polavarapu, Alexander Urban, and Jochen Feldmann — Chair for Photonics and Optoelectronics, Department of Physics, Ludwig-Maximilians-Universität (LMU), Amalienstaße 54, 80799 Munich, Germany

During recent years organic/inorganic halide perovskites have become a promising candidate for photovoltaic applications and also show a huge potential for light emitting applications. In case of two dimensional crystals quantum confinement affects the optical properties. Here, we present results on individual nanocrystals. Perovskites fabricated with varying halide content and geometry are embedded in a polymer matrix film to prevent degradation. Dark field photoluminescence and scanning electron beam measurements on individual spots of the sample are carried out. This yields a direct link between shape, halide composition and photoluminescence of these particles.

HL 80.13 Thu 18:15 H2

Luminescence blue-shift with decreasing size of perovskite needles. — •Amala Elizabeth and Katrin F.Domke — Molecular Spectroscopy Department,Max Planck Institute for Polymer Research, Mainz, 55128, Germany

Despite revolutionizing the photovoltaic industry by helping create highly efficient thin film solar cells, many intrinsic properties of organometallic halide perovskites still remain unknown. A complete understanding of the interplay of size, structure and electronic nature in determining the optical properties of thin film perovskites is crucial to fully exploit them for solar cell applications.

We studied methylammonium lead iodide perovskite thin films of ordered needles of varying submicron size. Energy-dispersive X-ray and IR spectroscopies reveal that the needles are chemically identical. While crystallinity is preserved in all samples, XRD and Raman spectra show a relative increase in the crystalline lead iodide content with decreasing needle size. Interestingly, we observe a blue-shift of 40 meV in both luminescence peak position and UV-vis absorption onset with decreasing needle size. Here, we discuss possible origins of the unexpected band gap increase with decreasing perovskite needle size, such as methyl ammonium cation orientational ordering [1] and lead iodide content [2].

References:
1. C. Quarti et al., J.Phys.Chem Lett. 5 (2014), 279-284.
2. Q.Shen et al., Nano Lett. 14 (2014), 4158-4163.

HL 81: Topological Insulators I (Joint session of DS, HL, O and TT, organized by HL)

Time: Thursday 14:45–17:15 Location: H10

HL 81.1 Thu 14:45 H10

Topological Dirac Semimetal in strained HgTe — •Tomáš Rauch[1], Steven Achilles[1], Jürgen Henk[1], and Ingrid Mertig[1,2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle (Saale), Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, D-06120 Halle (Saale), Germany

HgTe, one of the most intensively investigated materials in the context of topological insulators, is a semimetal with zero energy band gap when considered as a three-dimensional material. Applying uniaxial strain in [001] direction changes the situation dramatically [1]. Under compressive strain HgTe becomes a strong topological insulator featuring typical Dirac cone shaped surface states at the $\overline{\Gamma}$ point of the surface Brillouin zone. On the other hand, applying a tensile strain makes HgTe a topological Dirac semimetal with a pair of doubly-degenerate Dirac cones located along the k_z axis of the bulk Brillouin

zone.

By combined *ab initio* and tight-binding electronic structure calculations we investigate the bulk and surface electronic properties of three-dimensional HgTe in the topological Dirac semimetal phase. This includes calculating the bulk band structure, topological invariants, and the electronic structure of the (100) surface, at which the associated non-trivial surface states emerge.

[1] T. Rauch *et al.*, Phys. Rev. Lett. **114**, 236805 (2015)

HL 81.2 Thu 15:00 H10

Tight-Binding Approach towards an Effective Model for InAs/GaSb Quantum Wells — •Matthias Sitte[1], Karin Everschor-Sitte[1], and Allan MacDonald[2] — [1]Johannes Gutenberg-Universität Mainz, Institut für Physik, Staudingerweg 7, 55128 Mainz — [2]The University of Texas at Austin, Department of Physics, 2515 Speedway, Austin, TX 78712-1192

Topological insulators have attracted a great deal of attention as a new quantum state of matter in the last decade. The first realizations of 2D TIs were HgTe/CdTe quantum well heterostructures, but in recent years another class of semiconductor heterostructures — namely InAs/GaSb quantum wells — was shown to yield 2D TIs as well. Compared to the HgTe/CdTe-based systems they have many advantages, most prominently a continuously tunable band structure via external electric fields and stronger proximity coupling to superconductors. We perform empirical tight-binding calculations on these systems to study how topological properties are changed by varying external control parameters such as electric fields or well thicknesses.

HL 81.3 Thu 15:15 H10

Negative Magnetoresistance of $TlBi_xSb_{1-x}Te_2$ — •Oliver Breunig, Zhiwei Wang, Fan Yang, Alexey Taskin, and Yoichi Ando — II. Physikalisches Institut, Universität zu Köln

In the family of the ternary II-V-VI_2 compounds several materials have been identified as topological insulators. In the n-type $TlBiTe_2$ a topological surface state has been found, yet it is hardly accessible for transport studies due to the overlap with the bulk bands. Theoretical studies suggest that upon substituting Bi by Sb a narrow bulk band gap opens while preserving a single Dirac cone at the Γ point, leading to a possible realization of a bulk-insulating system with an exposed Dirac point.

Single crystals of $TlBi_xSb_{1-x}Te_2$ were grown by a modified Bridgman technique using high-purity starting materials. They were characterized by ICP/EDX as well as transport measurements. For intermediate values x we find insulating transport properties and a surprisingly strong negative magnetoresistance. We present our crystal growth results of $TlBi_xSb_{1-x}Te_2$ and discuss the origin of the observed large negative magnetoresistance.

HL 81.4 Thu 15:30 H10

Landau level spectroscopy of the 3D topological insulator Sb_2Te_3 — •Stefan Wilfert[1], Oliver Storz[1], Paolo Sessi[1], Thomas Bathon[1], Konstantin Kokh[2], Oleg Evgen'evich Tereshchenko[2], and Matthias Bode[1] — [1]Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Novosibirsk State University, 630090 Novosibirsk, Russia

Sb_2Te_3 is a prototypical three-dimensional topological insulator (TI) with intrinsic *p*-doping, which leads to a Dirac point lying well above the Fermi level [1]. We performed energy-dependent quasi-particle interference mapping and scanning tunnel spectroscopy in high magnetic fields up to 12 T on this compound, where both methods allow to obtain the energy dispersion. In contrast to the much more studied TIs Bi_2Te_3 [2] and Bi_2Se_3 [3], Sb_2Te_3 shows Landau levels with both negative and positive Landau level indices. This enables to analyze in more detail the energetic broadening of the Landau levels, which may lead to a better understanding of the physical limits of quantum coherence in this type of materials.

[1] C. Seibel *et al.*, Phys. Rev. Lett. **114**, 066802 (2015).
[2] Y. Okada *et al.*, Phys. Rev. Lett. **109**, 166407 (2012).
[3] T. Hanaguri *et al.*, Phys. Rev. B **82**, 081305 (2015).

30 min. Coffee Break

HL 81.5 Thu 16:15 H10

Aharonov-Bohm effect in the 3D topological insulator HgTe — •Johannes Ziegler[1], Dmitriy Kozlov[1,2,3], Dmitry Kvon[2,3], Nikolay Mikhailov[2], Sergey Dvoretsky[2], and Dieter Weiss[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Germany — [2]A.V. Rzhanov Institue of Semiconductor Physics, Novosibirsk, Russia — [3]Novosibirsk State University, Russia

We present our progress in the investigation of the Aharonov-Bohm effect in ring and nanowire structures, fabricated from high-mobility strained 80 nm HgTe films with a wet etching technique. The nanostructures are equipped with topgates to allow tuning of the Fermi level E_f and are measured in a dilution cryostat.

The focus lies on Topological Insulator nanowires, where it is expected that the magnetic flux Φ through the wire leads to both Φ_0 and $\Phi_0/2$ periodic oscillations [1]. Φ_0 ($= h/e$) periodic oscillations are expected to occur in the ballistic regime for a large range in E_f. For ballistic devices, both minima and maxima of the conductance are expected at $\Phi = \Phi_0/2$ with varying E_f. In the case of diffusive transport, Φ_0 periodic oscillations are expected for E_f close to the Dirac point, while tuning E_f away from the Dirac Point leads to $\Phi_0/2$ ($= h/2e$) periodic oscillations.

[1] J.H. Bardarson *et al.*, Phys. Rev. L **105**, 156803 (2010)

HL 81.6 Thu 16:30 H10

Emergence of quantum spin Hall and half-topological states at Graphene/TMDC heterostructures — •Denis Kochan, Martin Gmitra, Petra Högl, and Jaroslav Fabian — Institute for Theoretical Physics, University of Regensburg, Germany

We discuss orbital and spin-orbital proximity effects emerging in graphene deposited on a monolayer transition-metal dichalcogenides (TMDCs: MoS2, MoSe2, WS2, WSe2) and analyze the impact on spin transport in such graphene/TMDC heterostructures. First-principles investigations show that graphene on MoS2, MoSe2, and WS2 has a topologically trivial band structure, while graphene on WSe2 exhibits inverted bands. The essential low energy physics can be well described by a symmetry inspired realistic tight-binding Hamiltonian. We predict topologically protected helical edge states for graphene zigzag nanoribbons on WSe2, demonstrating the emergence of the quantum spin Hall effect. Our model also features "half- topological states", which are protected against time-reversal disorder on one edge only. Unlike in pristine graphene, the proximity spin-orbit coupling in graphene on TMDCs is significant (orders of meV), making the predicted effect testable experimentally.

This research was supported by DFG SFB 689, GRK 1570 and by the EU Seventh Framework Programme under Grant Agreement No. 604391 Graphene Flagship.

HL 81.7 Thu 16:45 H10

Chiral Magnetic Effect in an Interacting Weyl Semimetal — •Matthias Puhr, Semen Valgushev, and Pavel Buividovich — Universität Regensburg, D-93053 Regensburg, Deutschland

We present results of a mean-field study of the chiral magnetic effect in a simple model of a parity-breaking Weyl semimetal. Our model is given by the lattice Wilson-Dirac Hamiltonian with on-site repulsive interaction and a constant chiral chemical potential term. We find a non-trivial behaviour of the chiral magnetic conductivity (CMC) and observe an increase, a decrease and even a change of sign depending on the interaction strength. The absolute value of the CMC never exceeds the value for the non-interacting gapless Hamiltonian. Our model exhibits a phase transition to a phase with spontaneously broken parity (Aoki phase, axionic insulator phase) and we observe a strong suppression of the CMC in the parity broken phase.

HL 81.8 Thu 17:00 H10

Negative magneto-resistivity in finite-size samples of Weyl semimetals — Pavel Buividovich, Matthias Puhr, and •Semen Valgushev — University of Regensburg, Regensburg, Germany

We numerically study Chiral Magnetic Effect and magneto-resistivity in a slab of parity-breaking Weyl semimetal modeled by Wilson-Dirac hamiltonian with open boundary conditions and subjected to the external magnetic field parallel to the boundaries. We find that the density of CME current is locally non-zero and strongly localized near the boundaries, where it approaches conventional value $j = \mu_5 B/2\pi^2$. We calculate the magneto-resistivity in a physical setup when parallel magnetic and electric fields are applied to the sample and discuss our results in the context of recent experiments on negative magneto-resistivity in Weyl semimetals.

HL 82: Semiconductor Lasers II

Time: Thursday 14:45–15:30 Location: H13

HL 82.1 Thu 14:45 H13

Coaxial GaAs-AlGaAs core multishell nanowire lasers with epitaxial gain control — •Philipp Zimmermann[1], Thomas Stettner[1], Bernhard Loitsch[1], Markus Döblinger[2], Gerhard Abstreiter[1], Gregor Koblmüller[1], and Jonathan J. Finley[1] — [1]Walter Schottky Institut and Physik Department, Technische Universität München, Garching, Germany — [2]Department of Chemistry, Ludwig-Maximilians-Universität München, Munich, 81377, Germany

Semiconductor nanowires (NW) open up promising routes towards ultra-small, coherent light sources integrated on silicon. NWs act as natural Fabry-Perot cavities and have sufficient modal high reflectivity at the end facets, to facilitate lasing. Lasing has recently been demonstrated from conventional GaAs-AlGaAs core shell NWs up to room-temperature with emission in the near infrared [1]. For improved gain characteristics and lower threshold it is desirable to incorporate low-dimensional systems within the NW geometry. Here, we present single-mode lasing from radial single and multiple GaAs quantum wells (QWs) as active gain media in a GaAs-AlGaAs core-multishell NW. When subject to optical pumping lasing emission with a distinct s-shaped input-output characteristics and emission energies associated with the confined QWs are observed. The low temperature performance shows a reduced threshold power density for 7 coaxial QWs compared to a single QW in a NW with the same diameter, which confirms that gain characteristics can be optimized by epitaxial design [2]. [1] B. Mayer, et al. Nature Comm. 4, 2961 (2013). [2] T. Stettner, P. Zimmermann, et al., in review (2015).

HL 82.2 Thu 15:00 H13

InP-based tunable narrow linewidth laser array for use as local oscillator in coherent communication — •Annette Becker[1], Vitalii Sichkovskyi[1], Marko Bjelica[2], Florian Schnabel[1], Anna Rippien[1], Bernd Witzigmann[2], and Johann Peter Reithmaier[1] — [1]Institut für Nanostrukturtechnologie und Analytik, CINSaT, Universität Kassel, Deutschland — [2]Computational Electronics and Photonics, CINSaT, Universität Kassel, Deutschland

Reference lasers are a key element for high-capacitance coherent optical communication. These lasers need to be narrow linewidth widely tunable DFB lasers.

InP based quantum dot (QD) material developed for 1.55 μm enables tailoring of device properties, like low linewidth enhancement factor (α-factor) favourable for such an application. Theoretical considerations taking into account the quasi zero-dimensional nature of the active zone, clearly predict a strong reduction of the laser linewidth by appropriate tailoring the QD material design.

By adjusting growth parameters and QD layer numbre, the gain function could be tailored to be more symmetric, resulting in considerable reduction of the α-factor. Intrinsic linewidths of less than 200 kHz could be achieved. By arranging the lasers in an array, the tuning range could be extended to meet the demands of coherent communication systems.

HL 82.3 Thu 15:15 H13

Characterization of Multimode Semiconductor Lasers by Intensity and Wavefront Analysis — •Inga-Maria Eichentopf and Martin Reufer — Hochschule Ruhr West, Institut Naturwissenschaften, Mülheim an der Ruhr, Germany

In recent years wavefront measurements using a Shack-Hartmann Sensor became an established way to analyze the beam quality of laser sources. With the detection of the wavefront deformation a change of the modal composition can be recorded instantaneously. While this method is well established for nearly Gaussian laser beams, the wavefront analysis of broadarea semiconductor lasers requires a detailed understanding of the composition of the laser modes. For our investigations we utilize lasers emitting light in the near infrared based on the material system of GaAs. For this type of laser the number and structure of optical modes is affected by thermal as well as electric effects inside the active medium. Spectral information is recorded over the position at the laser facet by means of a spectrometer. Moreover the intensity distribution of the optical near and far field is monitored for a variation of diode currents. To describe the structure of the laser modes the measured intensity distributions are associated with a composition of Hermite Gaussian Modes gained by a simulation software.

HL 83: Focus Session: Functionalization of Semiconductors II

Organizers: Kerstin Volz, Sangam Chatterjee (Universität Marburg), Michael Dürr (Universität Giessen)

Time: Thursday 14:45–17:15 Location: H16

Invited Talk HL 83.1 Thu 14:45 H16

Electronic properties and applications of functionalized wide gap semiconductors — •Martin Stutzmann — Walter Schottky Institut and Physics Department, Technical University of Munich, 85748 Garching, Germany

Wide band gap semiconductors such as SiC, GaN and diamond are well suited for applications in bioelectronics and photochemistry due to their stability, their particular surface chemistry, and the possibility to change their work function by surface termination, alloying, or substitutional doping. In addition, inorganic, organic or biological surface functionalization can be used to enhance the specific properties for the targeted application. In this presentation we will review some recent examples of such applications: specific enzyme-based biosensors, the detection of cellular action potentials with electrolyte-gated field effect transistors, bio-photovoltaics with supported bacterial reaction centers, and the electronic control of photocatalytic reactions.

HL 83.2 Thu 15:15 H16

Frequency Conversion Properties of SnS-Clusters — •Nils W. Rosemann[1], Jens Eussner[2], Ulrich Huttner[1], Andreas Beyer[1], Kerstin Volz[1], Stephan W. Koch[1], Mackillo Kira[1], Stefanie Dehnen[2], and Sangam Chatterjee[1] — [1]Faculty of Physics and Materials Science Center, Philipps-Universität Marburg, Renthof 5, D-35032 Marburg, Germany — [2]Faculty of Chemistry and Materials Sciences Center, Philipps-Universität Marburg, Hans-Meerwein-Straße, D-35043 Marburg, Germany

Clusters based on at least one element of the chalcogenide family exhibit a large variety of physical properties. These arise mainly due to their diverse assembly of the cluster atoms resulting in highly complex electronic landscapes. Hence, such materials are expected to show an intriguing linear response and even more so significant nonlinear optical properties. Here, we present a SnS-based cluster that exhibits an extreme optical nonlinearity.

30 min. Coffee Break

HL 83.3 Thu 16:00 H16

Functionalization of III/V semiconductor surfaces with small organic molecules — •Patrick Vogt — Institut für Festkörperphysik, TU Berlin, Hardenbergstr. 36, 10623 Berlin; Germany.

Hybrid materials consisting of interfaces between organic layers and solid semiconductors form the basis for novel applications in sensing, biophysics and nanotechnology. The understanding of the fundamental properties that determine the interaction between organic materials and semiconductor surfaces, however, is still insufficient. This presentation summarizes our current understanding of the functionalization of differently reconstructed, carefully prepared GaAs, InP and GaP (001) surfaces with organic reagents. The functionalization is characterized by x-ray photoelectron spectroscopy, scanning tunneling microscopy, and by reflectance anisotropy spectroscopy in a spectral range between 1.5 and 5 eV.

HL 83.4 Thu 16:30 H16

Diethyl Ether on Si(001) - An Experimental Study on Adsorption Configurations and Energy Barriers — •Marcel Reutzel[1], Gerson Mette[1], Marcus Lipponer[1], Michael Dürr[1,2], and Ulrich Höfer[1] — [1]Philipps-Universität, 35037 Marburg — [2]Justus-Liebig Universität, 34392 Gießen

The functionalization of semiconductor surfaces with organic molecules has attracted much interest, especially with respect to the challenges arising from the miniaturization in semiconductor device physics. It is thus important to understand the basic adsorption processes of different functional groups on these surfaces.

Here, we present an experimental study of the adsorption configurations and the underlying potential energy curve of diethyl ether on Si(001): At low temperature, diethyl ether adsorbs in a datively bonded intermediate state, as observed by means of STM and XPS experiments. By thermal activation, the ether is cleaved; covalently attached Si-C_2H_5 and Si-O-C_2H_5 fragments are observed on two neighboring dimer rows [*J. Phys. Chem. C* **119**, 6018 (2015)]. Using optical second-harmonic generation, the surface mediated ether cleavage reaction was followed in realtime. Conversion rates were measured as a function of surface temperature; the barrier $\epsilon_a = 0.38 \pm 0.05$ eV ($\nu_a = 10^{4\pm1}$ s^{-1}) was determined. Using molecular beam techniques, the initial sticking probability was measured as a function of surface temperature. From the difference between binding energy ϵ_d and conversion barrier ϵ_a, the binding energy $\epsilon_d = 0.62 \pm 0.08$ eV ($\nu_d = 10^{7\pm1.3}$ s^{-1}) was determined [*J. Phys. Chem. Lett.* **6**, 3971 (2015)].

HL 83.5 Thu 16:45 H16

Ab initio study on precursor reactivity in CVD growth: GaP on Si — •Andreas Stegmüller and Ralf Tonner — Fachbreiech Chemie, Philipps-Universität, 35032 Marburg

Successful growth of high-qualtiy III/V semiconductor materials via CVD or MOVPE is (kinetically) constrained by precursor decomposition chemistry and transport.[1] As *in situ* experimental evidence is scarce DFT calculations were applied being an important means to grasp elementary processes during growth.

The molecular reactivity of commonly applied precursors triethylgallane (TEGa), tertiary butylphosphine (TBP) and higher homologues was screened and fundamental mechanisms were elucidated.[2,3] The insight gained can be utilized to optimize the decomposition behaviour by chemical design in order to reduce energy barriers and, thus, growth temperatures necessary for growth of metastable materials.[4] The influence of the Si substrate on precursor decomposition was investigated for various alkyl compounds of groups 13 and 15 (III/V) applying periodic models of the hydrogen-passivated Si(001)H surface.

[1] A. Brauers, J. Cryst. Growth, 107, 281-289, 1991.
[2] Andreas Stegmüller et al., Phys. Chem. Chem. Phys., 16, 17018-17029, 2014.
[3] Andreas Stegmüller et al., Inorg. Chem., 54, 6363-6372, 2015.
[4] Andreas Stegmüller et al., Chem. Vap. Depos., 21, 161-165, 2015.

HL 83.6 Thu 17:00 H16

***In situ* controlled MOVPE-preparation of As-modified Si(100) surfaces and single-domain GaP heteroepitaxy** — •Oliver Supplie[1,2], Matthias M. May[1,2], Agnieszka Paszuk[1], Andreas Nägelein[1], Peter Kleinschmidt[1], Sebastian Brückner[1,2], and Thomas Hannappel[1,2] — [1]TU Ilmenau, Institut für Physik, FG Photovoltaik — [2]HZB, Institute Solar Fuels

III-V/Si(100) tandem absorber structures are promising for high-efficiency direct solar watersplitting [1]. MOVPE-processing commonly involves arsenic, either supplied directly via precursors or in form of residuals. Annealing of Si(100) in TBAs and background As results in an As-modified surface with a characteristic reflection anisotropy spectroscopy (RAS) signal. We show that its spectral features emerge at different stages of a two-step annealing process. LEED patterns of the final surface show a preferential A-type, (1×2) reconstructed surface with dimer rows in parallel to the step edges. These are also clearly visible in STM images. XPS evidences the presence of As at the surface, but also atomic exchange across the interface. Subsequent pseudomorphic GaP heteroepitaxy leads to single-domain GaP/Si(100) surfaces, which are free of antiphase disorder. The sublattice orientation of the GaP film is inverted compared to GaP grown on H-terminated Si [2]. The atomic structure of the heterointerface is more complex than in the abrupt Si-P case [3] for As-free systems.

[1] M. M. May et al., *Nat. Commun.* **6**, 8256 (2015).
[2] O. Supplie et al., *Phys. Rev. B* **90**, 235301 (2014).
[3] O. Supplie et al., *J. Phys. Chem. Lett.* **6**, 464 (2015).

HL 84: Novel Functional Materials I

Time: Thursday 14:45–17:30 Location: H17

Invited Talk HL 84.1 Thu 14:45 H17

Resonant plasmonic nanoantennas for mid-infrared spectroscopy and sensing — •Frank Neubrech and Harald Giessen — 4th Physics Institute and Research Center SCoPE, University Stuttgart, Stuttgart

Plasmonic nanoantennas confine electromagnetic fields at infrared wavelengths to volumes of only a few cubic nanometers, resulting in huge local fields in the vicinity of the resonantly excited metal particles. These near fields are used to enhance the infrared vibrational bands of molecular monolayers and thus enable a spectroscopic detection with ultra-high sensitivity.[1,2] In the presentation, we will report on fundamental aspects of the vibrational enhancement in surface-enhanced infrared spectroscopy,[3,4] applications to infrared chemical imaging and sensing in life sciences, such as in-situ protein sensing. Additionally, we will present a combination of the above mentioned concept with a high power and broadband mid infrared laser source to further lower the detection limit in infrared spectroscopy.[5]

[1] F. Neubrech et al., Phys. Rev. Lett. **101**, 157403 (2008).
[2] D. Dregely et al., Nat. Commun. **4**, 2237 (2013).
[3] S. Bagheri et al., Adv. Opt. Mater. **11**, 1049 (2014).
[4] S. Bagheri et al., ACS Photonics **2**, 779 (2015).
[5] T. Steinle et al., Opt. Express **23**, 11105 (2015).

HL 84.2 Thu 15:15 H17

Tunable Coulomb-oscillations in improved CoPt nanoparticle based field-effect transistors — •Hauke Lehmann, Svenja Willing, Mirjam Volkmann, and Christian Klinke — Institut für Physikalische Chemie, Universität Hamburg, Grindelallee 117, 20146 Hamburg, Germany

Metallic nanoparticles offer possibilities to build and improve basic electrical devices. The role of a semiconductor bandgap is adopted by the Coulomb energy gap due to the charging of the single particles capacities. Thus, it is required to keep the nanoparticles individualized by tunnel barriers, while a merging of the particles would render them metallic again.

We synthesize monodisperse CoPt nanoparticles by colloidal chemistry. Those particles are deposited via the Langmuir-Blodgett technique as highly-ordered homogeneous monolayers onto substrates with predefined gold electrodes. Additional structuring of the films yields stripes from individual nanoparticles. A local back-gate electrode is employed underneath the channel to influence the transport. This enables good electrostatic control over individually addressable devices without interferences from a dielectric capping layer. It has been found, that the gate electrode is most effective underneath a channel of comparable width, while the position of the gate electrode allows to shift the oscillations. Temperature and applied bias voltage in turn adjust the number of charge carriers in the system. Understanding the influences of the various parameters allows to precisely tailor the system's properties to the needs of future applications.

HL 84.3 Thu 15:30 H17

Highly Mismatched GaAs1-xNx and Ge1-xSnx Alloys Prepared by Ion Implantation and Ultrashort Annealing — •Shengqiang Zhou — Helmholtz-Zentrum Dresden Rossendorf, Dresden, Germany

Doping allows us to modify semiconductor materials for desired properties such as conductivity, bandgap, and/or lattice parameter. A small portion replacement of the highly mismatched isoelectronic dopants with the host atoms of a semiconductor can result in drastic variation of its structural, optical, and/or electronic properties. Here,

the term 'mismatch' describes the properties of atom size, ionicity, and/or electronegativity. In this talk, we present the fabrication of two kinds of highly mismatched semiconductor alloys, i.e., Ge1-xSnx [1] and GaAs1-xNx [2]. The results suggest an efficient above-solubility doping induced by non-equilibrium methods of ion implantation and ultrashort annealing. Pulsed laser melting promotes the regrowth of monocrystalline Ge1-xSnx, whereas flash lamp annealing brings about the formation of high quality GaAs1-xNx with room temperature photoluminescence. The bandgap modification of Ge1-xSnx and GaAs1-xNx has been verified by optical measurements of spectroscopic ellipsometry and photoluminescence, respectively. In addition, effective defect engineering in GaAs has been achieved by flash lamp annealing, by which a quasi-temperature-stable photoluminescence at 1.3 um has been obtained [3, 4]. [1] K. Gao, et al., APL 105, 042107 (2014); [2] K. Gao, et al., APL 105, 012107 (2014); [3] K. Gao, et al., JAP 114, 093511 (2013); [4] S. Prucnal, et al., Opt. Express, 20, 26075 (2012).

HL 84.4 Thu 15:45 H17

Disentangling bulk from surface contributions in the electronic structure of black phosphorus — •Evangelos Golias, Maxim Krivenkov, and Jaime Sánchez-Barriga — Helmholtz-Zentrum Berlin für Materialien und Energie, Elektronenspeicherring BESSY II, Albert-Einstein Str. 15, 12489 Berlin, Germany

Most recently, black phosphorus (BP) has come into focus as a promising material for future applications in nanoelectronic devices due to its unique electronic and transport properties. Here, we use angle-resolved photoemission spectroscopy (ARPES) in conjunction with ab-initio calculations within the framework of density-functional theory (DFT) to disentangle surface from the bulk contributions in the electronic structure of BP. We find good agreement between our theoretical predictions for the intra and interlayer energy-momentum dispersions and the experimentally obtained three-dimensional band structure of this material. Our results provide compelling evidence for the existence of surface-resonant states near the top of the valence band which can play an important role in the performance of electronic devices based on BP.

30 min. Coffee Break

HL 84.5 Thu 16:30 H17

Optoelectronic and charge transport properties of Ta_3N_5 from first principles — •Juliana Morbec[1,2] and Giulia Galli[1] — [1]Institute for Molecular Engineering, University of Chicago, USA — [2]Department of Physics, University of Duisburg-Essen, Germany

Tantalum nitride (Ta_3N_5) is considered a promising material for photoelectrochemical water splitting due to its suitable band gap ($\sim$ 2.1 eV) for visible light absorption and favorable band-edge positions for water splitting. However, Ta_3N_5 photoanodes have been shown to exhibit poor performance, probably due to their rapid photodegradation and to limitations in their charge transport properties. Using first-principles calculations we carried out a detailed study of the optoelectronic and charge transport properties of crystalline Ta_3N_5 [1,2]. We present an analysis of the optoelectronic properties of Ta_3N_5 [1], showing that this material is highly anisotropic, with heavy holes in several directions, pointing to low mobilities. We also discuss the polaronic contributions to the hole and electron mobilities and the effect of stress and substitutional impurities on the electronic structure of Ta_3N_5 [2]. We show that the overall large effective masses of electrons and holes may be reduced with applied strain.

[1] Juliana M. Morbec, Ieva Narkeviciute, Thomas F. Jaramillo, and Giulia Galli, Phys. Rev. B 90, 155204 (2014).
[2] Juliana M. Morbec and Giulia Galli, 2015 (submitted).

ACKNOWLEDGMENTS: This work was supported by the National Science Foundation under the NSF Center CHE-1305124 for CCI Solar Fuels.

HL 84.6 Thu 16:45 H17

Assessment of first-principles structure optimisations, their impact on the band structures, and relative stability of polytypes in GaSe and InSe semiconductors — •Andrei Postnikov[1], Juliana Srour[1,2], Michael Badawi[1], and Fouad El Haj Hassan[2] — [1]Université de Lorraine, LCP-A2MC, Metz, France — [2]Université Libanaise, Faculté des Sciences, Beirut, Lebanon

Lattice parameters of β, γ, δ and ε polytypes of III-VI semiconductors GaSe and InSe are optimised in a sequence of first-principles (within the density functional theory) calculations, done with WIEN2k [1] and VASP [2] codes in comparison, the both being applied with a number of exchange-correlation (XC) "flavours". An underestimation of the van der Waals (vdW) gap between the Se-(cation)-(cation)-Se double layers is largely corrected by inclusion of the vdW interaction according to the (semiempirical) Grimme scheme. A critical analysis is done of different XC types in what regards their impact on the accuracy of the structure prediction and on the fine placement of the valence / conduction bands. The band structures are discussed with respect to their relation to those in chalcopyrite-type $Cu(Ga,In)Se_2$ compounds [3] and in the hexagonal In_2Se_3. For both binary compounds studied, different polytypes are ordered according to their energetic preference.

1. The WIEN2k code, `http://www.wien2k.at` .
2. The VASP code, `http://www.vasp.at` .
3. J.Srour, M. Badawi, F. El Haj Hassan, and A. V. Postnikov, to be published in phys.stat.solidi (c).

HL 84.7 Thu 17:00 H17

Electronic structure calculations for carbon nanotubes under strain — •Christian Wagner[1,3], Jörg Schuster[2], Michael Schreiber[3], Andre Schleife[4], and Thomas Gessner[1,2] — [1]Center for Microtechnologies, TU Chemnitz, Germany — [2]Fraunhofer Institute ENAS, Chemnitz, Germany — [3]Institute of Physics, TU Chemnitz, Germany — [4]Department for Materials Science, University of Illinois at Urbana-Champaign, USA

Carbon nanotube (CNT) optics is an active field of research and is becoming increasingly interesting for applications. CNTs show unique properties upon strain: Under load, their band gap is opening or closing (depending on the CNTs' chirality) which makes them suitable for electronic and optical strain sensing at the nano scale. Further, they could operate as strain-tunable emitters.

We present results of electronic structure calculations for strained CNTs: we employ density functional theory (DFT) for ground states, GW approximation for a correct description of the fundamental gap, and we solve the Bethe-Salpeter-equation for the optical polarization function.

Our results are strain-dependent band gaps and the derived deformation potentials for different CNT chiralities. The strain-induced shift of exciton-related peaks is quantified. This requires cutting off the Coulomb interaction of periodic images in our supercell approach. The strain parameters derived here can be used for large-scale device modeling and is compared to available literature data.

HL 84.8 Thu 17:15 H17

Cubic scaling GW: towards fast quasiparticle calculations — •Peitao Liu[1,2], Merzuk Kaltak[1], Jiri Klimeš[1], and Georg Kresse[1] — [1]University of Vienna, Faculty of Physics and Center for Computational Materials Science, Sensengasse 8/12, A-1090 Vienna, Austria — [2]Institute of Metal Research, Chinese Academy of Sciences, Shenyang 110016, China

Within the framework of the full potential projector-augmented wave (PAW) methodology, we present a promising low scaling GW implemention. It allows for quasiparticle calculations with a scaling that is cubic in the system size and linear in the number of k points used to sample the Brillouin zone. This is achieved by calculating the independent particle polarizability in real space and imaginary time via contraction over the Green's functions of occupied and unoccupied states. The Fourier transformation of the polarizability from the imaginary time to frequency domain is done by a very efficient discrete Fourier transformation with only a few nonuniform grid points. Fast Fourier transformations are used to go from real space to reciprocal space and vice versa. The analytical continuation from the imaginary axis to the real axis is done by exploiting the Thiele's reciprocal difference method. Finally, the method is applied successfully to predict the quasiparticle energies and spectral functions of typical semiconductors (Si, SiC, GaAs and ZnO) and metals (Na, Al, Pd, and $SrVO_3$). The results are compared with conventional standard GW calculations. Good agreement is achieved, highlighting the power of this method.

HL 85: Focus Session: Physics and Application of Emergent 2D-semiconductors and their Heterostructures 2

Atomically thin two-dimensional materials have advanced to the point where they are becoming highly appealing for the study of novel quantum physics and for constructing emergent photonic, electronic and photochemical devices using tailored 2D-heterostructures. The most prominent monolayer 2D material, graphene, has a bandstructure in its pristine form without an electronic bandgap. In contrast, monolayers of transition metal dichalcogenides (TMDCs) tend to be direct gap semiconductors with a bandgap in the visible to near-infrared spectral range. Moreover, the two-dimensional nature of these monolayered semiconductors give rise to very strong excitonic effects, even at ambient conditions and their strong light-matter interactions and spin-valley properties make them highly interesting for e.g. opto-valleytronics and novel coherent light sources. Intriguingly, TMDC crystals can host strongly localized excitons, which result in the possibility to emit quantum light. In this symposium the current status and prospects of the very rapidly evolving field of TMDC research will be summarised including materials properties and synthesis and the exploration of phenomena such as quantum light emission, coherent laser action, spinor excitonics and cavity quantum electrodynamics.

Organizers: Sven Höfling (U Würzburg), Christian Schneider (U Würzburg) and Jonathan Finley (WSI München)

Time: Thursday 15:00–17:00 Location: H8

Topical Talk HL 85.1 Thu 15:00 H8

Bright and dark excitons in transition metal dichalcogenide monolayers — Cedric Robert[1], Gang Wang[1], Aslihan Suslu[2], Bin Chen[2], Sije Yang[2], Sarah Alamdari[2], Iann Gerber[1], Thierry Amand[1], Sef Tongay[2], Bernhard Urbaszek[1], and •Xavier Marie[1] — [1]Universite de Toulouse, INSA-CNRS-UPS, LPCNO, 135 avenue de Rangueil, 31077 Toulouse cedex, France — [2]School for Engineering of Matter, Transport and Energy, Arizona State University, Tempe, AZ 85287, USA

Highly crystalline Mo(1-x)WxSe2 has been synthetized to show engineering of the direct optical bandgap and the spin-orbit (SO) coupling in ternary alloy monolayers. We have investigated the impact of the tuning of the SO splitting on the optical and polarization properties. In particular, we have measured the effect of tuning of the conduction band SO splitting on the bright versus dark exciton state population i.e. photoluminescence (PL) intensity. We show that the MoSe2 PL intensity decreases as a function of temperature by an order of magnitude, whereas for WSe2 we measure surprisingly an order of magnitude increase over the same temperature range (T=4-300K). The ternary material shows a trend between these two extreme behaviors [1]. These results are interpreted on the basis of the reversal of the sign of the spin-orbit splitting in the CB for MoSe2 and WSe2 leading to different temperature dependences of the emission yield. The additional role of the electron-hole exchange interaction on the bright/dark exciton states splitting will also be discussed on the basis of ab-initio calculations. [1] G. Wang, et al, Nature Com. 6, 10110 (2015)

Topical Talk HL 85.2 Thu 15:30 H8

Exciton fine structure in transition-metal dichalcogenides monolayers — •Mikhail Glazov — Ioffe Institute, St.-Petersburg, Russia

Strong spin-orbit interaction in transition-metal dichalcogenides monolayers (TMDCs) such as MoS_2 or WSe_2 results in the spin-valley locking effect: The states of electrons and holes in $\mathbf{K}_\pm$ valleys of the Brillouin zone are spin-split. This makes spin and valley dynamics of charge carriers and their complexes, neutral and charged excitons, in TMCDs non-trivial and interesting. In my talk, an overview of recent theoretical results on exciton and trion fine structure in TMDCs is given. It is shown that the spin/valley dynamics of bright exciton doublet is governed by the long-range exchange interaction between an electron and a hole. The latter provides efficient spin depolarization mechanism of excitons. The developed theory is illustrated by comparison with recent experimental results on time-resolved polarized photoluminescence and Kerr-rotation spectroscopy.

Topical Talk HL 85.3 Thu 16:00 H8

Photonics and polaritonics with van der Waals heterostructures — •Alexander Tartakovskii — Department of Physics and Astronomy, University of Sheffield, Sheffield, S3 7RH, UK

Monolayer films of van der Waals crystals of transition metal dichalcogenides (TMDCs) are direct band gap semiconductors exhibiting excitons with very large binding energies and small Bohr radii, leading to a high oscillator strength of the exciton optical transition. Together with graphene as transparent electrode and hexagonal boron nitride (hBN) as an insulator, TMDC monolayers can be used to produce so-called van der Waals heterostructures. Here we use this approach to make electrically pumped light-emitting quantum wells (LEQWs) and single-photon emitters. We combine this new technology with optical microcavities to demonstrate control of the emitter spectral properties and directionality, making first steps towards electrically injected TMDC lasers. By embedding MoSe2/hBN structures in tuneable microcavities, we enter the regime of the strong light-matter interaction and observe formation of exciton-polaritons. We demonstrate that the magnitude of the characteristic anti-crossing between the cavity modes and the TMDC excitons can be enhanced by embedding a multiple-QW structure, containing two TMDC monolayers separated by an hBN barrier. This work opens a new avenue in the use of van der Waals crystals and heterostructures with a potential for polariton devices operating at room temperature.

Topical Talk HL 85.4 Thu 16:30 H8

van der Waals Epitaxy of 2D materials — •Sefaattin Tongay — Arizona State University, USA

Van der Waals (vdW) epitaxy is a common technique used for production of 2D materials systems. Owing to their chemically passivated surfaces, vdW epitaxy does require any lattice match and a number of 2D transition metal dischalcogenide (TMDCs) and post-transition metal chalcogenides (PTMCs) can be deposited onto various oxide surfaces. Since the underlying substrate and 2D materials weakly interact with each other, vdW epitaxy anticipated to produce 2D systems with material properties closely similar to that of exfoliated ones. This talk will focus on how underlying substrates influence the material properties through interation with 2D layered materials, and introduce colossal band renormalization in some unique systems.

HL 86: Oxide Semiconductors for Device and Energy Applications 2

Time: Thursday 15:00–16:45 Location: H11

HL 86.1 Thu 15:00 H11

How Seebeck coefficient measurements help determine oxide transport properties — •Alexandra Papadogianni[1], Oliver Bierwagen[1], Mark E. White[2], James S. Speck[2], Zbigniew Galazka[3], Kelvin H. L. Zhang[4], Yingge Du[4], and Scott A. Chambers[4] — [1]Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5-7, D-10117 Berlin, Germany — [2]Materials Department, University of California, Santa Barbara, California 93106, USA — [3]Leibniz-Institut für Kristallzüchtung, Max-Born-Straße 2, D-12489 Berlin, Germany — [4]Pacific Northwest National Laboratory, Richland, Washington 99352, USA

Measuring the Hall effect is a common and convenient method to investigate the electrical transport properties of thin samples, providing us with an estimate of integral sheet carrier concentration. In low-mobility p-type semiconducting oxides, such as the Sr-doped $LaCrO_3$, however, Hall measurements fail. For such instances, studying thermoelectric properties, namely the Seebeck coefficient, can be a simple alternative, which provides us with the carrier type and volume carrier concentration. A combination of Seebeck and Hall measurements can moreover be used for estimating the actual thickness of a carrier system within a semiconductor. As an example, an application on n-type SnO_2 shows how this method can help distinguish bulk carriers, with homogeneous depth distribution, from sheet carriers accumulated within a thin layer.

HL 86.2 Thu 15:15 H11

Metal incorporation and reaction-kinetics for the molecular beam epitaxial growth of $(Ga_xIn_{1-x})_2O_3$ — •Patrick Vogt and Oliver Bierwagen — Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5–7, 10117 Berlin, Germany

This contribution presents the metal incorporation and reaction-kinetics study of the plasma-assisted molecular beam epitaxial (MBE) growth of the transparent semiconducting oxide alloy $(Ga_xIn_{1-x})_2O_3$. By using MBE, an impinging Ga- (Φ_{Ga}), In- (Φ_{In}), and oxygen-flux (Φ_O) react amongst others to $(Ga_xIn_{1-x})_2O_3$ on a heated, single-crystalline substrate under ultra-high vacuum conditions. The data obtained were measured *in-situ* by a laser reflectometry (LR) set-up and a line-of-sight quadrupole mass spectrometer (QMS) or *ex-situ* by energy dispersive X-ray spectroscopy (EDX). The LR allowed measuring the growth-rate (ρ), the QMS enabled identifying the species that desorbed off the substrate which are not incorporated into the alloy, and the EDX measurements revealed the In incorporation x and the reciprocal Ga incorporation 1-x.

We present the growth rate dependencies of the binary grown In_2O_3 and Ga_2O_3 as function of growth temperature (T_G). Furthermore, we show the dependence of ρ and x for the ternary grown alloy on T_G, the metal-to-oxide ratio ($r_{MeO} = (\Phi_{In} + \Phi_{Ga})/\Phi_O$) , and the In-to-Ga ratio ($r_{InGa} = \Phi_{In}/\Phi_{Ga}$).

The measured discrepancy of ρ for the binary grown oxides compared to x for the ternary grown alloy can be explained by the different adhesion energies for In and Ga on the $(Ga_xIn_{1-x})_2O_3$ surfaces.

HL 86.3 Thu 15:30 H11

Application of Cr_2O_3 and Cr_2O_3:Mg as a Buffer Layer in Organic Solar Cells — •Daragh Mullarkey[1], Elisabetta Arca[1], Linda Cattin[2], Jean Christian Bernède[3], and Igor Shvets[1] — [1]School of Physics and CRANN, Trinity College Dublin, University of Dublin, Ireland — [2]Université de Nantes, Institut des Matériaux Jean Rouxel, France — [3]Université de Nantes, MOLTECH-Anjou, France

The use of undoped Cr_2O_3 and p-type Cr_2O_3:Mg as an anode buffer layer in organic solar cells is explored. The effects of buffer layer thickness, roughness, and growth conditions on the properties of the solar cell were studied. These effects were investigated for solar cells grown on both indium tin oxide and fluorine doped tin oxide. In both cases, Cr_2O_3 and Cr_2O_3:Mg were found to improve the efficiency of the solar cell.

The band offsets between the anode material and the buffer layer, as well as between the buffer layer and the organic absorber were studied by X-ray Photoelectron Spectroscopy (XPS) and Ultra Violet Photoelectron Spectroscopy (UPS). The efficiency of the solar cells is discussed in terms of the experimentally determined band alignment.

HL 86.4 Thu 15:45 H11

TiO2 laminated Silicon microstructures based stable photocathode for water splitting — •Chittaranjan Das[1], Massimo Tallarida[2], and Dieter Schmeisser[3] — [1]Angewantde Physik / Sensorik ,BTU Cottbus-Senftenberg, Germany — [2]ALBA-Barcelona — [3]Angewantde Physik / Sensorik ,BTU Cottbus-Senftenberg, Germany

The photoelectrochemical (PEC) water splitting is one of the most efficient ways to obtain hydrogen from water using solar power which can be used as carbon free fuel. The PEC device can bedesigned using semiconducting material that will convert solar radiation to H2. Silicon can be one of the best choices for PEC due to its success in solar cells technology. There are certain issues with Si such as stability in electrochemical medium [1] and higher surface reflectance (25%) which limits the Si as an ideal candidate for PEC technique [2].

In the present work we addressed these issues by surface structuring and laminating the surface with metal oxide. The microstructuring of Si was done by electrochemical method. The Si microstructure photocathode was stabilized by thin layer of ALD grown TiO2 film. The microstructuring and lamination of Si photocathode by ALD layer of TiO2 decreased the reflectance ofthe surface and shift the onset potential towards anodic direction by 350 mV with a prolonged stability over 60 hours[3].

[1] C. Levy-Clement, J. Electrochem. Soc 1991, 12, 69 [2] J. Oh, et al. Energy Environ. Sci., 2011, 4, 1690 [3] C. Das, et al. Nanoscale 2015,7, 7726

HL 86.5 Thu 16:00 H11

Optical and Magneto-Optical Investigation of Normal and Disordered $ZnFe_2O_4$ in Relation to Magnetic Properties — •Vitaly Zviagin[1], Peter Richter[2], Yogesh Kumar[1], Israel Lorite[1], Michael Lorenz[1], Dietrich R.T. Zahn[2], Georgeta Salvan[2], Pablo Esquinazi[1], Marius Grundmann[1], and Rüdiger Schmidt-Grund[1] — [1]Universtät Leipzig, Institut für Experimentelle Physik II, Linnéstr. 5, Germany — [2]Technische Universtät Chemnitz, Semiconductor Physics, Reichenheiner Str. 70, Germany

We present the magneto-optical dielectric tensor of normal and disordered $ZnFe_2O_4$ grown at different temperatures on MgO (100) and $SrTiO_3$ (100) substrates by pulsed laser deposition. Optical transitions in the diagonal element of the dielectric function, obtained by spectroscopic ellipsometry, are identified as transitions from O_{2p} to Fe^{3+} 3d and 4s bands. Via the off-diagonal element, obtained by magneto-optical Kerr effect spectroscopy, the observed features are confirmed to be similar to the mentioned transitions. One transition in particular, namely a transition from O_{2p} to tetrahedrally coordinated Fe^{3+} cation, located at $\sim 3.5\,eV$, suggests disorder of the normal crystal structure. Its amplitude is highest for the sample grown at the lowest temperature in both the diagonal and off-diagonal elements of the dielectric tensor. Furthermore, the overall magnetic response, measured by SQUID, is highest for the sample grown at the lowest temperature, suggesting that the presence of Fe^{3+} on the tetrahedral sites is directly related to the ferrimagnetic order of the crystal due to the dominating nature of the oxygen mediated coupling between the two lattice sites.

HL 86.6 Thu 16:15 H11

Monitoring Proton Diffusion in Thin Films of Tungsten Oxide — •Simon Burkhardt[1], Sabrina Darmawi[1], Matthias T. Elm[1,2], and Peter J. Klar[1] — [1]I. Physikalisches Institut, Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, 35392 Gießen — [2]Physikalisch-Chemisches Institut, Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 17, 35392 Gießen

The reversible change of the optical properties of materials due to the electrochemical insertion of ions is called electrochromism. Tungsten-VI oxide (WO_3) and its electrochromic properties have been intensively studied since 1969 as a model system which nowadays can be found in applications like smart window systems or other coated glasses. However fundamental questions concerning the colouration mechanism are still under discussion. A combination of electrochemical proton insertion and *in situ* UV/Vis-transmission spectroscopy is applied to provide new insights. With the developed set up it is not only possible to investigate the time-dependence of the colouration behaviour, but it also allows a spatially resolved analysis of the colouration process and

thus the ion diffusion in electrochromic thin films. To investigate the diffusion of protons, thin films of WO_3 are deposited on TCO-coated substrates via electron beam evaporation and coated with a structured PMMA layer to enable local ion insertion. Significant differences in the colouration behaviour of amorphous and crystalline WO_3 films can be observed which will be compared with a simulation of lateral 1D diffusion processes.

HL 86.7 Thu 16:30 H11

Oxygen Vacancies in the Ultrathin SiO_2 Interfacial Layer of High-K/Metal Gate CMOS Devices — •Florian Lazarevic[1,2], Roman Leitsmann[1,2], Philipp Plänitz[1], and Michael Schreiber[2] — [1]MATcalc, AQcomputare GmbH, Annaberger Str. 240, 09125 Chemnitz, Germany — [2]Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany

We study oxygen vacancy defect levels in ultrathin SiO_2 layers in metal-oxide-semiconductor devices. First principles calculations were performed to model a $Si/SiO_2/HfO_2$ gate stack and a SiO_2 bulk reference system. The extremely thin SiO_2 layer thickness and dissimilar structural and electronic properties of the adjacent layers (namely Si and HfO_2) result in a degeneration and stabilization of certain SiO_2 bulk defects. We find that partial H passivation of the vacancies additionally stabilizes defects energetically which are related to the leakage current in CMOS devices. Furthermore the incorporation of F atoms has a large influence on the stability of H passivated SiO_2 defects.

HL 87: Transport: Molecular Electronics and Photonics 2 (Joint session of CPP, DS, HL, MA, O and TT, organized by TT)

Time: Thursday 15:00–16:00 Location: H23

HL 87.1 Thu 15:00 H23

First-principles calculation of the thermoelectric figure of merit for [2,2]paracyclophane-based single-molecule junctions — •Marius Buerkle[1], Fabian Pauly[2], and Yoshihiro Asai[1] — [1]AIST Tsukuba — [2]University Konstanz

Here we present a theoretical study of the thermoelectric transport through [2,2]paracyclophane-based single-molecule junctions [1]. Combining electronic and vibrational structures, obtained from density functional theory (DFT), with nonequilibrium Green's function techniques allows us to treat both electronic and phononic transport properties at a first-principles level. Paracyclophane derivatives offer a great flexibility in tuning their chemical properties by attaching different functional groups. We show that, for the specific molecule, the functional groups mainly influence the thermopower, allowing us to tune its sign and absolute value. We predict that the functionalization of the bare paracyclophane leads to a largely enhanced electronic contribution ZelT to the figure of merit. Nevertheless, the high phononic contribution to the thermal conductance strongly suppresses ZT. Our work demonstrates the importance to include the phonon thermal conductance for any realistic estimate of the ZT for off-resonant molecular transport junctions.

[1] M. Buerkle et al., PRB **91**, 165419 (2015)

HL 87.2 Thu 15:15 H23

Switching the conductance of a molecular junction by proton transfer — •Dominik Weckbecker, Pedro B. Coto, Chriszandro Hofmeister, and Michael Thoss — Institut für Theoretische Physik, Staudtstraße 7/B2, 91058 Erlangen, Germany

The idea of designing switches or diodes using single molecules has motivated intensive experimental and theoretical research on the conductance properties of these systems. In particular, it has been demonstrated that a molecular junction may be used as a nanoswitch if the molecular bridge has two stable states with different conductance that can be reversibly transformed into each other [1]. In this contribution, we explore the possibility of switching a molecular junction using a proton transfer reaction triggered by an external electrostatic field [2]. The study uses transport theory based on first-principles electronic structure calculations [2,3] and considers molecular junctions with graphene or gold as material for electrodes. We show that for the systems investigated, proton transfer can be used for the reversible interconversion between two states, which exhibit different degrees of delocalization of the π-electrons and therefore very different conductance.

[1] S. J. van der Molen et al., J. Phys.: Cond. Mat. **22**, 133001 (2010)
[2] C. Hofmeister et al., J. Mol. Model. **20**, 2163 (2014)
[3] M. Brandbyge et al., PRB **65**, 165401 (2002)

HL 87.3 Thu 15:30 H23

Design rules for molecular electronics: Diarylethene molecules und derivatives — •Lokamani Lokamani[1], Torsten Sendler[1], Peter Zahn[1], Sibylle Gemming[1,2], and Artur Erbe[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf e.V., 01314 Dresden, Germany. — [2]Instiute of Physics, Technische Universität, 09107 Chemnitz, Germany.

Diarylethenes, a class of photosensitive molecules which exhibit photochoromism, can be switched between open- and closed-ring isomers. In break-junction experiments diarylethene derivatives[1] in open and closed-ring forms can be distinguished by a low and high conductance state respectively with a difference in current levels of about one order of magnitude. In addition, these molecules exhibit stable electrical characteristics in both conductance states. Here, we study the electronic transport properties of such derivatives at the level of single molecules. In particular, we analyze the effect of various electron accepting and donating groups on the conductance properties of single molecules attached to gold electrodes. We explore the underlying design rules for molecular electronics comparing break-junction experiments and the theoretical investigations on diarylethene molecules and derivatives.

[1] T. Sendler et al., Advanced Science **2**, 1500017 (2015)

HL 87.4 Thu 15:45 H23

Experimental investigation of the role of electron-phonon-coupling on the Mott critical behavior in the organic charge-transfer salts κ-(BEDT-TTF)$_2$X — •E. Gati[1], M. Garst[2], R.S. Manna[1], U. Tutsch[1], B. Wolf[1], S. Hartmann[1], L. Bartosch[3], T. Sasaki[4], H. Schubert[1], J.A. Schlueter[5], and M. Lang[1] — [1]Physikalisches Inst., Goethe Uni, SFB/TR49, Frankfurt, DE — [2]Inst. f. Theo. Physik, Universität zu Köln, DE — [3]Inst. f. Theo. Physik, Goethe Uni, FfM, DE — [4]IMR, Tohoku University, Sendai, Japan — [5]Materials Science Division, Argonne National Laboratory, USA

The Mott transition is one of the key phenomena of strongly correlated electron systems. Of fundamental interest is the determination of its critical behavior and the underlying universality class. Despite intensive experimental efforts, the universality class is still unresolved. A key aspect, which has not been addressed in these approaches, is the role of electron-phonon-coupling as it is supposed to alter the critical properties to Landau criticality [1]. We will present thermal expansion studies under pressure [2] on the organic charger-transfer salt κ-(BEDT-TTF)$_2$Cu[N(CN)$_2$]Cl. This technique is a very sensitive tool to detect critical behavior [3] as well as influences of the lattice on the electronic subsystem [1]. Our results clearly show a breakdown of Hooke's law of elasticity which is a direct evidence for significant electron-phonon-coupling. Furthermore, we will discuss its effect on the critical exponents determined by this thermodynamic probe.

[1] Zacharias et al., PRL **109**, 176401 (12)
[2] Manna et al., Rev. Sci. Instrum. **83**, 085111 (2012)
[3] de Souza et al., PRL **99**, 0370031 (2007)

HL 88: Frontiers of Electronic Structure Theory: Focus on Topology and Transport V

Time: Thursday 15:00–18:15 Location: H24

HL 88.1 Thu 15:00 H24

Zero-point renormalization of the electronic structure: trends across chemical and structural space — •Honghui Shang[1], Christian Carbogno[1], Patrick Rinke[1,2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — [2]Aalto University, Helsinki, Finland

The importance of the renormalization of the electronic structure due to the zero-point nuclear motion (ZPR) has been discussed since long [1,2], but only recent advances in the first-principles treatment of electron-phonon coupling (EPC) enabled an accurate assessment of this effect for simple, prototypical materials, e.g., diamond [3] and Si [4]. However, it is largely unknown how chemical and structural properties affect the ZPR. To shed light on this question, we compute the EPC and ZPR for the octet binaries in both the zincblende and NaCl structure. Computationally, this is achieved by exploiting our recent implementation of density-functional perturbation theory in real-space, which provides considerable computational advantages with respect to numerical costs, parallelization, and especially scalability with respect to the number of atoms. We demonstrate the validity of our implementation by comparing with existing studies and finite difference results, investigate the trends across chemical/structural space, and critically discuss the role of the exchange-correlation functional.

[1] P. B. Allen and V. Heine, J. Phys. C **9**, 2305 (1976).
[2] M. Cardona, Solid State Commun. **133**,3 (2005).
[3] F. Giustino,*et.al.* Phys. Rev. Lett. **105**, 265501 (2010).
[4] S. Poncé, *et.al.* J. Chem. Phys. **143**, 102813 (2015).

HL 88.2 Thu 15:15 H24

All-Electron Many-Body Approach to X-Ray Absorption Spectroscopy — •Christian Vorwerk, Caterina Cocchi, and Claudia Draxl — Institut für Physik, Humboldt-Universität zu Berlin, 12489 Berlin, Germany

We present an all-electron approach of the many-body perturbation theory to describe X-ray absorption spectroscopy (XAS) in solid-state materials. In this formalism, the electron-hole interaction is explicitely included by solving the Bethe-Salpeter equation. A fully relativistic description of core states, as implemented in the all-electron full-potential code `exciting`[1], enables the explicit treatment of the effects of spin-orbit coupling in the spectra. We investigate the XAS for prototypical systems, such as TiO_2 and MgO, considering excitations from oxygen K and metal L edges. Our results, in good agreement with experiments, allow us to gain insight into the nature of the core-level excitations of these materials.

[1] A. Gulans et al., J. Phys. Condens. Matter 26, 363202 (2014).

HL 88.3 Thu 15:30 H24

Cohesive properties from all-electron RPA total energies — •Markus Betzinger[1], Christoph Friedrich[1], Andreas Görling[2], and Stefan Blügel[1] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Germany — [2]Lehrstuhl für Theoretische Chemie, Universität Erlangen-Nürnberg, Germany

We present an all-electron implementation of the RPA total energy within the full-potential linearized augmented plane-wave (FLAPW) method. An incomplete basis-set correction (IBC) [1] is employed to improve the convergence of the total energy with respect to the basis-set and the number of unoccupied states. To some extent the IBC incorporates an infinite number of bands and enables a virtually exact treatment of the core electrons.
We demonstrate that the core electrons give rise to a sizeable contribution to the RPA total energy. Their individual contribution is comparable to that of the valence electrons. All-electron RPA lattice constants and bulk moduli are shown for a set of prototype materials and compared to experimental results. An excellent agreement with experiment is observed.
[1] M. Betzinger *et al.*, Phys. Rev. B (accepted, 2015); **88**, 075130 (2013); **85**, 245124 (2012).

HL 88.4 Thu 15:45 H24

Explicitly correlated self consistent field theory — •Christian Lasar and Thorsten Klüner — Universität Oldenburg

Explicitly correlated correlation methods are an interesting field of current research since they are able to drastically improve the otherwise slow basis set convergence of conventional correlation methods. Therefore, chemical accuracy can be achieved with rather small basis sets.[1] The new correlation method presented in this contribution has already been developed for two-electron systems a long time ago[2]. We present the generalization of this ansatz to N-electron systems.

The basic idea is to augment a single slater-determinant with an explicitly correlated prefactor which then takes care of the correlation effects and the basis set convergence. Another interpretation of this ansatz would be a contracted CISD with orbital optimization in a complete basis set. The contraction is achieved by the explicitly correlated prefactor whose choice therefore defines the possible accuracy of the method. In principle, the generalization to any pair method i.e. CCSD and MP2 will be possible.

The big advantage of this kind of ansatz for the wave function is the drastic reduction of matrix elements needed for the optimization of the wave function. As a result, the presented method will be applicable to large molecules.

[1] Chem. Rev. 112, p. 4 (2012) [2] J. Chem. Phys. 99, p. 8830 (1993)

HL 88.5 Thu 16:00 H24

Representing energy landscapes by combining neural networks and the empirical valence bond method — •Sinja Klees[1], Ramona Ufer[2], Volodymyr Sergiievskyi[2], Eckhard Spohr[2], and Jörg Behler[1] — [1]Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D-44780 Bochum, Germany — [2]Lehrstuhl für Theoretische Chemie, Universität Duisburg-Essen, D-45141 Essen, Germany

In recent years, artificial neural networks (NNs) have become a powerful method to develop reactive interatomic potentials for large systems. However, the construction of NN potentials can become computationally very demanding due to the high dimensionality of the configuration space, which needs to be mapped by reference electronic structure calculations. Combining NN potentials with the empirical valence bond (EVB) method offers a promising approach to derive the potential energy of complex systems with substantially reduced effort, since the size of the reference structures can be strongly decreased. Preliminary results will be discussed and compared to density functional theory data.

HL 88.6 Thu 16:15 H24

CELL: a python package for cluster expansions with large parent cells — •Santiago Rigamonti[1], Maria Troppenz[1], Christopher Sutton[2], Luca M. Ghiringhelli[2], and Claudia Draxl[1] — [1]Humboldt-Universität zu Berlin — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft

The discovery of new materials for applications in areas such as energy harvesting, relies more and more on the accurate theoretical description of complex structures with large unit cells. The properties of interest are often tuned by substitutional dopants. Due to the vast configurational dopant space, a wide-spread approach is the cluster expansion (CE) technique. Most available CE codes are designed for alloys based on small parent cells, with usually 1 to 4 atoms. For the many important materials with much larger parent cells such approaches can't be applied. We devise an iterative scheme, based on efficient samplings of the configurational space, avoiding full structure enumerations. CELL consists of several modules that can be used independently, enabling to design CEs for specific purposes. Various CE schemes are available, offering ℓ_2 and ℓ_1 norms as penalization terms and different cross-validation strategies. Methods such as LASSO and split Bregman iteration are available for dealing with the ℓ_1 norm (compressive sensing). Access to finite-temperature properties and the characterization of phase transitions is possible through the Wang-Landau and diffusive nested sampling modules. Examples are presented for type-I thermoelectric clathrates, with 46 sites in the parent cell.

HL 88.7 Thu 16:30 H24

Structural and electronic properties of the thermoelectric clathrates $Ba_8Al_xSi_{46-x}$ and $Sr_8Al_xSi_{46-x}$ — •Maria Troppenz, Santiago Rigamonti, and Claudia Draxl — Humboldt-Universität zu Berlin

Clathrate compounds are promising candidates for high-efficiency thermoelectric applications. Their cage-like structure containing guest atoms allows for exploiting the idea of the phonon-glass electron-crystal and reaching a large figure of merit. We study $Ba_8Al_xSi_{46-x}$ and $Sr_8Al_xSi_{46-x}$ ($6 \leq x \leq 16$), where optimal electronic properties are expected close to the Zintl composition ($x = 16$). Cluster expansions on various quantities are performed, thus having access to ground-state as well as finite-temperature properties. A linear increase of the lattice constant with the number of Al substituents is obtained (0.019 Å per Al addition) confirming experimental observations (0.02 Å). The calculated bond distances between high-symmetry sites agree well with experiment for the full compositional range [1,2]. We find a close correlation between bond distances and fractional Al occupancies. This helps improving models used by experimentalists to estimate fractional occupancies. The substitutional configurations present an order-disorder transition around $600 - 900$ K, which is further analyzed applying the Wang-Landau method. An important finding is the semiconducting behavior of the low-temperature ordered phase at the Zintl composition, which points out the technological relevance of these compounds.

[1] J. H. Roudebush *et al.*; *Inorg. Chem.* **51**, 4161 (2012)
[2] M. Bobnar *et al.*; *Dalton Trans.* **44**, 12680 (2015)

HL 88.8 Thu 16:45 H24

***Ab-initio* calculation of Raman spectra of graphene-based materials** — •Albin Hertrich, Caterina Cocchi, Pasquale Pavone, and Claudia Draxl — Department of Physics, Humboldt-Universität zu Berlin, Germany

Raman scattering is an important non-destructive method for characterizing carbon-based materials. The main features of experimental Raman spectra of pristine graphene and graphite are the first-order G-band at ≈1580 cm^{-1} and the dispersive second-order 2D-band at ≈2700 cm^{-1}. We calculate first- and second-order Raman spectra fully *ab-initio* using the full-potential all-electron DFT package `exciting` [1], which allows for the calculation of both phonon dispersion, within the frozen-phonon approximation, and frequency-dependent dielectric tensors, from time-dependent DFT and the Bethe-Salpeter equation. In our approach [2], we expand the dielectric tensor with respect to the phonon normal coordinates. By taking its derivatives and by computing vibrational matrix elements, we calculate Raman scattering intensities. Applying this scheme to monolayer graphene, bilayer graphene, and graphite, we obtain the G-band in good agreement with experiment [3]. Furthermore, we explore the influence of both the stacking sequence and the laser energy on the 2D-band.

[1] A. Gulans *et al.*, J. Phys.: Condens. Matter **26**, 363202 (2014).
[2] C. Ambrosch-Draxl *et al.*, Phys. Rev. B **65**, 064501 (2002).
[3] A. C. Ferrari *et al.*, Phys. Rev. Lett. **97**, 187401 (2006).

HL 88.9 Thu 17:00 H24

Exciton dispersion in layered and 2D systems — •Francesco Sottile[1,2], Giorgia Fugallo[1,2], Pierluigi Cudazzo[1,2], and Matteo Gatti[1,2,3] — [1]Laboratoire des Solides Irradiés, École Polytechnique, CNRS, CEA-IRAMIS, Université Paris-Saclay, F-91128 Palaiseau, France — [2]European Theoretical Spectroscopy Facility — [3]Synchrotron SOLEIL, L'Orme des Merisiers, Saint-Aubin, Boîte Postale 48, F-91192 Gif-sur-Yvette, France

The study of the exciton dispersion is of paramount importance for all applications involving light harvesting, beside providing fundamental knowledge about exciton mobility and migration. Using state-of-the-art ab initio many-body approach, like the Bethe-Salpeter equation [1], we present a first principle study of exciton dispersions in layered materials and 2D systems. Results for the former systems (on the prototypical hBN and MoS2) have been recently confirmed by experiments carried out at the Synchrotron ESRF [2]. For the latter (2D) systems we investigate exciton dispersion in graphane and hBN. From our results we provide a general picture of the mechanisms governing the dispersion of neutral excitations in 2D systems, and of the role played by the confinement of the electronic charge in setting the exciton binding energy. In particular we found that due to the strongly reduced screening of the Coulomb interaction in low- dimensional materials, the binding energy of both Wannier and Frenkel excitons in the optical spectra is large and comparable in size[3]. [1] M. Gatti et al., Phys. Rev. B 88, 155113 (2013) [2] G. Fugallo et al. Phys. Rev. B 92, 165122 (2015) [3] P. Cudazzo et al. submitted to Phys. Rev. Lett.

HL 88.10 Thu 17:15 H24

Electronic structure of selected superheavy elements (Z>104) — •Hana Cencarikova[1] and Dominik Legut[2] — [1]Institute of Experimental Physics, SAS, Kosice, Slovakia — [2]IT4Innovations Center, VSB-TU Ostrava, CZ 708 33 Ostrava, Czech Republic

The electronic structure of selected super-heavy elements (Z>104) have been determined from the first-principle calculations based on the density functional method. To determine the ground-state structure we have calculated number of basic phases including the face-centered cubic, body-centered cubic, simple cubic as well as hexagonal closed packed structures. Our results were obtained using local density approximation for the exchange and correlation effects and without and with the spin-orbit interaction for the band states. The analysis has been focused on the determination of the electronic density of states, electronic band structure dispersion relation, mechanical properties (elastic constants) and selected thermodynamical properties.

HL 88.11 Thu 17:30 H24

Layer-resolved calculated vibrations at gold surfaces — •Andrei Postnikov[1] and Kamil Moldosanov[2] — [1]Université de Lorraine, LCP-A2MC, Metz, France — [2]Kyrgyz-Russian Slavic University, Bishkek, Kyrgyzstan

Vibration modes at (001), (011) and (111) surface of gold are calculated from first principles, using the Siesta method [1] and the frozen phonon approach. Calculations are done on thick slabs of moderate lateral size – (2×2) for (001), (2×3) for (011), (3×3) for (111). This allows to resolve the vibration patterns layer by layer into the depth, in dependence on the in-plane wavevector component, and discriminating the polarisation of vibration modes. One notes the softening of modes at the surface, and an appearance of specifically surfacial modes. The bulk behaviour is largely recovered from the 5th or 6th layer downwards.

This study was driven by an intention to grasp the properties of longitudinal acoustic modes propagating at some depth under the surface of gold nanoparticles, which were an important element of our recent work related to the mechanism of radiofrequency absorption and hence resulting heating of nanoparticles of $\gtrsim 5$ nm size [2]. Since it is difficult to meaningfully incorporate the diversity of the nanoparticles' shapes in a practical calculation, the vibrations beneath the most common facets occurring at the nanoparticles' surface were studied instead.

1. The Siesta method, `http://departments.icmab.es/leem/siesta/` .
2. A. Postnikov and K. Moldosanov, `http://arxiv.org/abs/1508.00735` .

HL 88.12 Thu 17:45 H24

Electronic structure, mechanical and thermodynamic properties of Actinium from first-principles — •Zuzana Grosmanova[1] and Dominik Legut[2] — [1]Nanotechnology, VSB-TU Ostrava, CZ 708 33 Ostrava, Czech Republic — [2]IT4Innovations Center, VSB-TU Ostrava, CZ 708 33 Ostrava, Czech Republic

In this work, the mechanical (elastic constants) and thermodynamic properties of actinium were investigated using first-principle calculations. Our results were obtained using density functional theory employing local density and general gradient approximation for the electronic exchange-correlation effects and including the spin-orbit interaction for the band states. The ground-state structure were determined among simple phases like the face-centered cubic, body-centered cubic, simple cubic as well as hexagonal closed packed structures.

HL 88.13 Thu 18:00 H24

Interaction of Tritium and Chlorine 36 with defects in Graphite: Insights from Theory — •Christoph Lechner[1], Philippe Baranek[1], and Holger Vach[2] — [1]EDF Lab Les Renardières, Avenue des Renardieres, F-77818 Moret-sur-Loing Cedex, France — [2]CNRS-LPICM, Ecole Polytechnique, F-91128 Palaiseau Cedex, France

In order to optimize the waste management of nuclear graphite used in power plants, it is important to understand the properties of the activated impurities it contains, such as tritium and chlorine 36. Therefore, a computational study of the interaction of tritium and chlorine 36 with defects in graphite has been achieved at the density functional theory (DFT) level by using the functionals PBE and PBE0 with Grimme's D3 dispersion correction. The physisorption and chemisorption of atomic and molecular hydrogen or chlorine on graphite surfaces, (001), (100), and (110) with or without mono- and divacancies, have been investigated. The stabilities of the formed complexes are interpreted in terms of the formation energy. To obtain insight into the nature of the bonding a population analysis of the systems has been performed. While the bonding of hydrogen is mostly covalent for

chemisorption and van der Waals for physisorption, the behavior of chlorine is much more complex. Depending on the defect site, both, dominantly covalent and dominantly charge transfer bonding, is observed. Raman spectra for selected structures have been investigated, in order to evaluate, if the experimentally observed defect bands can be reproduced.

HL 89: Quantum Dots and Wires: Lasing

Time: Thursday 16:00–17:45 Location: H13

HL 89.1 Thu 16:00 H13

Sub- and Superradiance in Quantum-Dot Nanolasers — •Heinrich A.M. Leymann[1], Alexander Foerster[1], Christopher Gies[2], Marc Assmann[3], Christian Schneider[4], Martin Kamp[4], Sven Höfling[4], Manfred Bayer[3], Frank Jahnke[2], and Jan Wiersig[1] — [1]Otto-von-Guericke-Universität Magdeburg Postfach 4120 39016 Magdeburg — [2]Institut for Theoretical Physics University of Bremen P.O. Box 330 440 28334 Bremen, Germany — [3]Experimentelle Physik 2 Technische Universität Dortmund Otto-Hahn-Straße 4 D-44227 Dortmund Germany — [4]Technische Physik Am Hubland 97074 Würzburg

We investigate the influence of radiative coupling between emitters in quantum-dot (QD) nanolasers. For typical lasers with tens to hundreds of active QDs, a strong impact of sub- and superradiance (SR) on laser characteristics is demonstrated. It is shown that radiative coupling enhances spontaneous emission such that significantly fewer emitters are required to reach the lasing threshold [1]. The SR coupling can seemingly change the β-factor by an order of magnitude. Experimental results show a direct connection between superradiant pulse emission and distinctive changes in the photon correlation function which is in excellent agreement with the theoretical results. Calculations are based on a microscopic laser theory for the coupled multi-QD-cavity-photon system [2].

[1] Phys. Rev. Applied **4**, 044018 (2015).
[2] Phys. Rev. B **89**, 085308 (2014).

HL 89.2 Thu 16:15 H13

Imaging the lasing emission of semiconductor nanowires — •Walter Dickmann[1], Max Riediger[1], Robert Röder[1], Robert Buschlinger[2], Carsten Ronning[1], and Ulf Peschel[2] — [1]Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — [2]Institut für Festkörpertheorie und Optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

The forthcoming limitations of conventional on-chip electronic circuits make the development of miniaturized photonic circuits desirable, which should be driven by coherent nanoscale light sources. Semiconductor nanowires are very promising as such functional device, because they provide efficient waveguiding in sub-wavelength diameter scales as well as lasing above a material dependent threshold. The emission features of single ZnO NWs are investigated in a head-on setup, as they highly affect the coupling efficiency into envisaged photonic circuits. Direct imaging of the far-field emission allows the characterization of the transverse mode(s) as well as their polarization features. This is realized by calculating the Stokes parameters from Fourier mappings of the far field. The measured intensity distributions are unambiguously assigned to the respective transverse lasing modes in agreement with FDTD simulations: For NW diameters below 180 nm, only the fundamental mode HE11 lases, while in thicker NWs additionally the TE01 mode contributes significantly.

HL 89.3 Thu 16:30 H13

Strain induced tunable semiconductor nanowire lasers — •Maximilian Zapf[1], Lisa Schade[1], Robert Röder[1], Karl Winkler[2], Alois Lugstein[2], and Carsten Ronning[1] — [1]Institute of Solid State Physics, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — [2]Institute of Solid State Electronics, TU Wien, Floragasse 7, A-1040 Vienna, Austria

Semiconductor nanowire (NW) lasers are a promising approach for the future miniaturization of optoelectronic devices. An emerging goal of research on nanoscale laser systems is the ability to tune the emission spectrally, which is achieved within semiconductor nanowires by inducing strain. Both the possibility of a strain induced bandgap modulation and laser oscillations in semiconductor NWs have been proven in several studies [Wei et al., Nano letters 12, 4595 (2012) ; Geburt et al., Nanotechnology 23, 365204 (2012)]. This has recently raised the idea of combining both efforts, aiming for lasing in strain tunable devices. Such devices were fabricated by placing NWs on a structured low refractive index substrate in a way that both NW ends are fixed, while the middle part is bridging a length tunable gap. Strain is applied by bending the sample macroscopically with a home built stage, which provides uniaxial strain to the gap area of the NW. Nanowire lasing measurements were conducted as a function of the applied strain, which lead to changes in the emission spectra as well as in the gain/loss ratio of the laser device. Furthermore, the device geometry enables the realization of strain switchable photonic waveguides.

15 min. Coffee Break

HL 89.4 Thu 17:00 H13

Lasing at arbitrary frequencies with atoms with broken inversion symmetry and an engineered electromagnetic environment — •Michael Marthaler[1], Martin Koppenhöfer[1], Karolina Słowik[1,2], and Carsten Rockstuhl[1] — [1]Karlsruhe Institute of Technology — [2]Instytut Fizyki, Uniwersytet Mikołaja Kopernika

We consider a two level system with both a transversal and longitudinal coupling to the electromagnetic field. If the longitudinal coupling is sufficiently, strong multi-photon transitions become possible. We assume that the electromagnetic environment has a spectrum with a single sharp resonance which serves as a lasing cavity. Additionally the electromagnetic environment should have a very broad peak at a frequency which differs form the sharp resonance. We use the polaron transformation, and derive a rate equation which can describe the dynamics of our system. Lasing at the frequency of the sharp mode is possible if the energy difference of the atomic transition is similar to the sum of the frequencies of both peaks in the spectral function. This allows for the creation of lasing over a large frequency range.

HL 89.5 Thu 17:15 H13

Pump-probe quantum state tomography in quantum-dot amplifiers: Theory and experiment — •Fabian Böhm[1], Nicolai B. Grosse[1], Nina Owschimikow[1], Roland Aust[2], Benjamin Lingnau[2], Mirco Kolarczik[1], Kathy Lüdge[2], and Ulrike Woggon[1] — [1]Institut für Optik und Atomare Physik, Technische Universität Berlin, Germany — [2]Institut für Theoretische Physik, Technische Universität Berlin, Germany

Optical quantum state tomography is a method which allows to reconstruct a quantum state by obtaining it's corresponding Wigner function. It can be used to infer the state's density matrix and thus the full quantum information such as the photon number distribution or correlation function can be obtained. We apply this technique to an In(Ga)As quantum-dot optical amplifier and investigate how the coherent state of an ultrashort probe pulse tuned to the quantum dot ground state is transformed by passing through the device. Combination with a probe pulse tuned to the excited state gives access to the dynamics of population inversion and device gain on a sub-picosecond scale as well as the amplified and spontaneous emission noise relative to the quantum noise limit in the amplifier. We experimentally study depletion and recovery mechanisms in the population inversion for varying pump currents and compare them with predictions from a theoretical model for semiconductor amplifiers.

HL 89.6 Thu 17:30 H13

Ultrafast optical pulse modulation in hybrid silicon nitride/colloidal quantum dot systems — •Christian Ulbrich[1], Bastian Herzog[1], Pieter Geiregat[2,3], Yunpeng Zhu[3], Yücel Kaptan[1], Mirco Kolarczik[1], Zeger Hens[2], Dries van Thourhout[3], Ulrike Woggon[1], and Nina Owschimikow[1] — [1]Institut für Optik und Atomare Physik, Technische Univeristät Berlin, Germany — [2]Physics and Chemistry of Nanostructures Group, Faculty of Science, Department of Inorganic and Physical Chemistry,

Ghent Univeristy, Belgium — [3]Photonics Research Group, Faculty of Engineering and Architecture, Department of Information Technology, Ghent Univeristy, Belgium

To explore the prospects for the integration of quantum dots with silicon photonics, we investigate the effect of colloidal PbS quantum dots coated onto SiN waveguides on the optical properties of the waveguides. The quantum dots are coupled to the waveguide mode via the evanescent field. In heterodyne detected pump-probe experiments we study (cross)-amplitude and -phase modulation of a probe pulse induced by optical pumping of intra- and interband transitions of the quantum dots.

HL 90: Poster III

Topics: Organic-inorganic perovskite semiconductors, Graphene, Oxide Semiconductors other than ZnO, Organic photovoltaics and electronics, Quantum information systems, Carbon: Diamond, nanotubes

Time: Thursday 16:00–19:00 Location: Poster A

HL 90.1 Thu 16:00 Poster A

In Situ Raman Spectroscopy for the Characterization of Plasma Textured Black Silicon — •Maria Gaudig[1,2], Jens Hirsch[1,3], Dominik Lausch[3], Paul-T. Miclea[2,3], Alexander N. Sprafke[2], Norbert Bernhard[1,3], and Ralf B. Wehrspohn[2,4] — [1]Anhalt University of Applied Sciences, Technologies of Photovoltaics Group, Bernburger Str. 55, D-06366 Köthen — [2]Martin Luther University Halle-Wittenberg, Institute of Physics, Group mikroMD, Heinrich-Damerow-Str. 4, D-06120 Halle (Saale) — [3]Fraunhofer Center for Silicon Photovoltaics CSP, Otto-Eißfeldt-Straße 12, D-06120 Halle (Saale) — [4]Fraunhofer Institute for Mechanics of Materials IWM, Walter-Hülse-Str. 1, D-06120 Halle (Saale)

Black silicon (b-Si) promises with its extremely low reflectivity to become a real alternative to wet chemical textured silicon in the PV industry. In this work, the nano texturing is realized with a maskless SF6/O2 plasma etch process. We showed different plasma textures with absorption about 95 % and effective lifetimes in the microsecond, which is adequate for solar cells. However, the physical understanding behind the b-Si formation is still insufficient. To clarify the creation of these small nano-needles by a maskless process, we applied Raman spectroscopy, which provides information about the surface roughness, stress or amorphous silicon formation and the chemical composition on the surface. A Raman probe is constructed inside the plasma etch chamber. Transient Raman spectra were measured and evaluated. In this contribution, we will show the results of these in situ measurements and our conclusions concerning the b-Si formation.

HL 90.2 Thu 16:00 Poster A

Improved Selenization Process of Wet-Chemically Fabricated Cu2ZnSn(S,Se)4 Absorbers for Thin-Film Solar Cells — •Markus Neuwirth[1], Huijuan Zhou[1], Mario Lang[1], Niklas Mathes[1], Thomas Schnabel[2], Erik Ahlswede[2], Michael Powalla[2,3], Heinz Kalt[1], and Michael Hetterich[1] — [1]Institute of Applied Physics, Karlsruher Institut für Technologie (KIT), 76131 Karlsruhe — [2]Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg (ZSW), 70565 Stuttgart — [3]Light Technology Institute, Karlsruher Institut für Technologie (KIT), 76131 Karlsruhe

Solar cells based on Cu2ZnSn(S,Se)4 (CZTSSe) are promising since they only comprise environmentally friendly and earth-abundant elements. However, their conversion efficiency is still too low to be competitive and especially good reproducibility of high-efficiency devices is a major issue. Our fabrication approach for CZTSSe consists of a cheap and simple solution-based process that spares toxic solvents such as hydrazine. Optimizing the selenization process of the doctor-bladed precursors led to a significantly improved reproducibility and energy conversion efficiencies of up to 7

HL 90.3 Thu 16:00 Poster A

Kelvin Probe Force Microscopy Studies of CIGS Solar Cells — •Jasmin Seeger[1], Zhenhao Zhang[2,4], Wolfram Witte[3], Michael Powalla[2,3], Heinz Kalt[1], and Michael Hetterich[1] — [1]Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [2]Light Technology Institute, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [3]Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg (ZSW), 70565 Stuttgart, Germany — [4]Present address: Singulus Technologies AG, 63796 Kahl am Main, Germany

$Cu(In,Ga)Se_2$ (CIGS) is a well-established absorber material for thin-film solar cells, achieving conversion efficiencies of up to 21.7%. In order to further improve this performance, a detailed understanding of the potential distribution (width of the space charge region etc.) in these devices is essential. Of particular interest are the impact of alternative buffer materials or a variation of the gallium content of the absorber on the device performance. To study this impact we investigate the surface as well as the cleaved edge of CIGS solar cells utilizing Kelvin Probe Force Microscopy (KPFM). The contact potential difference (CPD) is studied through the complete structure, partly even on illuminated operating devices. The results are correlated with complementary data such as I-V characteristics and give insights into loss mechanisms in CIGS solar cells.

HL 90.4 Thu 16:00 Poster A

Time-resolved photoluminescence in $Cu_2ZnSn(S,Se)_4$ solar cells — •Mario Lang[1], Alexander Opolka[1], Christoph Krämmer[1], Tobias Abzieher[2], Thomas Schnabel[2], Erik Ahlswede[2], Michael Powalla[2,3], Heinz Kalt[1], and Michael Hetterich[1] — [1]Insitute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [2]Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg, 70565 Stuttgart, Germany — [3]Light Technology Institute, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany

Solar cells made of $Cu_2ZnSn(S,Se)_4$ (CZTSSe) offer a high potential for commercial application. So far efficiencies up to 12.6% have been achieved, but the material suffers from its high open-circuit voltage deficit. The origin of this huge deficit is still an open question, but can probably be attributed to the complex defect structure of the material. Spectrally as well as time-resolved photoluminescence (TRPL) are suitable methods to gain information about the defect structure and can be used to further study the physical recombination mechanisms in CZTSSe solar cells. In this contribution we investigate the decay dynamics and loss mechanisms by time-resolved photoluminescence in dependence of excitation power and temperature.

HL 90.5 Thu 16:00 Poster A

State-Filling Versus Screening of Electrostatic Potential Fluctuations in $Cu_2ZnSn(S,Se)_4$ thin-film solar cells — Christian Zimmermann[1], Christoph Krämmer[1], Mario Lang[1], •Tobias Renz[1], Tobias Abzieher[2], Thomas Schnabel[2], Erik Ahlswede[2], Michael Powalla[2,3], Christian Huber[1], Heinz Kalt[1], and Michael Hetterich[1] — [1]Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [2]Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg, 70565 Stuttgart — [3]Light Technology Institute, KIT

$Cu_2ZnSn(S,Se)_4$ (CZTSSe) is a promising alternative for the well-established absorber material $Cu(In,Ga)Se_2$ in thin-film solar cells. However, the efficiency of CZTSSe devices is still not competitive and essentially limited by an insufficient open-circuit voltage. Excitation power-dependent photoluminescence (PL) measurements show a "blue-shift" of the PL maximum by 15–20 meV/decade. This is often explained by a screening of electrostatic potential fluctuations caused by charged defects. In literature, electrostatic potential fluctuations are often held accountable for the low V_{OC}. In this contribution we investigate excitation-power dependent PL at 10K. We can show by analyzing the whole PL lineshape that the observed "blue-shift" is rather dominated by filling of defect states than by a screening of electrostatic potential fluctuations.

HL 90.6 Thu 16:00 Poster A

Characterization of absorber and buffer layers in $Cu_2ZnSn(S,Se)_4$ solar cells by electroreflectance — •Nicolas Schäfer[1], Christoph Krämmer[1], Christian Huber[1], Mario

Lang[1], Tobias Abzieher[2], Thomas Schnabel[2], Erik Ahlswede[2], Michael Powalla[2,3], Heinz Kalt[1], and Michael Hetterich[1] — [1]Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [2]Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg, 70565 Stuttgart, Germany — [3]Light Technology Institute, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany

$Cu_2ZnSn(S,Se)_4$ (CZTSSe) is a promising thin-film solar cell absorber material. One of its main advantages compared to the well-established $Cu(In,Ga)Se_2$ (CIGS) is the absence of expensive and environmentally problematic indium and gallium. However, especially the achieved open-circuit voltages are still a problem and the CdS buffer adopted from the CIGS device architecture may not be optimal. In our study we use electromodulated reflectance (ER) to study the band structure of both the CZTSSe absorber and buffer. In this context the impact of post-annealing procedures and the application of alternative buffer layers on the absorber/buffer interface is of particular interest.

HL 90.7 Thu 16:00 Poster A

Co-evaporation of alternative buffer layers in CZTSSe solar cells — •Max Reimer[1], Markus Neuwirth[1], Lwitiko Mwakyusa[1], Michael Wolfstädter[1,2], Erik Ahlswede[2], Michael Powalla[2,3], Heinz Kalt[1], and Michael Hetterich[1] — [1]Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [2]Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg, 70565 Stuttgart, Germany — [3]Light Technology Institute, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany

$Cu_2ZnSn(S,Se)_4$ (CZTSSe) has drawn wide interest as an alternative absorber layer in thin-film solar-cells due to its composition of environmentally friendly and low-cost materials. However, CZTSSe solar cells suffer from their low open-circuit voltage and hence from a low efficiency. The solar cell structure of CZTSSe solar cells is mainly adopted from the well-established $Cu(In,Ga)Se_2$ solar cells and thus CdS is typically used as buffer layer. The CdS buffer layer could be one limiting factor for the low open-circuit voltage due to a non-optimal band alignment between the buffer and the absorber. It also reduces the short-circuit current since its band gap is too small, leading to parasitic absorption. In this study we co-evaporate different II-VI semiconductors as alternative buffer layers on CZTSSe solar cells. The buffer layers are analysed concerning their capability as suitable buffer layers for CZTSSe solar cells.

HL 90.8 Thu 16:00 Poster A

Wet-Chemical Processing of CdS and Alternative Buffer Layers for $Cu_2ZnSn(S,Se)_4$ Solar Cells . — •Lwitiko Mwakyusa[1], Markus Neuwirth[1], Niklas Mathes[1], Mario Lang[1], Thomas Schnabel[2], Erik Ahlswede[2], Michael Powalla[2,3], Bryce Richards[3,4], Heinz Kalt[1], and Michael Hetterich[1] — [1]Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [2]Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg (ZSW), 70565 Stuttgart, Germany — [3]Light Technology Institute, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [4]Institute of Microstructure Technology, Karlsruhe Institute of Technology (KIT), 76344 Karlsruhe, Germany

Solar cells based on $Cu_2ZnSn(S,Se)_4$ (CZTSSe) are promising since they only comprise environmentally friendly and earth-abundant elements. However, their device architecture which has been adopted from $Cu(In,Ga)Se_2$ (CIGS) is not yet optimal. This holds in particular for the CdS buffer. In this contribution we study the fabrication of alternative buffer layers, especially that of (Cd,Zn)S and their impact on the performance of CZTSSe solar cells.

HL 90.9 Thu 16:00 Poster A

X-Ray Absorption of Kesterite-Based Materials Studied from First Principles — •Archana Manoharan[1], Lorenzo Pardini[1], Karsten Hannewald[1,2] und Claudia Draxl[1,2] — [1]Humboldt-Universität zu Berlin, Institut für Physik und IRIS Adlershof, Zum Groβen Windkanal 6, 12489 Berlin, Germany. — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany.

The kesterite material Cu_2ZnSnS_4 (CZTS) and its Ge-substituted derivative Cu_2ZnGeS_4 (CZGS) are considered as good absorber material for photovoltaic applications. Here, we study the X-ray absorption spectra of CZTS and CZGS by solving the Bethe-Salpeter equation of many-body perturbation theory on top of density-functional theory. The *ab-initio* calculations are carried out using the all-electron full-potential code `exciting`. Special emphasis is put on comparative studies of the sulfur K and $L_{2,3}$ edges in CZTS and CZGS as well as in its stable binary phase ZnS. A detailed analysis and interpretation of the observed spectral signatures, in particular, the Coulomb interaction between core hole and conduction electrons is performed.

HL 90.10 Thu 16:00 Poster A

Laser-induced shockwave delamination: A non-thermal structuring method of functional thin films — •Pierre Lorenz[1], Tomi Smausz[2,3], Tamas Csizmadia[2], Lukas Bayer[1], Martin Ehrhardt[1], Klaus Zimmer[1], and Bela Hopp[2] — [1]Leibniz-Institut für Oberflächenmodifizierung e. V., Permoserstraße 15, 04318 Leipzig, Germany — [2]Department of Optics and Quantum Electronics, University of Szeged, H-6720 Szeged, Dóm tér 9, Hungary — [3]MTA-SZTE Research Group on Photoacoustic Spectroscopy, University of Szeged, H-6720 Szeged, Dóm tér 9, Hungary

Shock-wave-induced film delamination (SWIFD) as non-thermal laser patterning process enables a gentle film removal and offers therefore a great potential for application. At the SWIFD, the localized removal of the functional thin films is induced by a shock wave which is produced by a laser ablation with 25 ns and 248 nm laser pulses applied to the rear side of the substrate. Different film / substrate combination was tested e.g. copper indium gallium selenide (CIGS) solar cell stacks on polyimide and steel carrier foil and indium tin oxide (ITO) on polyethylene terephthalate (PET). The morphology and the composition of the structures were analysed by optical and scanning electron microscopy (SEM) and by energy-dispersive X-ray spectroscopy (EDX), respectively. Furthermore, the mechanism of SWIFD was analyzed by shadowgraph experiments and this will allow improvements of the physical understanding, modelling and process optimization.

HL 90.11 Thu 16:00 Poster A

Impact of gas exposure on electronic properties of methylammonium lead iodide films — •Bernd Epding[1,3], Christian Mueller[1,2,3], Robert Lovrincic[2,3], and Wolfgang Kowalsky[1,2,3] — [1]Kirchhoff-Institut für Physik, Universität Heidelberg, Germany — [2]Institut für Hochfrequenztechnik, TU Braunschweig, Germany — [3]Innovation Lab, Heidelberg, Germany

Over the last few years the power conversion efficiency of organometal-halide perovskite (such as $CH_3NH_3PbI_3$) based solar cells has skyrocketed at an unprecedented rate to values around 20%. This is even more impressive if we take into account that such high efficiencies can be reached for various cell designs, made from different precursor materials, for both solution and vacuum processed absorber layers. Even though very good devices can already be manufactured, the exact mechanisms, which lead to good charge carrier mobility and extraction, are still not fully understood.

We focus in this work on a comparison between perovskite layers (and solar cells based thereon) in different surrounding atmospheres to investigate the role of intercalated water [1]. Scanning Kelvin probe microscopy was performed under different atmospheric conditions. Thereby we are able to map electronic and structural properties with high spatial resolution. Together with IV measurements, this allows us to directly correlate the obtained data to device performance.

[1] C. Mueller et al., Chem. Mater., 2015, 27 (22), p. 7835-7841

HL 90.12 Thu 16:00 Poster A

Stabilization of $CH_3NH_3PbI_3$ in Humid Air by Partial Substitution of Iodide by Bromide — •Raffael Ruess, Martina Stumpp, and Derck Schlettwein — Institute of Applied Physics, Justus Liebig University Giessen, Heinrich-Buff-Ring 16, D-35392 Giessen, Germany.

Thin films of methylammonium lead halides $CH_3NH_3Pb(I_{1-x}Br_x)_3$ were prepared onto FTO substrates and exposed to humid air in the dark. To characterize the stability of the materials, UV-vis spectra were acquired at fixed intervals, accompanied by X-ray diffraction, energy dispersive X-ray spectroscopy, scanning electron and confocal laser scanning microscopy. Two different degradation mechanisms were observed. It was confirmed that bromide slowed down the formation of PbI_2. Furthermore, it was found that the formation of the perovskite monohydrate phase was successfully suppressed, presumably caused by stronger hydrogen bonding interactions between the organic cation and bromide ions. The use of an increased bromide content in methylammonium lead halide absorbers is discussed for the application in perovskite solar cells.

HL 90.13 Thu 16:00 Poster A

Lasing in lead iodide perovskite thin films on distributed feedback gratings — •Mareike Stulz[1,2], Philipp Brenner[1], Aina Quintilla[1], Holger Röhm[1], Ian Howard[3], Alexander Colsmann[1], Heinz Kalt[2], and Uli Lemmer[1] — [1]Light Technology Institute, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [2]Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [3]Institute of Microstructure Technology, Karlsruhe Institute of Technology (KIT), 76344 Eggenstein-Leopoldshafen, Germany

Hybrid organic-inorganic perovskites have recently shown great potential as gain material for laser devices with the advantages of solution processability, wavelength tunability and high stability [1]. Furthermore, the low trap densities and high charge carrier mobilities might enable electrically pumped gain in this material.

We prepared thin films of Methylammonium lead iodide ($CH_3NH_3PbI_3$) on corrugated substrates by solution-based spincoating or doctor blading. Matching the film thickness and grating period enabled optically pumped distributed feedback single mode lasing at room temperature. Additionally, the modal net gain of the perovskite thin films was measured with the variable stripe length method.

[1] Xing et al. Nature Materials 13, 476-480, 2014.

HL 90.14 Thu 16:00 Poster A

Radiative loss mechanisms in hybrid trihalide perovskite films — •Robert Hanfland, Fabian Meier, Christoph Baumbach, and Carsten Deibel — Institut für Physik, Technische Universität Chemnitz, 09126 Chemnitz, Germany

During the last few years, hybrid trihalide perovskite based solar cells showed an impressive ascent of efficiency and recently reached values beyond 18 %. Recombination mechanisms as the main loss mechanism control the dynamics of photoluminescence (PL) and play an important role for further improvement of efficiency.

We investigated the recombination mechanisms in hybrid trihalide perovskite films by using a confocal setup for PL measurement. The measured transients were analysed using models with different recombination mechanisms such as direct or trap assisted recombination. Other processes like multiple trapping are included as well. We discuss the dominant recombination mechanisms in view of its implications on the device performance.

HL 90.15 Thu 16:00 Poster A

Electronic structure of lead halide perovskite — •Daniel Niesner[1,2], Tyler J. S. Evans[1], Bryan J. Kudisch[1], Prakriti P. Joshi[1], Kiyoshi Miyata[1], Xiaoxi Wu[1], M. Tuan Trinh[1], Haiming Zhu[1], Manuel Marks[1], and X.-Y. Zhu[1] — [1]Department of Chemistry, Columbia University, New York, NY 10027, USA — [2]Festkörperphysik, FAU Erlangen-Nürnberg, D-91058 Erlangen, Germany

Angle-resolved photoelectron spectroscopy (ARPES) and two-photon photoelectron spectroscopy give insight into the valence and conduction band electronic structure of semiconductors. Doping levels can directly be extracted. Experiments require samples with well-defined surfaces. We report the preparation of high-quality polycrystalline thin films of $(CH_3NH_3)PbI_3$ on native silicon oxide on Si(111), sapphire, and PbSe(001). The (110) crystalline axis is orientated along the surface normal. Surface roughness is 1 nm. ARPES data are in semiquantitative agreement with band structure calculations. The valence band is located 1.5 ± 0.1 eV below the Fermi level E_F. The films on oxide surfaces are highly to degenerately n-doped, with the conduction band minimum up to 0.08 eV below E_F. Photoemission techniques are combined with optical spectroscopy taking into account the Burstein shift resulting from the high doping level. The band gap is 1.535 ± 0.030 eV, in good agreement with the reported value for single-crystalline $(CH_3NH_3)PbI_3$.

HL 90.16 Thu 16:00 Poster A

The influence of fabrication process and substrate material on electrical characteristics of methylammonium lead iodide — •Tim Helder[1,2], Christian Mueller[1,2,3], Wolfgang Kowalsky[1,2,3], and Robert Lovrincic[2,3] — [1]KIP, Universität Heidelberg, Germany — [2]InnovationLab, Heidelberg, Germany — [3]IHF, TU Braunschweig, Germany

Research interest in halide perovskites such as $CH_3NH_3PbI_3$ as photovoltaic materials has increased continuously in the last years due to an increase of solar cell efficiencies to over 20%. This development is even more impressive if we take into account the possibilities in variation of substrates, precursor materials and fabrication methods. Despite all these efforts we still lack in understanding fundamental processes in solar cells based on these materials.

Herein we present Kelvin Probe measurements to investigate the impact of fabrication processes on the work function of $CH_3NH_3PbI_3$ layers. Therefore we deposited $CH_3NH_3PbI_3$ by spincoating and vacuum evaporation. Moreover, we varied the process parameters of single process steps (e.g. annealing) as well as the substrate materials (e.g. PEDOT, TiO_2, Au). Thereby we are able to directly investigate the impact of single changes in the fabrication process on the electrical behavior of the perovskite layer. We will discuss implications of our results for solar cell performance.

HL 90.17 Thu 16:00 Poster A

Charge dynamics of Organometal Trihalide Perovskite using broadband transient absorption technique — •Yajun Gao[1], Tobias Schnier[2], Kestutis Budzinauskas[1], Jingyi Zhu[1], Selina Olthof[2], Klaus Meerholz[2], and Paul Loosdrecht[1] — [1]Physics Institute II, University of Cologne, Zülpicher street 77, 50937, Cologne, Germany — [2]Physical Chemistry, University of Cologne, Luxemburger street 116, 50939, Cologne, Germany

Organometal trihalide perovskites provide a promising alternative for photovoltaic applications, with the highest solar cell power conversion efficiency of 19.3% as reported in 2014. The precise mechanism of power conversion in these materials is currently not well understood. In this work, we address this issue using visible and near-infrared broadband transient absorption (TA) spectroscopy, which can discriminate between free charges and excitons, to study the ultrafast charge generation in organometal trihalide perovskite CH3NH3PbI3 films. Charge selectivity is achieved by observing the transient response of charge-selective extraction layers, PCBM for electrons and spiro-OMeTAD for holes, spin-coated on the perovskite film. In addition to the response of the charge-selective layers, additional TA features show up which are attributed to free charges in the perovskite film. We use these experiments to determine the diffusion length of excitons and free carriers in the perovskite film, a property which is of central importance to the functionality of perovskite based solar cell devices.

HL 90.18 Thu 16:00 Poster A

Temperature-dependent absorption measurements and photoluminescence spectroscopy of mixed organic-inorganic halide perovskite films — •Angelika Schulz[1], Fabian Ruf[1], Nadja Giesbrecht[2], Matthias Handloser[2], Pablo Docampo[2], Heinz Kalt[1], and Michael Hetterich[1] — [1]Institute of Applied Physics, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [2]Department of Chemistry and Center for NanoScience, University of Munich (LMU), 81377 München, Germany

Organic-inorganic halide perovskites show an outstanding performance as absorber material in solar cells due to their strong absorption coefficient, low non-radiative carrier recombination and simple low-cost production methods. With temperature-dependent absorption measurements and photoluminescence spectroscopy from 10 K to room-temperature we can gain information on structural and optical properties of the material system which is important for a better understanding of the physical processes in the absorber material. In this contribution we study $CH_3NH_3Pb(I_{1-x}Br_x)_3$ and investigate the composition-dependent band-gap variation which is useful for band-gap tuning in solar cells. The material system undergoes a phase transition from the low-temperature orthorhombic phase to the tetragonal phase at 150-165 K depending on the halide composition. On the basis of the temperature-dependent absorption and photoluminescence measurements above 170 K, where the tetragonal phase seems to be stable, an upper limit for the exciton binding energy of methyl ammonium lead iodide can be estimated.

HL 90.19 Thu 16:00 Poster A

Electrical Characterization of Methylammonium Tin Iodide Layers as Photovoltaic Absorbers — •Jonas Horn, Manuel Weiss, Christoph Richter, and Derck Schlettwein — Justus-Liebig-Universität Gießen, Institut für Angewandte Physik, Heinrich-Buff-Ring 16, D-35392 Gießen, Germany.

The preparation of absorber layers composed of methylammonium tin iodide ($CH_3NH_3SnI_3$) in a two-step process was investigated. The material may serve as a less toxic alternative to $CH_3NH_3PbI_3$ as active material in perovskite solar cells. Tin(II) iodide layers prepared by physical vapor deposition on microstructured Au electrode arrays on SiO_2/Si were converted to $CH_3NH_3SnI_3$ by reaction with a spin-

coated solution of methylammonium iodide. The perovskite particles were over 200 nm in size and the films reached almost complete surface coverage. The material absorbs over a broad part of the solar spectrum, broader even than $CH_3NH_3PbI_3$. An average resistivity of 26 Ohm cm was measured, characteristic of semiconducting rather than metallic $CH_3NH_3SnI_3$, which speaks in favor of the suitability for photovoltaic applications. The excellent stability of the resistivity, at least within the inert atmosphere of the glove box, and the independently proven stability of the film structure even after contact to air show the good prospects for applications as absorber layers in perovskite solar cells.

HL 90.20 Thu 16:00 Poster A

Characterisation of photoluminescence and absorption in hybrid perovskite thin films — •Seth Niklas Schumann, Sebastian Reichert, Alexander Wagenpfahl, and Carsten Deibel — Fakultät für Naturwissenschaften, TU Chemnitz, D-09126 Chemnitz

In the last few years the organic-inorganic hybrid perovskite solar cells came to attention due to their impressive power conversion efficiency increase to above 20 %. They also are expected to have low manufacturing cost. To take advantage of the potential the hybrid perovskites have to offer for photovoltaics we need to characterise the active layer regarding layer homogeneity and optical properties. For our active layers we used the $CH_3NH_3PbI_3$ material system which we processed using the interdiffusion approach. We optimized the processing parameters to obtain homogeneous and pinhole free thin films. We characterised these thin films using photoluminescence, absorption and excitation spectroscopy.

HL 90.21 Thu 16:00 Poster A

Influence of preparation parameters on film morphology and charge transfer in doped organic semiconductors investigated by IR spectroscopy — •Sebastian Beck[1,2], Lars Müller[2,3], Vipilan Sivanesan[1,2], and Annemarie Pucci[1,2] — [1]Universität Heidelberg, Kirchhoff-Institut für Physik — [2]InnovationLab GmbH, Heidelberg — [3]Technische Universität Braunschweig, Institut für Hochfrequenztechnik

Molecular orientation as well as a homogeneous dopant distribution are known to be important for efficient charge transfer (CT) in doped organic semiconductors. Both properties can be varied in a certain range by changing preparation parameters. In this study, the influences of different preparation parameters on film morphology and CT in doped organic semiconductors are investigated. In films deposited onto a cooled substrate in vacuum a reduced diffusion of the evaporated molecules on the substrate surface occurs. The reduced thermal energy of the deposited molecules freezes non-equilibrium molecular orientations of dopant and matrix molecules which prevent efficient CT. During warming up to room temperature a molecular rearrangement takes place facilitating CT in the doped layer. This effect is studied and identified by means of in-situ IR spectroscopy. The morphologies of solution processed thin films are varied by spin coating doped layers from solvents with different polarities and evaporation temperatures. Observed differences in UV-Vis spectra of doped P3HT solutions and thin layers prepared from these solutions indicate a pre-definition of the thin film morphology already in the liquid phase.

HL 90.22 Thu 16:00 Poster A

Improving electron injection and stability of metal electrodes in organic electronic devices with self-assembled monolayers on printing-relevant time-scales — •Sabina Hillebrandt[1,2], Milan Alt[2,3], Janusz Schinke[2,4], Malte Jesper[5], and Annemarie Pucci[1,2] — [1]Heidelberg University, KIP — [2]InnovationLab GmbH, Heidelberg — [3]Karlsruhe Instiute of Technology, LTI — [4]TU Braunschweig, Inst. f. Hochfrequenztechnik — [5]Heidelberg University, OCI

In organic semiconductor devices charge injection at the interface is important for the device performance. Charge injection can be improved by controlling the energy alignment at the interfaces, especially between metal contact and organic semiconductor. The thickness of these layers has to be very well defined to avoid any insulating or doping effects. Self-assembled monolayers (SAMs) in this case offer a beneficial way to produce such layers.

In our studies we work with molecules that allow a work function (WF) reduction of about 1.2eV on Gold and Silver contacts. Effects on the WF shift due to molecular orientation are investigated by IR reflection-absorption spectroscopy, the WF is investigated by Kelvin Probe measurements and photoelectron spectroscopy. Devices are fabricated focussing on printing feasibility and the improvement of device life time.

HL 90.23 Thu 16:00 Poster A

Transient localization in rubrene — •Michael Geiger[1], Andrea Rohwer[1], Martin Dressel[1], Ute Zschieschang[2], Hagen Klauk[2], Teresa Schmeiler[3], and Jens Pflaum[3] — [1]1. Physikalisches Institut, Universität Stuttgart, Germany — [2]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [3]Experimentelle Physik VI, Universität Würzburg, Germany

Rubrene single crystals consist of van der Waals bound polycyclic aromatic hydrocarbons. Intrinsically, rubrene is an insulator, but can become conductive by e.g. field-effect doping. As such rubrene single crystals have shown highest room-temperatur hole mobilities of about 20 cm^2/Vs. Due to these properties rubrene has gained attention over the last years and appears to be a promising candidate for electronic applications such as field effect transistors (FETs) in active matrix displays.

We study the fundamental mechanisms that govern charge carrier transport in rubrene and that are still under debate. In particular, by the thermal motion of molecules the electronic wave function can localize on time scales corresponding to these molucular vibrations and charge transport has to be modelled by transient localization. To verify this theory for organic semiconductors we measure the hole mobility as a function of temperature in FETs composed of ultra pure rubrene crystals as active transport layer and compare the results to calculations [1]. In the next step we investigate these FETs by IR spectroscopy to trace the dynamical behaviour of charges and their excitation by pulsed lasers.

[1] S. Fratini, S. Ciuchi & D. Mayou, Phys. Rev. B 89, 235201 (2014)

HL 90.24 Thu 16:00 Poster A

Accessing charge transfer dynamics in Merocyanine:PCBM blends using NIR-VIS transient absorption spectroscopy — •Kestutis Budzinauskas[1], Lena Wysocki[1], Dirk Hertel[2], Klaus Meerholz[2], and Paul H.M. van Loosdrecht[1] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77 50937 Köln — [2]Institut für Physikalische Chemie, Universität zu Köln, Luxemburger Str. 116, 50939 Köln

Merocyanine based dyes are good model materials to investigate charge generation mechanisms in donor:acceptor blend systems. The power conversion efficiency of organic solar cells is a complex parameter, which usually strongly depends on microscopic processes involving for instance interfacial charge transfer states and the formation of long lived triplet states. Fundamental understanding of these effects is critical in order to design new high conversion efficiency solar cells. Here, we study these processes on their intrinsic timescale using time resolved VIS-NIR spectroscopy methods. We focus on the charge formation dynamics in solution processed merocyanine:PCBM blends as well as in merocyanine single crystals and extract quantitative information on the charge transfer dynamics between different excited species.

HL 90.25 Thu 16:00 Poster A

Temperature Dependent Charge-Transfer-State Spectroscopy of Organic Solar Cells — •Clemens Göhler and Carsten Deibel — Institut für Physik, Technische Universität Chemnitz, 09126 Chemnitz, Germany

In nowadays often used bulk-heterojunction solar cells, the separation of excitons is aided by adding an acceptor material to the absorbing donor, forming an interfacial state at which charge transfer can take place. This charge-transfer or CT-state can be excited directly with sub-bandgap photons and serves as the main radiative recombination pathway when the solar cell is used as a light emitting diode.

By examining both effects via external quantum efficiency (EQE) and electroluminescence (EL) spectroscopy, one can learn more about the nature of charge-carrier separation and recombination in organic solar cells, which are considered main effects for the losses in the open-circuit voltage (V_{oc}).

To contribute, we examine both the EQE and EL of organic solar cells with varying V_{oc} as a function of the ambient temperature to reduce homogeneous broadening of the CT-absorption and emission lines. Thus, we have an access to the Marcus Theory's molecular reorganization energy and their influence on the V_{oc}-losses.

HL 90.26 Thu 16:00 Poster A

Characterisation of loss mechanisms in hybrid trihalide perovskite solar cells — •Sebastian Reichert, Seth Niklas Schu-

mann, Alexander Wagenpfahl, and Carsten Deibel — Fakultät für Naturwissenschaften, TU Chemnitz, D-09126 Chemnitz

Organic-inorganic trihalide perovskite solar cells belong to the most significant developments in the field of photovoltaics in the last years and seem to be a good bet at satisfying the need for high efficiencies and low manufacturing cost.

To take advantage of the potential of these hybrid solar cells, the loss mechanism which occurs within the active layer need to be understood. We therefore measure current–voltage characteristics for a range of perovskite ($CH_3NH_3PbI_3$) solar cells with different processing parameters. We investigate the photoluminescence transients on corresponding thin films without electrodes. The loss mechanisms are modeled by fitting the obtained data to the continuity equation for excitons and charge carriers. We finally correlate the found recombination losses to the extracted solar cell parameters.

HL 90.27 Thu 16:00 Poster A

The Influence of Morphology and Interface Treatment on Organic 6,13 bis(triisopropylsilylethynyl)-Pentacene Field-Effect Transistors — •Daniel Bülz, Franziska Lüttich, Sreetama Banerjee, Georgeta Salvan, and Dietrich R. T. Zahn — Semiconductor Physics, Technische Universität Chemnitz, Germany

For the development of electronics, organic semiconductors are of great interest due to their adjustable optical and electrical properties. Aiming for simpler fabrication processes, we investigate TIPS-pentacene organic field effect transistors (OFETs) made from solution with different techniques. Because of the different deposition methods, the TIPS-pentacene thin films exhibit different morphologies in terms of crystal size and homogeneity of the substrate coverage. Additionally, the interface treatment is known to have a strong influence on the threshold voltage, eliminating trap states of silicon oxide at the gate electrode and thereby changing the electrical switching response of the transistors. We therefore investigate the influence of interface treatment using either octadecyltrichlorosilane (OTS) or a simple cleaning procedure with acetone, ethanol, and deionized water. The transistors consist of prestructured OFET substrates including gate, source, and drain electrodes, on top of which TIPS-pentacene dissolved in a mixture of tetralin and toluene is deposited by spray-, or spin-coating. The OFETs are characterized by means of optical microscopy (in order to determine the overall quality of the sample, i.e. crystal size and coverage of the channel region) and electrical transport measurements.

HL 90.28 Thu 16:00 Poster A

Confocal photoluminescence measurements of the charge transfer state in diluted bulk heterojunctions — •Martin Streiter, Alexander Wagenpfahl, and Carsten Deibel — Institut für Physik, Technische Universität Chemnitz, 09126 Chemnitz, Germany

The understanding of recombination mechanisms at donor-acceptor interfaces is of high importance for improving organic solar cells, as they determine the open circuit voltage and influence the photocurrent. In order to investigate the local properties of charge transfer (CT) states in view of nongeminate losses, we studied diluted bulk heterojunction films.

Photoluminescence spectroscopy was performed using a confocal laser scanning microscopy setup with cryostat sample stage to collect spatially resolved CT emission with sub-micron resolution. Spin coated TAPC-C_{60} and TAPC-PCBM films with less than 1 mol% acceptor concentration were studied. We investigated the connection between structural information, e.g. acceptor material cluster formation, to CT emission and discuss the results with respect to thermal activation and energetic disorder.

HL 90.29 Thu 16:00 Poster A

Solution Processed TIPS-pentacene/Au Hybrid Trench Devices for Light Sensing Applications — •Sreetama Banerjee[1,2], Daniel Bülz[1], Danny Reuter[2], Karla Hiller[2], Dietrich R. T. Zahn[1], and Georgeta Salvan[1] — [1]Semiconductor Physics, Technische Universität Chemnitz, Germany — [2]Zentrum für Mikrotechnologien, Technische Universität Chemnitz, Germany

Organic-inorganic hybrid electronics can combine the advantages offered by either organic or inorganic materials individually and thereby exhibit enhanced performance. In this work, we present 6,13-bis (triisopropylsilylethynyl)-Pentacene solution-processed planar type organic/inorganic hybrid devices with trench isolated gold electrodes. Devices with organic channel dimensions of 100 nm - 260 nm were fabricated by UV lithography and drop-coating using a TIPS-pentacene solution. The electrical characterization of such devices was carried out with and without illumination to check for possible applications of such devices in light sensing. Three different laser lines (325 nm, 514.7 nm, and 632.8 nm) were used for illuminating the sample. It was observed that the photocurrent and photo-switching response time increases with the photon energy. Devices with smaller channel length showed higher photocurrents and faster switching behaviour. This observation is in agreement with the presence of space charge limited currents as a main transport mechanism.

HL 90.30 Thu 16:00 Poster A

Efficient dissociation of charge transfer states in PTB7-based organic solar cells — •Marina Gerhard[1], Andreas P. Arndt[2], Ian A. Howard[3], Mühenad Bilal[1], Arash Rahimi-Iman[1], Uli Lemmer[2,3], and Martin Koch[1] — [1]Faculty of Physics and Materials Sciences Center, Philipps-Universität Marburg, 35032 Marburg, Germany — [2]Light Technology Institute, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany — [3]Institute of Microstructure Technology, Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany

In organic solar cells, interfacial charge transfer (CT) states can either act as precursors for free charges or possess trapping character, enhancing geminate recombination. Here, we present a study on the polymer PTB7, blended with the fullerene derivative $PC_{71}BM$, where we investigate interfacial recombination by means of time-resolved photoluminescence[1]. Our results on the temperature- and energy-dependent decay dynamics suggest that there is a kinetic competition between charge separation and CT recombination. We find low activation barriers for CT quenching in the range of $k \cdot T$ at room temperature, indicating that the CT states are only weakly bound. This is consistent with our recent experimental work on field-induced CT quenching. Furthermore, we observe that the nanomorphology has a strong influence on the efficiency of charge separation, because the CT emission yield is much higher after selective excitation of the polymer rather than for preferential excitation of pure fullerene domains.

[1] J. Phys. Chem. C, DOI: 10.1021/acs.jpcc.5b09842 (2015)

HL 90.31 Thu 16:00 Poster A

Revealing spin pair processes in organic solar cells — •Alexander J. Kupijai, Florian G. Schaeble, Martin Stutzmann, and Martin S. Brandt — Walter Schottky Institut und Physik-Department, Technische Universität München, Am Coulombwall 4, 85748 Garching

Further improvements of the efficiency of organic solar cells are expected e.g. from advances in chemistry and the optimization of charge carrier transport. We have previously demonstrated that pulsed electrically detected magnetic resonance (pEDMR) and especially electron double resonance (ELDOR) can be used to identify polaron pair recombination as the rate-limiting spin-dependent charge transport mechanism in P3HT/PCBM solar cells at 10 K. We have shown that these multi-frequency measurements can be extended to solar cells containing other polymers such as PCDTBT, where the same polaron pair recombination is observed, suggesting that this recombination is typical for organic solar cells at low temperatures. At room temperature the situation is different, as the negative polaron peak vanishes. Instead, a signal at lower magnetic fields is tentatively attributed to polarons in PEDOT:PSS, which is used as a hole transport layer in the solar cell studied. Again, we use single- and multi-frequency pEDMR techniques to identify the pair processes leading to spin-dependent transport in order to provide information for an optimization of overall solar cell efficiencies.

HL 90.32 Thu 16:00 Poster A

Multilayer fullerene-free organic solar cells with low energy losses — •Vasileios Christos Nikolis, Donato Spoltore, Johannes Benduhn, Felix Holzmüller, Christian Körner, and Koen Vandewal — Institut für Angewandte Photophysik, Technische Universität Dresden, George-Bähr-Str. 1, 01069 Dresden, Germany

The generation of free charge carriers at interfaces between organic electron donors (D) and electron acceptors (A) can be very efficient, enabling organic solar cells with external quantum efficiencies (EQE) higher than 80 % and internal quantum efficiencies (IQE) approaching 100 %. On the other hand, recombination of free charge carriers at the D-A interface reduces the open-circuit voltage, and overall power conversion efficiency (PCE) of photovoltaic devices comprising such interfaces.

In this study, we introduce an optimization route in order to improve the V_{oc} in multilayer organic solar cells. The deposition of an ultrathin interlayer between D and A creates a discontinuous layer which reduces the D-A interface area and thus free carrier recombination, while keeping a high free carrier generation yield. Investigating a series of interlayers and multilayer device architectures, we achieve PCE's $> 7.5\,\%$. Most notably, this strategy enables a V_{oc} of 1.18 V with a peak external quantum efficiency of 78 % at 1.77 eV (700 nm). Such high quantum efficiencies combined with the very low voltage losses below 0.59 V are unprecedented for organic solar cells. Furthermore, this work provides clear pathways for the minimization of photon energy losses by manipulation of the organic photovoltaic device architecture.

HL 90.33 Thu 16:00 Poster A

Ab-initio simulations of vacancy-impurity complexes in carbon allotropes — •Alejandro Martinez-Soria Gallo[1,2], Andreas Grueneis[1], Helmut Fedder[2], Thomas Gruber[1], and Joerg Wrachtrup[2] — [1]Max Planck Institut für Festkörperforschung, Stuttgart, Germany — [2]3rd physics institute, University of Stuttgart, Stuttgart, Germany

Nitrogen Vacancy defects in diamond have become over the last years an important candidate for a bulk room temperature quantum information processing device. In this poster we investigate the feasibility of approximate density functional theory calculations for describing optical and electronic properties for several vacancy-impurity complexes in different carbon allotropes.

HL 90.34 Thu 16:00 Poster A

Quantum technology application with the silicon-vacancy centre in diamond — •Andreas Dietrich[1], Kay Jahnke[1], Lachlan Rogers[1], Junichi Isoya[2], Fedor Jelezko[1], and Alexander Kubanek[1] — [1]Institute for Quantum Optics, University Ulm, Germany — [2]National Institute for Materials Science, Namiki, Tsukuba, Ibaraki, Japan

Colour centres in diamond appeared as important and valuable quantum systems for emerging quantum technologies, including the fields of quantum processing, quantum key distribution quantum communication, information processing, quantum meteorology and many more. Recently a new color centre showed up to be promising in the fields of single photon generation, flying qubit entanglement and quantum repeater, the silicon vacancy center (SiV^-) in diamond. Latest work on SiV^- has shown its exceptional and promising spectral properties. These qualities leads to efforts to apply these system in quantum technologies. Nevertheless for these purposes some features and effects are still not fully understand. We show how our progress leads to a deeper understanding and to more sophisticated applications of the silicon vacancy centre in diamond.

HL 90.35 Thu 16:00 Poster A

FPGA based measurements of optical properties of silicon-vacancy (SiV) centers in diamond — •Simon Rupp[1], Andreas Dietrich[1], Andrea Kurz[1], Kay Jahnke[2], Lachlan Rogers[1], Junichi Isoya[1], Fedor Jelezko[1], and Alexander Kubanek[1] — [1]Institute for Quantum Optics, University Ulm, Germany — [2]National Institute for Materials Science, Namiki, Tsukuba, Ibaraki, Japan

In the last decades, colour centres in diamond has shown perfect optical properties for quantum information processes. Especially, the silicon-vacancy (SiV) centers with high brightness, narrow bandwidth and spectral stability can be used as an excellent source of indistinguishable single photons. To observe and control the optical properties of such colour centres in real time, a suitable system is required. The FPGA (Field Programmable Gate Array) technology has the ability to implement physical parallel and independent processes in real time. Furthermore, independent tasked can be processed simultaneously on a FPGA which can't be achieved with commercial devices. This gives us the possibility to measure and control the optical properties of silicon-vacancy (SiV) centers in diamond with FPGA technology.

HL 90.36 Thu 16:00 Poster A

Mechanical tuning of nuclear spins in Si — •Moritz P.D. Pflüger, David P. Franke, and Martin S. Brandt — Walter Schottky Institut and Physik-Department, Technische Universität München, Am Coulombwall 4, 85748 Garching, Germany

Nuclear spins of ionized donors in silicon have many properties that make them interesting for quantum computing applications, especially as a quantum memory. They are compatible with silicon technology, scalable, and possess very long coherence times [1]. However, due to their good isolation, it is difficult to address them selectively. This becomes possible for heavier donors, such as ^{75}As, via their quadrupole moment which interacts with electric field gradients which in turn can be tuned by applying elastic strain to the host crystal [2].

We measure pulsed electrically detected electron nuclear double resonance of arsenic-doped silicon, a technique allowing to observe nuclear magnetic resonance phenomena via monitoring the change in conductivity. We extend earlier experiments by applying stress to the samples via piezoelectric actuators, discuss the resonance shifts achievable, and explore the influence of strain on the decoherence of the $^{75}As^+$ nuclear spins.

[1] M. Steger, K. Saeedi, M. L. W. Thewalt, J. J. L. Morton, H. Riemann, N. V. Abrosimov, P. Becker, and H.-J. Pohl, Science **336**, 1280 (2012).

[2] D. P. Franke, F. M. Hrubesch, M. Künzl, H.-W. Becker, K. M. Itoh, M. Stutzmann, F. Hoehne, L. Dreher, and M. S. Brandt, Phys. Rev. Lett. **115**, 057601 (2015).

HL 90.37 Thu 16:00 Poster A

Influence of ^{29}Si nuclear spins on the coherence of ionized phosphorus donors in silicon — •Andreas M. Rauscher, David P. Franke, and Martin S. Brandt — Walter Schottky Institut and Physik-Department, Technische Universität München, Am Coulombwall 4, 85748 Garching, Germany

The fragility of quantum mechanical states is one of the main obstacles for the physical implementation of quantum bits (qubits). Promising candidates for the latter are the spins of impurities in silicon. In this case, the interaction with ^{29}Si nuclear spins generally acts as the main source of decoherence. Removing this isotope in isotopically controlled ^{28}Si, a record-breaking coherence time of 39 minutes for $^{31}P^+$ nuclear spins has been achieved[1]. Using pulsed electrically detected magnetic resonance (pEDMR) and electron nuclear double resonance (ENDOR), we are able to access the nuclear spin states of both $^{31}P^+$ and ^{29}Si in γ-irradiated silicon with natural isotope composition, based on spin pairs formed between donors and irradiation defects (SL1)[2]. Here, we apply hyperpolarization techniques demonstrated on $^{31}P^+$[3] to ^{29}Si coupled to SL1 and the possibility to use this approach to systematically study the effects of ^{29}Si spins on the decoherence of $^{31}P^+$ nuclei.

[1] Kamyar Saeedi et al., Science **342**, 830 (2013)
[2] David P. Franke et al., Phys. Rev. B **89**, 195207 (2014)
[3] Felix Hoehne et al., Phys. Rev. Lett. **114**, 117602 (2015)

HL 90.38 Thu 16:00 Poster A

Optical spectroscopy of vacancy related defects in silicon carbide generated by proton irradiation — •C. Kasper[1], H. Kraus[2,1], A. Sperlich[1], D. Simin[1], T. Makino[2], S.-I. Sato[2], T. Ohshima[2], G. V. Astakhov[1], and V. Dyakonov[1,3] — [1]Experimental Physics VI, Julius Maximilian University of Würzburg, 97074 Würzburg — [2]Japan Atomic EnergyAgency, Takasaki, Gunma, Japan — [3]ZAE Bayern, 97074 Würzburg

Defects in silicon carbide (SiC) received growing attention in recent years[1,2,3,4], because they are promising candidates for spin based quantum information processing. In this study we examine silicon vacancies in 4H-SiC crystals generated by proton irradiation. By the use of confocal microscopy the implantation depth of Si vacancies for varying proton energies can be verified.

An important issue is to ascertain the nature and distribution of the defects. For this purpose, we use the characteristic photoluminescence spectrum of Si vacancies, whose intensity is proportional to the defect density. Using xyz-scans, where the photoluminescence at each mapping point is recorded, one can thus determine the vacancies nature and their distribution in the SiC crystal. Additionally we verify the nature of the examined defects by measuring their uniquely defined zero-field-splitting by using ODMR associated with defect spins.

[1] H. Kraus et al., Nature Phys. 10, 157 (2014)
[2] D. J. Chrystle et al., Nature Mater. 14, 160 (2015)
[3] M. Widmann et al., Nature Mater. 14, 164 (2015)
[4] A. Lohrmann et al., Nature Comm. 6, 7783 (2014)

HL 90.39 Thu 16:00 Poster A

Generation of Nitrogen Vacancy Centers in Diamond by Focused Ion Implantation — •Johannes Lang, Boris Naydenov, and Fedor Jelezko — Institut für Quantenoptik, Universität Ulm, Germany

The color center in diamond formed by a substitutional nitrogen and an adjacent vacancy (NV center) is amongst the most studied defects

in diamond and a promising candidate for different applications such as e.g. qubit spin registers in future quantum computers [1], or as magnetic and electric field sensors [2]. The targeted creation of these NVs is essential for the described applications [3]. We present a UHV-setup for low energy focused ion implantation of nitrogen in order to create NV centers. By adjusting the implantation energy and fluence, the generation depth of up to 20 nm below the surface of the diamond substrate, as well as the NV density and position can be controlled.

[1] J. Scheuer et al., New J. Phys. 16 093022 (2014) [2] C. Müller et al., Nat. Comm., 5 4703 (2014) [3] J. Meijer et al., Appl. Phys. Lett. 87, 261909 (2005)

HL 90.40 Thu 16:00 Poster A

Mechanical and vibrational properties of strained carbon nano-materials — •Alexander Croy[1], Christian Wagner[2], and Jörg Schuster[3] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Center for Microtechnologies, TU Chemnitz, Germany — [3]Fraunhofer Institute ENAS, Chemnitz, Germany

The introduction of carbon nanomaterials, like carbon nanotubes and graphene, into modern nano-electronic architectures is a wide field of application-oriented research — and requires reliable, non-destructive and fast characterization techniques to quantify defects and (local) strain. Optical spectroscopy, such as Raman spectroscopy, to indirectly probe phonons (vibrations), play a major role in this field.

Thus, a detailed understanding of the influence of defects and strain on Raman spectra is required, but the full *ab-initio* description of the coupled optical and phonon interaction is usually not feasible. Therefore, the problem is restricted to the main contribution by phonons — which are typically calculated by means of molecular dynamics (MD).

To maintain *ab-initio* accuracy, we compare the elastic properties of ideal and defective carbon nanostructures obtained by density functional calculations and different carbon force-fields. Within (static) numerical stretching experiments, we focus in particular on nonlinear contributions in the stress-strain-relation. Using MD calculations we study the strain- and defect dependence of the dominant phonon modes, i.e., their frequencies and life-times. Finally, we discuss consequences for Raman spectra.

HL 90.41 Thu 16:00 Poster A

Characterization of diamondoids by Raman spectroscopy — •Dominique B. Schuepfer[1], Andrey A. Fokin[2], Peter R. Schreiner[2], and Peter J. Klar[1] — [1]Institute of Experimental Physics I, Justus Liebig University Giessen, Germany — [2]Institute of Organic Chemistry, Justus Liebig University Giessen, Germany

Diamondoids, like adamantane, are the smallest building blocks of diamonds and are currently used to form new molecules by linking these sp^3-bonded units to larger cages. Raman spectroscopy is used to characterize various diamondoids as well as the newly formed materials. In particular, in wavelength and polarization dependent Raman experiments the number of modes and their corresponding signal intensity vary, allowing to study the symmetry characteristics and scattering propabilities of the Raman active modes. The vibrational structure of diamondoids and the more complicated coupled diamondoid molecules give insight into the molecule symmetry and electronic structure. Beside this fundamental point of view diamondoids are of great interest as propellant for radiofrequency ion thrusters, because they are available in abundance and match the required properties. Raman spectroscopy could be used to characterize the residual components of the thruster propellant.

HL 90.42 Thu 16:00 Poster A

Investigations into Optoelectronic Properties of Carbon Nitrides for Solar Hydrogen Production — •Filip Podjaski[1], Juan Galisteo-López[2], Brian Tuffy[1], Katharina Schwinghammer[1], Hernán Míguez[2], and Bettina V. Lotsch[1,3] — [1]Max-Planck-Institute for Solid State Research, Stuttgart, Germany — [2]Institute of Material Science of Sevilla, Sevilla, Spain — [3]Department of Chemistry, University of Munich (LMU), Munich, Germany

Since the discovery of water splitting on TiO2 under UV-illumination by Honda and Fujishima in 1970s, a lot of materials and cocatalysts have been investigated to produce hydrogen from water using sunlight. A recent discovery has shown that carbon nitrides, consisting only of abundant elements, are able to perform visible light-driven hydrogen evolution. Our research focuses on the understanding and enhancement of charge transfer properties in these semiconducting polymers that lead to improved hydrogen evolution. Time resolved photoluminescence measurements suggest the use of a more general approach than used nowadays in literature to describe the complex decay processes after photo-excitation. Our results reveal how the particle size, the presence of sacrificial donors and how cocatalysts attached to the surface influence the lifetimes of excited states. This findings may lead to a better understanding of the different environmental contributions in homogeneous catalysis and can be used to achieve better charge transfer properties using these materials in heterojunctions for visible light water splitting.

HL 91: Poster IIIb (Joint session of DS and HL, organized by HL)

Topics: Oxides, Two-dimensional materials, Epitaxial growth

Time: Thursday 16:00–19:00 Location: Poster A

HL 91.1 Thu 16:00 Poster A

Formation of polar oxide thin films and interfaces: Insights from ab initio simulations — •Marc Landmann, Eva Rauls, and Wolf Gero Schmidt — Theoretische Physik, Universität Paderborn, Warburg Straße 100, 33098 Paderborn

The layer quality of heteroepitaxial ZnO films widely suffers from the lack of suitable substrate materials. In order to reduce the defect density of ZnO films, caused by the substantial lattice mismatch with common substrates, the introduction of MgO buffer layers turned out to be beneficial. [1-3] In addition, the buffer-layer approach facilitates the polarity control of ZnO films due to the formation of metastable rock-salt interlayers in the MgO buffer layer [2] as well as the ZnO films itself [3].

Here, we have studied the growth process of polar ZnO films with and without inclusion of MgO buffer layers of varying thicknesses and morphologies by state-of-the-art density functional theory calculations. Our results provide new insights into the fundamental growth dynamics of ZnO and MgO thin films and interfaces as well as the driving forces behind surface polarity selection.

[1] M. W. Cho et al., Semicond. Sci. Technol. 20, 13 (2005) [2] H. Kato et al., Appl. Phys. Lett. 84, 4562 (2004) [3] H. T. Yuan et al., J. Cryst. Growth 312, 263 (2010)

HL 91.2 Thu 16:00 Poster A

Elastic properties and strain-tuning of single-layer phosphorene — Daniel Midtvedt[1,2], Caio H. Lewenkopf[3], and •Alexander Croy[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Chalmers University of Technology, Göteborg, Sweden — [3]Universidade Federal Fluminense, Niterói, Brazil

Phosphorene (or black phosphorus) has attracted a lot of interest in recent times. Its unusual puckered structure leads to interesting anisotropic elastic and electronic properties with promising potential applications. Moreover, single-layer phosphorene is a direct semiconductor, which makes this material a candidate to be used in (opto)electronic devices. An important question in this context is the strain-dependence of the electronic band-gap.

We calculate the elastic properties of single-layer phosphorene using the valence-force model of Kaneta et al [1] and the approach given in [2], which accounts for the non-Bravais lattice structure of the material. Using a two-orbital tight-binding model [3], we study the strain-induced band-gap modification. We compare our results with recent *ab initio* calculations.

[1] C. Kaneta et al, Solid State Commun. **44**, 613 (1982).
[2] D. Midtvedt et al, arXiv:1509.02365.
[3] J.-W. Jiang and H. S. Park, Phys. Rev. **B91**, 235118 (2015).

HL 91.3 Thu 16:00 Poster A

Time-resolved photoluminescence spectroscopy on vanadium-(IV)oxide nanostructures — •Konstantin Neuhaus[1], Celina Hellmich[1], Nils Rosemann[1], Marc K. Dietrich[2], Peter J. Klar[2], Angelika Polity[2], and Sangam Chatterjee[1] — [1]) Faculty of Physics and Materials Science Center, Philipps-Universität Marburg, Renthof 5, D-35032 Marburg, Germany — [2]) I. Physical Institute, Justus-Liebig University Giessen, Heinrich-Buff-Ring 16, D-35392 Gießen, Germany

Transitionmetal oxides show various intriguing phenomena which may be attributed to the complex interplay of various degrees of freedom such as electronic excitations, lattice vibration, and spin states of matter. Vanadium(IV)oxide for instance shows a metal-insulator transition at a lattice temperature of T_c=68°C which is accompanied by a change in the crystal structure. Here, we study the electro-optical response on VO_2 nanostructures. The microcrystalline samples are grown on various substrates by radio-frequency sputter-deposition and partially doped with Sr. The time-resolved photoluminescence characteristics are recorded for various lattice temperatures using a confocal streak-camera setup with high spatial resolution.

HL 91.4 Thu 16:00 Poster A

Magnetization dynamics of the Skyrmion cuprate Cu_2OSeO_3 — •Evgeniia Slivina[1], Prashant Padmanabhan[1], Rolf B. Versteeg[1], Petra Becker[2], and Paul H. M. van Loosdrecht[1] — [1]Physics Institute 2, University of Cologne, 50937 Cologne, Germany — [2]Institute for Crystallography, University of Cologne, 50939 Cologne, Germany

In chiral crystal structures, the competition between the Heisenberg exchange and Dzyaloshinskii-Moriya exchange leads to a helimagnetic ground state ordering. Interestingly, under the presence of an external magnetic field, the Zeeman interaction energy stabilizes the formation of topologically robust nanometer sized Skyrmion spin vortices. Recently, ultrafast inverse Faraday effect measurements have been used to address the fundamental magnetic relaxation processes of the Skyrmion lattice in the cuprate material Cu2OSeO3. Here, we extend upon these findings by employing the time-resolved magneto-optical Kerr effect (TR-MOKE). In addition, we investigate the time-domain dynamics of the weakly fluctuating regime at the boundary between the helical, conical, and paramagnetic phase.

HL 91.5 Thu 16:00 Poster A

Magnetization dynamics of the Skyrmion cuprate Cu_2OSeO_3 — •Evgeniia Slivina[1], Prashant Padmanabhan[1], Rolf B. Versteeg[1], Petra Becker[2], and Paul H. M. van Loosdrecht[1] — [1]Physics Institute 2, University of Cologne, 50937 Cologne, Germany — [2]Institute for Crystallography, University of Cologne, 50939 Cologne, Germany

In chiral crystal structures, the competition between the Heisenberg exchange and Dzyaloshinskii-Moriya exchange leads to a helimagnetic ground state ordering. Interestingly, under the presence of an external magnetic field, the Zeeman interaction energy stabilizes the formation of topologically robust nanometer-sized Skyrmion spin-vortices. Recently, ultrafast inverse Faraday effect measurements have been used to address the fundamental magnetic relaxation processes of the Skyrmion lattice in the cuprate material Cu_2OSeO_3. Here, we extend upon these findings by employing the time-resolved magneto-optical Kerr effect (TR-MOKE). In addition, we investigate the time-domain dynamics of the weakly fluctuating regime at the boundary between the helical, conical, and paramagnetic phase.

HL 91.6 Thu 16:00 Poster A

Nonlocal resistance in plasma hydrogenated graphene — •Tobias Völkl, Thomas Ebnet, Philipp Nagler, Tobias Korn, Christian Schüller, Dieter Weiss, and Jonathan Eroms — Institut für Experimentelle und Angewandte Physik, Universität Regensburg, Germany

Plasma hydrogenation was used to modify monolayer graphene with the intent to increase the spin orbit coupling strength in graphene. Raman spectroscopy was employed to extract the defect concentration and to characterize the hydrogenation process. Further, the temperature dependence of the hydrogen desorption was examined. Electrical transport measurements on an as fabricated sample showed large nonlocal resistances. The high value of the nonlocal resistance and the absence of any inplane magnetic field dependence of this resistance indicate that this signal is not caused by the spin-Hall effect.

HL 91.7 Thu 16:00 Poster A

Population inversion in Landau-quantized graphene — •Samuel Brem[1], Florian Wendler[1], and Ermin Malic[2] — [1]Technische Universität Berlin, Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, 10623 Berlin, Germany — [2]Chalmers University of Technology, Department of Physics, SE-412 96 Gothenburg, Sweden

In the presence of strong magnetic fields the linear band dispersion of graphene is quantized into non-equidistant Landau levels, which can be selectively excited and probed with circularly polarized light. The extraordinary arrangement of energy levels opens up the possibility to create a population inversion between optically coupled Landau levels of graphene [1]. This is an important prerequisite for the design of a highly tunable Landau level laser in the terahertz regime.

To prove that the predicted population inversion can be exploited to generate coherent laser light, a quantum optical investigation of Landau-quantized graphene in a cavity is performed. Based on the density matrix formalism combined with a tight-binding approach, we study the ultrafast dynamics of Dirac electrons in a magnetic field coupled to the photons in an optical cavity. This approach allows us to address the question whether the emission of coherent laser light in a graphene-based Landau level laser is possible.

[1] F. Wendler, and E. Malic, Sci. Rep. 5:12646 (2015)

HL 91.8 Thu 16:00 Poster A

THz Photoconductivity of Epitaxial Graphene and the Possible Opening of a Bandgap — •Markus Göthlich[1], Cay-Christian Kalmbach[2], Mattias Kruskopf[2], Klaus Pierz[2], Franz-Josef Ahlers[2], and Andreas Hangleiter[1] — [1]Institut für Angewandte Physik, Technische Universität Braunschweig, Mendelssohnstraße 2, D-38106 Braunschweig — [2]Physikalisch-Technische Bundesanstalt, Bundesallee 100, D-38116 Braunschweig

Due to it's Dirac like nature the Landau quantization in graphene is given by $E_n = \mathrm{sgn}(n)\sqrt{\Delta^2 + 2\hbar v_F^2 e\,|Bn|}$ with Landau level (LL) index n. This gives a nontrivial Shubnikov-de Haas-effect (SdH) depending on the magnetic field B and – different to conventional material systems – on the chemical potential. It also allows the observation of resonant inter-Landau-level transitions at different magnetic fields for a given transition energy as shown by Gusynin et al. (Phys. Rev. Lett. **98**, 157402 (2007)). Motivated by a simulation that shows that SdH measurements alone might not be able to distiguish between the effect of a bandgap and the effect of the chemical potential, we want to investigate here the influence of a possible opening of a band gap in epitaxial graphene on the cyclotron resonance. Therefore we use the change of the photoconductivity in the cyclotron resonance case in the SdH regime and in the THz spectral range ($\hbar\omega_{\mathrm{photon}} \approx 10\,\mathrm{meV}$) for epitaxial graphene on SiC. Our results can also be relevant for the detection of THz radiation by spectrally selective detectors based on cyclotron resonance in graphene.

HL 91.9 Thu 16:00 Poster A

Engineering the band structure and magnetism in edge corrugated zigzag graphene nanoribbons — •Prakash Parida[1] and Swapan K Pati[2] — [1]Institute for Theoretical Physics, University of Regensburg, D-93040 Regensburg, Germany — [2]Theoretical Sciences Unit, Jawaharlal Nehru Centre For Advanced Scientific Research, Bangalore 560064, India

Electronic structure and conductance properties of edge-corrugated zigzag graphene nanoribbons have been studied within the framework of p-orbital tight binding model with a mean field approximation to the Hubbard term. The results show that, both the band gap and magnetic moment increase with the depth of corrugation. Electric field modulates the carrier nature of mid-gap states to a great extent.

HL 91.10 Thu 16:00 Poster A

Towards biomedical sensing with chemically functionalized graphene FETs — •David Kaiser[1], Andreas Winter[1], Thomas Weimann[2], and Andrey Turchanin[1,3] — [1]Institute for Physical Chemistry, Friedrich Schiller University Jena, Lessingstr. 10, 07743 Jena, Germany — [2]Physikalisch-Technische Bundesanstalt, 38116 Braunschweig, Germany — [3]Jena Center for Soft Matter (JCSM), Philosophenweg 7, 07743 Jena, Germany

Graphene field-effect transistor (GFET) biosensors can intrinsically possess a very high sensitivity up to the fM level. However, this sensitivity is difficult to achieve in combination with high selectivity and specificity of the biomolecular binding events. Thus, covalent func-

tionalization of GFETs results in impairing the electronic structure of graphene, which significantly reduces the device mobility. The functionalization of graphene via physisorption typically causes larger distances between the analyte and graphene plane, which reduces the number of charge carriers induced in graphene per binding event. Both effects reduce sensitivity of GFET biosensors. To overcome these problems, we employ ultrathin (~ 1 nm) dielectric carbon nanomembranes (CNMs) to chemically functionalize GFETs without impairing the electronic performance. A CNM is placed on top of graphene in the manner of all-carbon van der Waals heterostructures and acts as an analyte-specific electrochemical transducer [1]. We present and analyze the electronic characteristics of the fabricated hybrid CNM/graphene FET arrays.

[1] M. Woszczyna et al. Adv. Mater. 26, 4831 (2014).

HL 91.11 Thu 16:00 Poster A

Quasi-classical ballistic transport in graphene antidot superlattices — •George Datseris, Ragnar Fleischmann, and Theo Geisel — Max Planck Institute for Dynamics and Self-Organization (MPIDS), 37077 Goettingen, Germany

Recent magneto-transport experiments have revealed that electrons in graphene can exhibit similar commensurability effects as those that have been observed in ballistic semiconductor devices. We therefore study quasi-classical models for transport in graphene monolayers patterned with antidot superlattices at magnetic fields below the quantum Hall regime. Using the first order approximation of the dispersion relation of graphene (i.e. the Dirac equation approximation) we reproduce the experimental findings. Progressing from this we explore parameter regions not yet studied in experiment and extend our model to include the quasi-classical dynamics generated by the second order approximation of the dispersion relation.

HL 91.12 Thu 16:00 Poster A

Magneto Transport Properties of Mesoscopic HOPG Graphite Flakes: Thickness Dependence — •Mahsa Zoraghi[1], José Barzola-Quiquia[1], Markus Stiller[1], Tobias Lühmann[2], and Pablo Esquinazi[1] — [1]Division for Superconductivity and Magnetism, Faculty of Physics and Earth Sciences, University of Leipzig, Linnestr. 5, D-04103, Germany — [2]Institute for Medicine Physics and Biophysics, University of Leipzig, 04107 Leipzig

The electrical transport properties of mesoscopic thin graphite flakes (HOPG) as function of temperature and magnetic field were investigated. Samples were measured in the range of 2 up to 310 K and magnetic fields of ±7 T. The temperature dependendent resistance $R(T)$ shows that samples thicker than ≈35 nm have metallic behavior and thinner samples show semiconducting-like behavior. The resistivity increases with decreasing sample thickness. We explained the $R(T)$ measurements using a model, which considers contributions in parallel. A contribution behaving like a 2DEG system formed at the interfaces of the crystals inside the sample; the other has a semiconducting behavior, which we attribute to the crystalline regions. The MR measurements show a thickness dependence, i.e. the change is reduced by reducing the thickness of the sample. Shubnikov de Haas (SdH) oscillations are more pronounced in thick samples, and show that the conductivity in our samples is dominated by two types of carriers. The results indicate that transport properties of bulk graphite are not intrinsic and depend on the interfaces. Raman results reveal that all of the samples have the same structural quality as of bulk HOPG.

HL 91.13 Thu 16:00 Poster A

The substrate dependence of localizing excitons in WSe2 monolayers — •Jhih-Sian Tu[1], Sven Borghardt[1], Florian Winkler[2], Detlev Grutzmacher[1], and Beata Kardynal[1] — [1]PGI-9, Forschungszentrum Juelich, Juelich, Germany — [2]ER-C, Forschungszentrum Juelich, Juelich, Germany

Monolayer transition-metal dichalcogenides (TMDs) have become new building blocks for two-dimensional (2D) heterestructures which are composed of monolayers of different materials bound with Van der Waals forces. In this study, the photoluminescence (PL) of WSe2 monolayers (ML) is compared with that of hexagonal-boron nitride (hBN)/WSe2 ML/hBN heterostructures. The samples were prepared by PDMS dry transfer of WSe2 MLs on target substrates (SiO2 or hBN). The PL measurements showed that encapsulation leads to a suppression of the free exciton emission and to a shift of the exciton emission energy. An impurity band emission, although present in all sample geometries, is also strongly modified by the encapsulation. It is present across the whole sample and takes a form of a set of sharp emission lines in wide wavelength range. These sharp emission lines are linearly polarized as in the case of the emission from the localized states in WSe2 on SiO2 or on hBN. Variations in geometries of measured samples allow the analysis of the data in terms of influence of external impurities, intrinsic defects and a surface strain caused by hBN encapsulation. We discuss the substrate choice for the control of photoluminescence from localized states in WSe2 ML.

HL 91.14 Thu 16:00 Poster A

Ab initio elasticity of Ga_2O_3 in the α and β phase — •Konstantin Lion, Dmitrii Nabok, Pasquale Pavone, and Claudia Draxl — Physics Department and IRIS Adlershof, Humboldt-Universität zu Berlin D-12489 Berlin

The transparent conducting oxide Ga_2O_3 has a wide band gap of about 4.4 - 4.8 eV. It is a very promising candidate in a number of applications, such as transparent electrodes for UV optoelectronic devices, semiconducting lasers and transparent electrodes in solar cells. Depending on the preparation, Ga_2O_3 can crystallize in 5 different structures, among them the monoclinic β and the hexagonal α phase. The structural and elastic properties of these phases are investigated from first principles using the full-potential all-electron code `exciting` [1]. The calculated lattice parameters are in good agreement with experimental and previously reported theoretical results. Second-order elastic constants of both phases are calculated using the tool `ElaStic` [2]. Furthermore the stability of these 2 phases is investigated by applying stability criteria, such as the Born criteria.

[1] A. Gulans *et al.*, J. Phys.: Condens. Matter **26**, 363202 (2014).
[2] R. Golesorkhtabar *et al.*, Comp. Phys. Commun. **184**, 1861 (2013).

HL 91.15 Thu 16:00 Poster A

PAMBE-Growth of SnO_2 — •Max Kracht, Alexander Karg, Jie Jiang, Jörg Schörmann, and Martin Eickhoff — I. Physikalisches Institut der JLU Gießen, Heinrich-Buff-Ring 16, D-35392 Gießen

The application of tin dioxide (SnO_2) as gas sensitive material or highly doped as a transparent conducting oxide has been investigated in detail. To further increase the application range of this non-toxic, chemically stable material and to gain further knowledge of the basic material properties, single crystalline thin films are required.

Plasma-assisted molecular beam epitaxy is a well established method to gain high quality crystalline films. Therefore SnO_2 thin films were grown by PAMBE on r-plane sapphire substrates. The influence of different growth parameters like substrate temperature or tin beam equivalent pressure on the structural and electrical film characteristics are investigated using high resolution X-ray diffraction (HRXRD), scanning electron microscopy (SEM), atomic force microscopy (AFM) and Hall measurements.

HL 91.16 Thu 16:00 Poster A

Group-IV doping of ion-beam sputtered Ga_2O_3 — •Philipp Schurig, Martin Becker, Fabian Michel, Angelika Polity, and Martin Eickhoff — 1st Physics Institute, Justus-Liebig-University Giessen, Giessen, Germany

For the last years the interest in transparent conductive materials stayed at a high level due to possible applications in the field of (opto-)electronics, for example as photoresistors/-diodes, high temperature sensors and solar cells. The thermodynamically most stable oxide of gallium, β-gallium oxide, has monoclinic crystal structure and a band gap of around 4.9 eV.

One requirement for the usage in electronics is a controllable carrier concentration, achievable by n-type doping with suitable elements as there are Sn, Si and Ge. With Ion-Beam-Sputtering from a Ga_2O_3 target Sn, Si and Ge doped samples were prepared. The substrate holder was heated to 650 °C during deposition and c-sapphire and quartz substrates were used.

Transmittance, X-Ray-Diffraction, Energy Dispersive X-Ray Spectroscopy and Scanning Electron Microscopy measurements were performed to characterize the deposited layers after deposition and to investigate the effect of a post-deposition anneal at temperatures of 1000 °C and above in oxidizing atmosphere. An improvement of the structural properties and a blue-shift of the optical absorption edge were observed.

HL 91.17 Thu 16:00 Poster A

An X-ray photoelectron spectroscopy (XPS) study on NiO/SnO_2 and SnO/SnO_2 heterojunctions — •Fabian Michel,

Benedikt Kramm, Martin Becker, Robert Hamann, Angelika Polity, Detlev M. Hofmann, and Martin Eickhoff — Justus-Liebig Universität Giessen, Germany

The energy band diagrams of different pn-heterojunctions were evaluated by X-ray photoelectron spectroscopy. The heterojunctions were fabricated by ion beam sputtering. The valence band and conduction band discontinuities of NiO/SnO_2 and SnO/SnO_2 were investigated using the common method of E.A. Kraut[1] and J.R. Waldrop[2] considering the position of the different core level signals and especially the related energy difference in the vicinity of the heterointerface. Using depth profiling via in situ Ar+ ion etching we made a qualitative analysis of the interfacial chemical state by estimating the modified Auger parameter and the relative concentrations of the photoelectron signals. We also investigated the challenging Ni 2p signal by decomposing the line structure and the satellite structure. Results will be discussed with respect to other metal oxide heterojunctions.

[1] Kraut, E. A.; Grant, R. W.; Waldrop, J. R. und Kowalczyk, S. P., Semiconductor core-level to valence-band maximum binding-energy differences: Precise determination by x-ray photoelectron spectroscopy. Phys. Rev. B, Aug. 1983, 28(4):1965

[2] Waldrop, J. R. und Grant, R. W., Measurement of AlN/GaN (0001) heterojunction band offsets by x-ray photoemission spectroscopy. Applied Physics Letters, 1996, 68(20):28792881

HL 91.18 Thu 16:00 Poster A

Energy Band Alignment of Novel p-type Transparent Conducting Oxides on Indium Tin Oxide — Emma Norton, Leo Farrell, Daragh Mullarkey, Igor Shvets, and •Karsten Fleischer — School of Physics and Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN), Trinity College, University of Dublin, Dublin 2, Ireland

Thin films of p-type Cr_2O_3:Mg have been produced by Molecular Beam Epitaxy (MBE) as well as amorphous, copper deficient p-type Cu_xCrO_2 deposited by a low temperature solution based method (spray pyrolysis). These thin films are deposited on top of commercial n-type Indium Tin Oxide substrate to produce transparent pn junctions. The band alignment of these two interfaces is studied using X-ray Photoelectron Spectroscopy (XPS) and Ultra Violet Photoelectron Spectroscopy (UPS). An estimate of the band discontinuities at the interfaces of ITO/Cr_2O_3:Mg and ITO/a-Cu_xCrO_2 are given. An emphasis is given to the fact that the Fermi level and work function position for both Cr_2O_3:Mg and a-Cu_xCrO_2 show changes with surface preparation and surface termination.

HL 91.19 Thu 16:00 Poster A

Noise spectroscopy on In_2O_3 films — •Bonito Thielert[1], Fariba Hatami[1], W. Ted Masselink[1], Oliver Bierwagen[2], and James S. Speck[3] — [1]Humboldt-Universität zu Berlin, Inst. für Physik, Newtonstr. 15, 12489 Berlin — [2]Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5-7, 10117 Berlin — [3]Materials Department, University of California, Santa Barbara, USA

How good is the quality of In_2O_3 layers? In order to answer this question, several In_2O_3 samples were grown using molecular-beam epitaxy on Y-stabilized ZrO_2(001) wafers. Mg-, Zn- and unintentionally doped samples were after growth thermally annealed in vacuum and in oxygen environment to change the compensating point defect concentration. The influence of doping and annealing of the electronic properties and the material quality were investigated by noise spectroscopy and Hall measurements. Our results show that most samples annealed in vacuum have 1/f noise with higher magnitude compared to samples annealed in oxygen environment. The estimated Hooge-factor [1] was between 10^{-2} and 10^{2} depending on the type of the doping and the annealing conditions. The Mg-doped sample annealed in oxygen environment has the lowest Hooge-factor of 10^{-2}. The value is more than one order lower than the reported value for the amorphous In_2O_3 [2]. The Sn-doped sample annealed in vacuum, on the other hand, has the highest Hooge-factor. The Hooge-factor will be qualitatively correlated to conductivity and the concentration of dopants and point defects.

[1] F. N. Hooge, Physica (Amsterdam) 60, 130 (1972) [2] R. E. Johanson, and S.O. Kasap, J. Vac. Sci. Technol. A 20, 1027 (2002)

HL 92: Postersession DS/HL

Presenters are kindly requested to be near their poster for at least one hour during poster session or leave a note about their availability for discussions.

Time: Thursday 16:00–19:00 Location: Poster A

HL 92.1 Thu 16:00 Poster A

Metallic Chains on Ge (001) Surface and Their Manipulation — •Deniz Aşan Acar[1], Umut Kamber[1], Dilek Yildiz[2], and Oğuzhan Gürlü[1] — [1]Istanbul Technical University, Istanbul, Turkey — [2]University of Basel, Basel, Switzerland

One dimensional, single atom thick wires present an exotic playground. We investigate the surface structure formed by adsorption of Pt and Au on Ge(001) surface. It is well known that upon annealing of Pt deposited Ge(001) surface at 1000 K atomic chains form along with two different types of terraces. Similar structures form due to Au deposition on Ge(001). In this study we have experimented on the co-deposition of Au and Pt on to Ge(001) surfaces. We will report on our findings related to the formation of novel atomic scale structures. (This study was funded by a TUBITAK 1001 project with grant number 112T818.)

HL 92.2 Thu 16:00 Poster A

Mask-less Selective Area Epitaxy of self-catalyzed GaN-microrods on silicon — •Christian Blumberg, Dennis Jansen, Werner Prost, and Franz-Josef Tegude — University Duisburg-Essen, Faculty of Engineering, Solid-State Electronics Department, Duisburg, Germany

3D GaN microrod structures offer the potential to fabricate electro-optical devices that may outperform their 2D counter parts. Promising candidates are the GaN/InGaN microrod-LEDs. These m-planar GaN/InGaN-LEDs are not limited by quantum-confined Stark effect at the GaN/InGaN interface (long charge-carrier lifetimes and less radiative efficiency at high intensities). A major issue by producing a macro sized usable LED from microrod-structures is the inhomogeneous distribution among the microrods: length, diameter and distance between each rod changes from rod to rod. As a result each rod-device has different electro-optical properties, which leads e.g. to a broadening of emission spectrum of a LED, consisting of parallel electric-powered microrod-LEDs. In order to reach a high homogeneity selective area epitaxy (SAE) of the rods is necessary. In this work we discuss the high-density seeding of rods on Si (111). We have developed a new method of the SAE for self-catalysed GaN-rods, which is based on pattering the Si-surface by nanoimprint technology. In contradiction to other methods for SAE we did not use a dielectric mask (like SiNx or SiOx). By adapting the Si-surface pattern (depth of etched holes and surface cleaning) and the epitaxial parameters (silane-flow and V/III) we were able to grow position controlled GaN-rods on Si.

HL 92.3 Thu 16:00 Poster A

Stability of misfit dislocations in axial-heteroepitaxial 3C-SiC/c-GaN nanopillars and nanomesas — •Thomas Riedl[1], Ricarda Kemper[1], Andras Kovacs[2], Doris Meertens[2], Donat As[1], and Jörg Lindner[1] — [1]University of Paderborn, Department of Physics, Warburger Straße 100, 33098 Paderborn, Germany — [2]Ernst-Ruska Centre for Microscopy and Spectroscopy with Electrons, FZ Jülich, 52425 Jülich

GaN represents the most important compound semiconductor for realization of highly efficient blue LEDs and lasers. The cubic modification of GaN (c-GaN) has attracted growing interest due to the absence of internal electric fields. For the fabrication of high-quality semiconductor devices defect-free epilayers are essential. One way to avoid defects arising due to misfit is to reduce the lateral dimension of the layer to the nanoscale, which leads to a purely elastic relaxation in three dimensions.

In order to investigate the effect of the lateral size of axial pillar or mesa shaped heterostructures on the stability of misfit dislocations for the 3C-SiC/c GaN system, we apply various analytic approaches based

on linear continuum elasticity theory. We find that the approaches of Glas and Ertekin predict the stability zone of misfit dislocations to exist at significantly smaller lateral dimensions and slightly larger layer thicknesses in comparison to the model of Zubia and Hersee. The former approaches yield a reasonable agreement with high-resolution TEM observations of c-GaN layers that have been grown on top of 3C-SiC mesa posts of different edge lengths.

HL 92.4 Thu 16:00 Poster A

Spectroelectrochemical Response of Half Cells for Solid-state Electrochromic Devices — •Christian Lupo[1], Yurong Su[2], Angelika Polity[2], and Derck Schlettwein[1] — [1]Institute of Applied Physics, Justus Liebig University Giessen, Heinrich Buff-Ring 16, 35392 Giessen, Germany. — [2]1st Physics Institute, Justus Liebig University Giessen, Heinrich Buff-Ring 16, 35392 Giessen, Germany

Electrochromic devices made by solid-state components only could provide longer lifetimes or faster switching speeds compared with currently produced devices ("smart windows", "smart mirrors") with polymeric or liquid electrolytes. Lithium phosphorous oxynitride ($LiPON$) is a promising candidate as a solid electrolyte for use in electrochromic devices. Thin films of $LiPON$ could replace the relatively thick electrolytes based on a Lithium salt in liquid or polymeric compounds because of a high chemical stability and good transparency of $LiPON$. In the present study, $LiPON$ is used in combination with tungsten oxide (WO_x) or nickel oxide (NiO), both well-known electrochromic materials which become colored upon chemical reduction or oxidation, respectively. On the way to an all-solid-state device, the first challenges consist in reaching a good ionic conducting solid electrolyte and well-working solid contacts. Electrochemical and spectroelectrochemical measurements are used to characterize the response and the coloration performance of electrochromic half cells consisting of combinations of $WO_x/LiPON$ or $LiPON/NiO$ solid layers prepared via combinations of sputtering and/or chemical bath deposition methods.

HL 92.5 Thu 16:00 Poster A

Spectroscopic Ellipsometry and MOKE as a Probe for Structural Properties of Spinel Oxide Thin Films — •Vitaly Zviagin[1], Peter Richter[2], Yogesh Kumar[1], Israel Lorite[1], Michael Lorenz[1], Daniel Spemann[1], Jan Meijer[1], Dietrich R.T. Zahn[2], Georgeta Salvan[2], Pablo Esquinazi[1], Marius Grundmann[1], and Rüdiger Schmidt-Grund[1] — [1]Universtät Leipzig, Institut für Experimentelle Physik II, Linnéstr. 5, Germany — [2]Technische Universtät Chemnitz, Semiconductor Physics, Reichenheiner Str. 70, Germany

Normal, disordered, and inverse spinel oxide ferrite and cobaltite thin films were grown at different temperatures on MgO (100), $MgAl_2O_4$ (100), and $SrTiO_3$ (100) substrates by pulsed laser deposition. Assigned electronic transitions visible in diagonal and off-diagonal elements of the dielectric tensor show a clear dependence on growth temperature corresponding to the crystal quality of the films. Silicon irradiation of $ZnFe_2O_4$ films caused inversion of normal spinel structure as well as lattice distortion with further treatment, clearly visible in the dielectric function. The $Zn_xFe_{3-x}O_4$ composition was found to contain defects such as presence of Fe^{2+} ions. Magneto-optical Kerr effect spectroscopy was employed to investigate magneto-optically active transitions, and in combination with spectroscopic ellipsometry we obtained detailed information of site occupancy related to crystal inversion and disorder. We relate optical properties to magnetic properties to show a direct correlation between site occupancy of tetrahedral sites by Fe^{3+} ions to saturation and remanence magnetization.

HL 92.6 Thu 16:00 Poster A

Growth-of p-type nickel oxide on different substrates and surface orientations — •Carsten Tschammer and Oliver Bierwagen — Paul-Drude-Institut, Hauvogteiplatz 5-7, 10117 Berlin, Germany

NiO belongs to the transparent semiconducting oxides with unintentional p-type conductivity. Currently, NiO is used in batteries and capacitors, and is considered for future applications in UV-detectors, all-oxide hetero pn-diodes, and organic solar cells. For the latter, NiO is an excellent candidate for an interfacial layer between the ITO anode and active organic layer, serving as electron blocking and hole transport layer. Doping NiO with Nitrogen as an acceptor should increase the p-type conduction.

Here NiO thin layers were grown by plasma-assisted MBE using RHEED as in situ monitoring tool. For the growth of well-defined NiO layer and surfaces MgO was chosen as substrate due to its common crystal structure and low lattice mismatch to NiO. Thus, NiO was grown on MgO(100), MgO(110), MgO(111) to help investigating the interface to the active organic layer on differently oriented surfaces. Growth on epitaxial ITO and In_2O_3 was performed to come closer to the solar cell application and application in pn-diodes, respectively. The film crystal and surface structure were investigated by AFM, XRD, XRR. The electronic properties were investigated by Raman, PL and transport measurements.

HL 92.7 Thu 16:00 Poster A

Intermediate tin oxide phases from first principles — Bianca Eifert and •Christian Heiliger — Institut für Theoretische Physik, Justus Liebig University Gießen, D-35392, Germany

The two stable tin oxides, SnO and SnO_2, are semiconductors with bandgaps of different types and sizes. Both of them are therefore of great interest for applications, and may even be used together for tin-only devices. It has also been known for over a century that when SnO disproportionates, mixed-valence oxides of other stoichiometries can be formed as intermediates. These phases are also accessible from elementary precursors, for instance through thin-film deposition techniques. The intermediate oxides have, however, eluded conclusive analysis in the past. Using density functional theory (DFT) and phonon calculations, we can predict the electronic structures and Raman spectra for different candidate crystal structures. Comparing these new insights with experimental results, we are now able to determine the identity and properties of the intermediate tin oxide.

HL 92.8 Thu 16:00 Poster A

Pseudomorphic growth and relaxation of alpha gallium oxide on sapphire substrate — •Zongzhe Cheng[1], Patrik Vogt[1], Robert Schewski[2], Oliver Bierwagen[1], Martin Albrecht[2], Achim Trampert[1], and Michael Hanke[1] — [1]Paul-Drude-Institut für Festkörperelektronik (PDI), Berlin, Germany — [2]Leibniz-Institut für Kristallzüchtung (IKZ), Berlin, Germany

Alpha phase gallium oxide is a transparent semiconducting material with an indirect wide band gap of around 5eV. The heteroepitaxial growth of alpha phase gallium oxide on insulating c-plane sapphire (band gap = 8.8ev) can be realized by molecular beam epitaxy since they have the same corundum crystal structure and small lattice mismatch (4.6% in a-axis and 3.3% in c-axis). However under ambient conditions, the beta phase gallium oxide with a monoclinic structure is thermodynamically more stable than the alpha phase, so normally beta phase gallium oxide starts to grow after a three atomic layer of alpha phase gallium oxide on the c-plane sapphire substrate in molecular beam epitaxy growth. So it is important to stabilize the growth of alpha phase gallium oxide trying to get pure alpha phase gallium oxide layer on the substrate in case of device applications (eg. 2deg). In this work, we use mainly synchrotron radiation and high resolution transmission electron microscopy in order to understand the pseudomorphic growth and relaxation of the alpha phase gallium oxide on c-plane sapphire substrate. In addition, an annealing experiment on a low-temperature-deposited amorphous gallium oxide layer is performed trying to crystallize the gallium oxide layer and stabilize the alpha phase.

HL 92.9 Thu 16:00 Poster A

Transmission Electron Diffraction on a really free-standing heterostructure and analysis of the resulting Moiré pattern — Marlene Adrian, •Arne Senftleben, Silvio Morgenstern, and Thomas Baumert — Institut für Physik und CINSaT, Universität Kassel, Heinrich-Plett-Straße 40, 34132 Kassel

The combination of various 2D layered materials in multilayer heterostructures arises great interest in the current science. Due to the large variety of electronic properties of the group of 2D layered materials the combination opens a new pathway towards ultrasmall electronic devices. In this contribution we present a preparation method to obtain free-standing samples of multilayer heterostructures and a full characterisation of their diffraction images. A 20 nm thick MoS_2–graphite heterostructure was produced and analysed with the methods presented. Additionally, the ultrafast lattice dynamics after optical excitation of the sample will be discussed.

HL 92.10 Thu 16:00 Poster A

Silicene-based spin-filter device: Impact of random vacancies — Cesar Nunez[1], Francisco Dominguez-Adame[2], Pedro Orellana[1], Luis Rosales[1], and •Rudolf A. Römer[3] — [1]Universidad Tecnica Federico Santa Maria, Valparaiso, Chile —

[2]Universidad Complutense, E-28040 Madrid, Spain — [3]University of Warwick, Coventry, CV4 7AL, UK

We propose a hybrid spin-filter device based on a silicene nanoribbon. A ferroelectric polymer grown on top of the nanoribbon splits spin-up and spin-down electron bands and gives rise to spin polarisation of the conductance. In particular, we study the effects of a random distribution of vacancies on the performance of this spin-filter device. Disorder induces Anderson localisation of electrons and we find that the localisation length strongly depends on the electron spin. By adjusting the Fermi level of the source contact, only electrons with one spin orientation can reach the drain contact because their localisation length is larger than the length of the device. Electrons with opposite spin are largely back-reflected. Electric conductance then becomes spin polarised and the device behaves as a quasi-half-metal. We conclude that a moderate concentration of vacancies has little impact on the spin-filter capabilities of the device, opening the possibility to using it as a tuneable source of polarized electrons.

HL 92.11 Thu 16:00 Poster A

Stacking different two-dimensional materials to fabricate a high mobility transistor — •Himani Arora[1,2], Gotthard Seifert[3], Gianaurelio Cuniberti[4], Manfred Helm[1,2], and Artur Erbe[1] — [1]HZDR, Bautzner Landstrasse 400, 01328 Dresden — [2]Technical University Dresden, Faculty of Mathematics and Natural Sciences, 01062 Dresden — [3]Technical University Dresden, Institute for Physical Chemistry and Electrochemistry, 01062 Dresden — [4]Technical University Dresden, Institute for Materials Science and Max Bergmann Centre of Biomaterials, 01062 Dresden

In recent years, several two-dimensional (2D) semiconducting materials like graphene, MoS2, WSe2, silicene, germanene etc. have been produced and studied. Their semiconducting properties allow the development of 2D structures, whose electronic properties can be tuned. By fabricating gate electrodes on the 2D materials, field effect transistors have been demonstrated. Further exciting possibilities open up when these materials are stacked together to achieve the desired application. The first series of experiments are carried out with graphene nanoribbons (GNRs) deposited on functionalized Si/SiO2 substrate. Prior to the deposition, the Si/SiO2 substrate is patterned with Ni alignment marks, to locate and characterize GNRs by AFM and Raman spectroscopy. Au electrodes are then fabricated on selected GNRs using electron beam lithography to measure the electrical transport properties. In future, the aim will be to fabricate a heterostructure by stacking different 2D materials, whose different properties can complement each other to fabricate a high mobility transistor.

HL 92.12 Thu 16:00 Poster A

Magnetic-field dependent photoluminescence measurements of WS_2 monolayers — •Jan Kuhnert, Simon Schmitt, Arash Rahimi-Iman, Ajanth Velauthapillai, and Wolfram Heimbrodt — Faculty of Physics and Materials Sciences Center, Philipps-Universität Marburg, Renthof 5, D-35032 Marburg, Germany

Layered transition-metal dichalcogenides have attracted great interest in the last few years. Thinned down to monolayers they exhibit outstanding optical properties caused by the direct band gap. Here we present photoluminescence measurements of tungsten disulfide monolayers at low temperatures (2 K) in the presence of an external magnetic field in Faraday geometry. In the monolayer limit the inversion symmetry is broken and spin and valley are coupled. The degeneracy between the two equivalent K and K' valleys is broken by applying external magnetic fields. This causes a Zeeman shift which has already been shown in similar layered transition-metal dichalcogenides (eg. MoSe2: 0,25 meV/T (1)). We show this field-dependent Zeeman splitting in tungsten disulfide at low temperatures (2 K) and find a surprisingly large splitting of 0,8 meV/T.

(1) Nature Physics 11, 141147 (2015)

HL 92.13 Thu 16:00 Poster A

Hydrogenation of Epitaxial Silicene Studied by *in situ* Raman Spectroscopy — •Dmytro Solonenko[1], Patrick Vogt[2], Ovidiu D. Gordan[1], and Dietrich R.T. Zahn[1] — [1]Semiconductor Physics, Technische Universität Chemnitz, D-09107 Chemnitz, Germany — [2]Institut für Festkörperphysik, Technische Universität Berlin, D-10623 Berlin, Germany

As silicene can be only grown epitaxially on a substrate like Ag(111) single crystals, the influence of the substrate on the 2D silicene properties have been extensively discussed in literature. It was shown that the electronic properties of epitaxial silicene are altered due to the significant interaction with the substrate but it still keeps a clear semimetallic character[1], as expected for ideal freestanding silicene. On the other hand, an electronic bandgap could be opened by applying an electric field perpendicular to the sheet, or via functionalization, *e.g.* by H-adsorption. In the latter case, controlled hydrogenation of freestanding silicene might open a bandgap up to the UV edge of the visible spectral region[2]. In order to examine if the silicene structure is preserved upon hydrogenation, we grew silicene monolayer sheets on Ag(111) substrate and hydrogenated them by supplying activated atomic H. *In situ* Raman spectroscopy study was carried out in order to follow structural changes of the silicene layer upon H-adsorption. We find that the silicene hydrogenation is reversible by heating the sample, at temperatures expected to be sufficient for breaking the H-Si bonds. [1] Johnson, N. W. *et al.*, *Adv. Func. Mat.* **24**, 5253-5259 (2014). [2] Osborn, T. H. *et al.*, *Chem. Phys. Lett.* **511**, 101 (2011).

HL 92.14 Thu 16:00 Poster A

Electrical properties of CVD Molybdenum disulfide — •Wajid Awan[1], Tommy Schönherr[1], Artur Erbe[1], Stefan Facsko[1], and Xinliang Feng[2] — [1]Helmholtz-Zentrum Dresden-Rossendorf — [2]Technische Universität Dresden

Two dimensional materials are attractive for the use in next-generation nanoelectronic devices as compared to one dimensional material because it is relatively easy to fabricate complex structures from them. Recently the layered 2D semiconducting Transition metal dichalcogenides came into the picture and got a place in a wide range of novel applications as well as in basic research. Strikingly, MoS_2 receives significant attention since it undergoes transition from indirect bandgap (bulk form) to a direct bandgap (1.2eV) semiconductor if thinned out to a single atomic layer. The bandgap is an essential property for tunable 2-D nanodevices. We performed electrical transport measurements at room temperature for CVD grown MoS_2 on SiO_2/Si substrate. Standard Electron beam lithography (EBL) was used to pattern Gold (Au) metal contacts on MoS_2 flakes. For the purpose of sample characterization, we performed the Atomic Force Microscopy (AFM) and Raman Spectroscopy techniques, respectively, which confirm that the thickness of the CVD grown MoS_2 triangular flakes corresponds to single layers. Low temperature characterization of the electrical properties of the layers elucidates the exact mechanisms of charge transport in the 2d-layers. This knowledge will be used to modify the electrical properties in a controlled way, for example by ion irradiation.

HL 92.15 Thu 16:00 Poster A

Molecular beam epitaxy growth and in situ analysis of transition metal dichalcogenides — •Avanindra Kumar Pandeya, Amilcar Bedoya Pinto, Ilya Kostanovskiy, Kai Chaang, and Stuart Parkin — Max Plank Institute for Microstructure Physics, Halle, Germany

Atomically thin transition metal dichalcogenides (TMDCs), layered materials which have captured great attention due to their tunable electronic properties [1], are commonly fabricated via exfoliation of high-quality bulk crystals. Although there has been tremendous progress in fabricating devices out of exfoliated heterostructures [2], there are other effects, such as spin transfer, that need atomically clean interfaces for an optimum harvesting. Our approach is to grow TMDCs layers by molecular beam epitaxy and assess the layer and interface quality using in-situ characterization (RHEED, LEED, XPS, AES and STM). The fabrication of high-quality TMDCs heterostructures by UHV methods opens new prospects for the design of interface-sensitive electronic and spintronic devices.

1. J. Kang, et al. Applied Physics Letters, 102, 012111 (2013)
2. C. Lee, et. al. Nature Nanotechnology 9, 676-681, (2014)

HL 92.16 Thu 16:00 Poster A

Si(553)-Au surface functionalized by small molecules — •Svetlana Suchkova[1], Eugen Speiser[1], Sandhya Chandola[1], Conor Hogan[2], Friedhelm Bechstedt[3], and Norbert Esser[1] — [1]Leibnitz-Institut für Analytische Wissenschaften - ISAS - e.V., Department Berlin, Schwarzschildstr. 8-10, 12489 Berlin, Germany — [2]Universita di Roma Tor Vergata, Via della Ricerca Scientifica 1, 00133 Roma, Italy — [3]Friedrich-Schiller-University Jena, Institut für Festkörpertheorie und optik, Helmholtzweg 3, 07743 Jena

We discuss the adsorption of toluene-3,4-dithiol molecules on the Si(553)-Au surface. In contrast to the highly reactive clean Si surface, Au-passivated surfaces offer the potential for a more selective adsorption, eventually yielding molecular layers that are essentially

self-ordered on the underlying silicon substrate. The calculations of Potential Energy Surface (PES) by Density Functional Theory (DFT) in combination with reflectance anisotropy spectroscopy (RAS) provide us with the information on molecular orientation on the surface.

HL 92.17 Thu 16:00 Poster A

Preparation-dependent viscoelastic properties of ultra-thin glass-forming polymer films. — •Pierre Chapuis[1,2], Anne Rubin[2], Freddy Anstotz[3], Paul Montgomery[3], and Günter Reiter[1] — [1]Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Germany — [2]Institut Charles Sadron, Strasbourg, France — [3]ICube/IPP, Strasbourg, France

Properties of ultra-thin glassy polymers films differ from bulk behavior. Many studies stated that it is a consequence of confinement and/or interfacial physics. Another possible explanation is suggested: the preparation process of the film by spin-coating entails an out-of-equilibrium state of the chains [1].

To give insight on this phenomenon we explore the influence of the preparation process of ultra-thin glassy freestanding polymer films on their viscoelastic response. Ultra-thin polymer films are obtained by spin-coating technique and transferred onto a silicone substrate containing an array of 5 μm. Using the nanobubble inflation method [2], a static pressure was applied and the resulting deformation was probed with time by 4D interferometric microscopy which is a non-contact method (3D + real time) developed at ICube.

We discuss the results of creep compliance measurements on poly(vinyl acetate) (PVAc) films of thicknesses below 100 nm for different molecular weights.

[1] M.Chowdhury et al., PRL 109, 136102 (2012) [2] P.A. O Connell et al., Science 18, 1750 (2005).

HL 92.18 Thu 16:00 Poster A

Transparent white AC/DC OLEDs — •Felix Fries, Markus Fröbel, Simone Lenk, and Sebastian Reineke — Institut für Angewandte Photophysik, Technische Universität Dresden, Germany

Future lighting applications will strongly benefit from transparent luminescent devices. In this contribution, we demonstrate transparent organic light-emitting diodes (OLEDs), which allow for flexible adjustment of the emission color. We extend the AC/DC concept, that was only recently presented for bottom-OLEDs, to transparent devices. Since two units are stacked on each other and the cathode of one is connected to the anode of the other, they can be addressed independently via an AC-signal. Comprising blue and yellow emission units leads to the possibility to tune the color between deep blue over cold and warm white to yellow emission.

Based on optical simulation, we build OLEDs that show an overall transparency of 62% when switched off and emit warm white light to both sides (top, bottom) with an overall power efficacy of 11.8 lm/W at a brightness of 1000 cd/m^2 when switched on. Moreover, devices without indium-tin oxide (ITO) are presented, which exclusively rely on highly transparent ultra-thin metal electrodes. These ITO-free devices achieve a power efficacy of 18.4 lm/W at 1000 cd/m^2 for warm white emission and 56% transmission.

Using an emitter combination providing red, green, and blue emission, we were also able to achieve a high color-rendering index (CRI) of 84, which further expands the range of possible applications for this promising device concept.

HL 92.19 Thu 16:00 Poster A

Influence of temperature on the interaction of excitons with electron-hole pairs in organic bulk heterojunction structures — •Jędrzej Szmytkowski — Faculty of Applied Physics and Mathematics, Gdańsk University of Technology, Gdańsk, Poland

Nowadays, a great attention is focused on organic photovoltaics. Bulk heterojunction structures based on donor-acceptor materials are treated as very promising systems to obtain high efficiencies of organic solar cells. The main effect which causes a loss of photocurrent is a recombination of charge carriers. Recently, it has been shown that an order of recombination depends on temperature. The aim of this work is to describe this process in the case when it occurs at a donor-acceptor interface due to excitons annihilation on electron-hole Langevin pairs. Additionally, a theoretical consideration based on the role of disorder is also presented.

HL 92.20 Thu 16:00 Poster A

Polarization-dependent Differential Reflectance Spectroscopy for real-time monitoring of organic thin film growth — •Andrea Navarro-Quezada, Markus Aiglinger, Ebrahim Ghanbari, Thorsten Wagner, and Peter Zeppenfeld — Institute of Experimental Physics, Johannes Kepler University, Altenbergerstr. 69, 4040 Linz, Austria

Optical spectroscopy is a powerful tool to study physical processes occurring in molecular thin films and at their interfaces with inorganic materials. In particular, differential reflectance spectroscopy (DRS) records the change in the reflectance of a surface upon physical or chemical modification. Therefore, it allows real-time monitoring of the deposition of organic thin films. In this work, we present an extended DRS setup that allows the simultaneous detection of both linear polarization states (s and p) of the reflected light [1]. The setup exhibits a signal to noise ratio better than 1000:1 as well as high signal stability, thus we detect changes in the reflectance in the order of 10^{-3}. As a proof of principle, we have implemented polarization-dependent DRS to monitor the growth of perfluoropentacene thin films on a Ag(110) single crystal in combination with photoelectron emission spectroscopy. From the analysis of the different DRS transients for s and p polarized light, we follow the alignment of the molecules on the Ag(110) surface during growth.

[1] A. Navarro-Quezada, M. Aiglinger, E. Ghanbari, Th. Wagner, and P. Zeppenfeld, *Rev. Sci. Inst.* 86, 113108 (2015)

HL 92.21 Thu 16:00 Poster A

Improved color stability of white OLEDs with tandem structure and new host material — •Yuan Liu[1,2], Zuo-Quan Jiang[1], and Liang-Sheng Liao[1] — [1]Institute of Functional Nano & Soft Materials, Soochow University, 215123 Suzhou, China; — [2]Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden, Germany;

Tandem structures can improve the efficiency and lifetime of organic light-emitting diodes (OLEDs) simultaneously. More importantly, this is also an effective strategy to reduce the color shift with increasing current density in white OLEDs. High performance tandem OLEDs require highly efficient emitting units along with an efficient charge generation layer. To improve the performance of single emitting unit, two novel host materials SF2BCz and SF3BCz which combine spirobifluorene and carbazole units via meta- and para-bonding are designed for phosphorescent OLEDs (PhOLEDs). The meta-linkage of spirobifluorene enables SF3BCz to possess high triplet energy, suitable energy levels, and good thermal stability. Blue PhOLEDs featuring SF3BCz as a host show high performance and low efficiency roll-off, with an efficiency of 41.4 cd/A (18.0%, 39.8 lm/W) at 100 cd/m2 and 39.7 cd/A (17.2%, 29.8 lm/W) at 1000 cd/m2. In addition, SF3BCz is adopted as a universal host for tandem white OLEDs, achieving an external quantum efficiency of 40% and a color stable emission spectrum.[1]

References: [1] Y. Liu, L. Cui, X. Shi, Q. Li, Z. Jiang and L. Liao, J. Mater. Chem. C, 2014, 2, 8736.

HL 92.22 Thu 16:00 Poster A

Controlling Nanostructures by Templated Templates: Inheriting Molecular Orientation in Binary Heterostructures — •Tobias Breuer and Gregor Witte — AG Molekulare Festkörperphysik, Philipps-Universität Marburg

Precise preparation strategies are required to fabricate nanostructures of specific arrangement. In bottom-up approaches, where nanostructures are gradually formed by piecing together individual parts to the final structure, the self-ordering mechanisms of the involved structures are utilized. In order to achieve the desired structures regarding morphology, grain size and orientation of the individual moieties, templates can be applied, which influence the formation process of subsequent structures. However, this strategy is of limited use for complex architectures, as the templates only influence the structure formation at the interface between the template and the first compound. Here, we discuss the implementation of so-called templated templates and analyze, in which extent orientations of initial layers are inherited in top layers of another compound to enable structural control in binary heterostructures. To that purpose we have prepared crystalline templates of the organic semiconductors pentacene and perfluoropentacene in different exclusive orientations. We observe that for templates of both individual materials the molecular orientation is inherited in the top layers of the respective counterpart.

[1] T. Breuer & G. Witte ACS Applied Materials & Interfaces 7 (36), 20485-20492 (2015)

HL 92.23 Thu 16:00 Poster A

Preparation and Characterization of Mixed Organic Thin

Films Containing Sexithiophene and Perfluorinated Sexithiophene — •Berthold Reisz, Simon Weimer, Rupak Banerjee, Christopher Lorch, Johannes Dieterle, Giuliano Duva, Alexander Hinderhofer, Alexander Gerlach, and Frank Schreiber — Universität, Tübingen, Deutschland

We study molecular mixed thin films of α-Sexithiophene (6T), a well known organic p-type semiconductor with high hole mobility, together with its perfluorinated counterpart, the so far rarely studied n-type tetradecafluoro-α-sexithiophene (PF6T). Thin films of this donor-acceptor system with various mixing ratios have been grown on several substrates in ultrahigh vacuum by coevaporation. The films have been examined with x-ray and ultraviolet photoelectron spectroscopy (XPS/UPS), atomic force microscopy (AFM), x-ray diffraction (XRD), absorption measurements and variable angle spectroscopic ellipsometry (VASE). Connections between mixing ratio, morphology, crystalline structure and optical properties are discussed, following previous studies [1].

[1] A. Hinderhofer, F. Schreiber. Organic-Organic Heterostructures: Concepts and Applications. ChemPhysChem, 13(3):628-643, 2012.

HL 92.24 Thu 16:00 Poster A

Surface morphology of vapor deposited chitosan thin films — •Maria Jose Retamal[1,3], Tomas Corrales[2], Marcelo Cisternas[3,6], Nicolas Moraga[3,6], Sebastian Gutierrez[4], Tomas Perez-Acle[4], Patrick Huber[5], and Ulrich Volkmann[3,6] — [1]Facultad de Química, PUC, Santiago, Chile — [2]IAI Universidad de Tarapacá, Arica, Chile — [3]CIEN-UC, Santiago, Chile — [4]DLab, Fundación Ciencia y Vida, Santiago, Chile — [5]Hamburg U. of Technology, D-21073 Hamburg, Germany. — [6]Instituto de Física, PUC, Santiago,Chile

Chitosan is a useful biopolymer with several industrial and biological applications. In spite of the many applications of chitosan, there is a lack of studies regarding the morphology and growth mechanisms of thin films of this biopolymer. We present a study of thin chitosan films prepared using PVD with in-situ ellipsometric monitoring. The prepared films are studied using AFM in order to correlate surface morphology with evaporation parameters. We find that the surface morphology of our final thin films depends both on the ellipsometric optical thickness as well as the evaporation rate. We find the correct evaporation parameters in order to obtain homogeneous thin films of chitosan, which are relevant for future chitosan based nano-devices. AFM images on samples prepared as a function of film thickness at constant evaporation rate, as well as AFM topographies of samples prepared as a function of evaporation rate for reaching identical film thickness show both very strong similarities to images reported as spinodal dewetting of thin metal and polymer films as a function of temperature.

HL 92.25 Thu 16:00 Poster A

XPS study of Tetraphenylporphyrin layers on Au(111) — •Peter Roese[1,2], Philipp Espeter[1,2], Christoph Keutner[1,2], Dominique Krull[1,2], Ulf Berges[1,2], and Carsten Westphal[1,2] — [1]Experimentelle Physik I, TU Dortmund, Otto-Hahn-Straße 4a, 44221 Dortmund, Germany — [2]DELTA, Technische Universität Dortmund, Maria-Goeppert-Mayer-Straße 2, 44221 Dortmund, Germany

Porphyrins are important building blocks of life. Furthermore, the interest in applying porphyrins as technical devices increased in recent years. Applications such as organic solar cells [1], organic LED's [2] or the usage of porphyrins as a photosensibilisator in cancer treatment [3] utilize the strong absorption properties of porphyrins in the visible spectrum. Here, we present the investigation of multilayers of metal-free meso-tetraphenylporphyrin (2HTPP) on an Au(111) surface using x-ray photoelectron spectroscopy (XPS) at the U55 beamline 11 at DELTA. In this study we report on a possible bonding between the molecules in the first interface layer to the Au(111) substrate while the upper molecule layers are deposited in their original form without bonding. References: [1] J. P. Collman et al., Chemical Reviews 104, 561 (2004). [2] J. M. Olson, Biochimica et Biophysica Acta (BBA) - Reviews on Bioenergetics 594, 33 (1980). [3] W. M. Campbell et al., The Journal of Physical Chemistry C 111, 11760 (2007).

HL 92.26 Thu 16:00 Poster A

Interface Analysis of PTCDI-C1 thin films on polycrystalline silver surfaces — •Guangcheng Huang, Carolin C. Jacobi, Julia Rittich, Cathy Jodocy, and Matthias Wuttig — I. Institute of Physics (IA), RWTH Aachen University, Aachen, Germany

Electronic devices based on organic thin films, such as organic solar cells (OSCs) and organic thin film transistors (OTFTs), have been greatly improved in the last decade. Understanding the interface effects between organic thin films and metal surfaces is one of the crucial steps to further improve these devices. The organic material N,N'-Dimethyl-3,4,9,10-perylenetetracarboxylic diimide (PTCDI-C1) is a promising n-type semiconductor for the application in OSCs and OTFTs. In this work, thin films of PTCDI-C1 are deposited by organic molecular beam deposition (OMBD) with varying film thicknesses onto polycrystalline silver surfaces. The energy level alignment and binding state between the metal surface and the organic molecule are determined in-situ by photoelectron spectroscopy (PES) and inverse photoelectron spectroscopy (IPES). In addition, the morphology of the organic thin films is investigated by atomic force microscopy (AFM) and the structure by X-ray diffraction (XRD).

HL 92.27 Thu 16:00 Poster A

Optical and Structural Properties of Thin Films of Difluoro-anthradithiophene — •Timo Storzer[1], Alexander Hinderhofer[1], Giuliano Duva[1], Alexander Gerlach[1], John E. Anthony[2], and Frank Schreiber[1] — [1]Universität Tübingen, Institut für Angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen — [2]Department of Chemistry, University of Kentucky, Lexington, Kentucky, 40506, USA

We report on the optical and structural properties of the novel functionalized anthradithiophene derivative difluoro-anthradithiophene (diF-ADT). Anthradithiophene (ADT) is isoelectronic with pentacene, which is one of the most studied organic semiconductors. A fluorinated anthradithiophene derivative with (triethylsilyl)ethynyl side groups (diF-TES-ADT) has been studied in recent years and showed high charge carrier mobilities in solution-cast thin-film transistors [1]. We present a study of thin films of diF-ADT prepared by organic molecular beam deposition (OMBD). We show how the growth conditions (e.g. substrate temperature, deposition rate) influence the optical and structural properties based on UV-Vis absorption, spectroscopic ellipsometry, photoluminescence (PL), X-ray reflectivity (XRR) and AFM measurements.

[1] Gundlach, D. J.; Anthony, J. E. et al., Nat. Mater. 2008, 7, 216.

HL 92.28 Thu 16:00 Poster A

Nanomechanical investigation of a thin-film multi-layered electroceramic/metal-organic framework optical device — •James P Best[1], Engelbert Redel[2], Hartmut Gliemann[2], Christof Wöll[2], and Johann Michler[1] — [1]EMPA, Thun, Switzerland — [2]KIT-IFG, Karlsruhe, Germany

Thin-film multilayer stacks of mechanically hard magnetron sputtered indium tin oxide (ITO) and mechanically soft highly porous surface anchored metal-organic framework (SURMOF) HKUST-1 were studied using nanoindentation. Crystalline, continuous, and monolithic surface anchored MOF thin films were fabricated using a liquid-phase epitaxial growth method. Control over respective fabrication processes allowed for tuning of the thickness of the thin film systems with a high degree of precision. It was found that the mechanical indentation of such thin films is significantly affected by the substrate properties; however, elastic parameters were able to be decoupled for constituent thin-film materials. For indentation of multilayer stacks, it was found that as the layer thicknesses were increased, while holding the relative thickness of ITO and HKUST-1 constant, the resistance to deformation was significantly altered. Such an observation is likely due to small, albeit significant, changes in film texture, interfacial roughness, size effects, and controlling deformation mechanism as a result of increasing material deposition during processing. Such effects may have consequences regarding the rational mechanical design and utilization of MOF-based hybrid thin-film devices.

HL 92.29 Thu 16:00 Poster A

Adsorption study of terephthalic and benzoic acids on HOPG with Metastable Induced Electron Spectroscopy (MIES) — •Marcel Marschewski[1], Harun Tas[2], Christian F. Otto[2], Wolfgang Maus-Friedrichs[1], Andreas Schmidt[2], and Oliver Höfft[3] — [1]Institut für Energieforschung und Physikalische Technologien, Technische Universität Clausthal, Deutschland — [2]Institut für Organische Chemie, Technische Universität Clausthal, Deutschland — [3]Institut für Elektrochemie, Technische Universität Clausthal, Deutschland

The adsorption behavior of benzoic acids on conducting interfaces like HOPG is of high interest for the understanding of the building mech-

anism of 2D and 3D frameworks on surfaces. Thus, the knowledge about the molecular orientation and the molecule-substrate interaction is of great importance. Here we present our results on the adsorption of 4-substituted benzoic acids (R = hydroxy-, methoxy-, propoxy-, pentyloxy- and decyloxy-chains) and terephthalic acid (TPA) on HOPG. The molecular films were studied with Metastable Induced Electron Spectroscopy (MIES) and Ultraviolet Photoelectron Spectroscopy (UPS(HeI)). For the TPA monolayer we find hints for a more planar orientation of the molecules. The benzoic acid molecules show a similar adsorption behavior on HOPG. For the 4-(decyloxy) benzoic acid we assume a possible reorientation of the alkyl chains after the first monolayer.

HL 92.30 Thu 16:00 Poster A

The study of interaction, nonlinear and dissipation effects in nanomembranes by investigating the dispersion relations of bending waves — •Fan Yang, Elke Scheer, and Reimar Waitz — Universitaetsstrasse.10 Fach 681, 78457 Konstanz, Germany

Deciphering the mode shapes of vibrations of nanopatterned membranes is paving the way for applications of nanoscale membrane which rely on particular properties of vibrational excitations. The mode shape of bending waves in thin silicon, silicon carbide, silicon nitride and ultrathin carbon nanomembranes is measured as a function of space and time, using a phase-shift interferometer with continuous and stroboscopic light [1,2]. We develop a method to obtain the contribution of the membrane itself, the eigen-frequencies and the Q factor of the membrane. The contributions of a superposition of the mode corresponding to the excitation frequency and several higher harmonics can be separated and be imaged up to the eighth harmonic of the excitation frequency. We can determine the dispersion relation of membrane oscillations in a frequency range from ground mode up to 12 MHz. The study of the temperature-dependent vibration behavior reveals an unexpected temperature dependence of the mechanical properties of a prestressed nanomembrane. At variance to expectations based on classical continuum mechanics we observe that Young's modulus increases with increasing temperature.

[1] R. Waitz, et al., Phys. Rev. B 86, 039904 (2012).
[2] X. H. Zhang, et al., Appl. Phys. Lett. 2015, 106(6): 063107.

HL 92.31 Thu 16:00 Poster A

Growth of pinholes in metal electrodes of organic photovoltaic cells — •Daniel Fluhr[1], Burhan Muhsin[1], Rolf Öttking[1], Roland Rösch[1], Marco Seeland[2], and Harald Hoppe[1] — [1]Center for Energy and Environmental Chemistry Jena (CEEC Jena) & Laboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, 07743 Jena, Germany — [2]Technische Universität Ilmenau, 98693 Ilmenau, Germany

Lifetime is still a major problem of organic photovoltaic (OPV) cells. There are many reasons for solar cell degradation varying from shunts induced by impurities or electromigration over photoinduced oxidation of active layer materials to corrosion and delamination of the metal contact both induced by oxygen or water ingress. One issue concerns so-called pinholes through the metal back electrode of the device. These pinholes offer pathways for ingress of water and oxygen which may attack the metal-organic interface by introducing delamination through formation of insulating metal oxides or hydrogen evolution. As charge injection and extraction is suppressed at delaminated areas, the active area taking part in power conversion - and hence the overall efficiency - becomes reduced. We investigated the influence of different environmental conditions on the reduction of the active area of the OPV cell. Spatially resolved measurements give information on location and size of insulated areas induced by pinholes in the metal back contact. Time resolved measurements during degradation of the devices revealed the dynamics and rate of growth of these individual defects.

HL 92.32 Thu 16:00 Poster A

Formation of noble metal thin films on P(VDF-TrFE) during DC-magnetron sputtering — Alexander M. Hinz[1], •Oleksandr Polonskyi[1], Franziska C. Löhrer[2], Volker Körstgens[2], Matthias Schwartzkopf[3], Stephan V. Roth[3], Peter Müller-Buschbaum[2], Thomas Strunskus[1], and Franz Faupel[1] — [1]CAU zu Kiel, Institut für Materialwissenschaft, LS Materialverbunde, 24143 Kiel, Germany — [2]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — [3]Deutsches Elektronensynchrotron DESY, 22607 Hamburg, Germany

In most devices using organic thin films as functional layers, e.g. organic solar cells, OLEDs or MEMS sensors, it is necessary to have an electrical contact with well-defined properties on these layers. This is often accomplished by depositing metallic electrodes onto the organic layers by physical vapour deposition (PVD) techniques. In order to control and predict the properties of the electrical contacts it is necessary to understand the interplay between the deposition process and the formation of the metallic electrodes. In this contribution we present the in-situ morphological characterization of Au thin film growth during the deposition by DC-magnetron sputtering onto P(VDF-TrFE). P(VDF-TrFE) is a versatile ferroelectric polymer used in many applications including transducers, actuators and sensors. The morphological information is obtained by grazing incidence small angle x-ray scattering (GISAXS). The in-situ information is compared with ex-situ information obtained by SEM.

HL 92.33 Thu 16:00 Poster A

Molecular order in dihexylsexithiophene thin film OFETs — Nina Zeilmann[1], Hans-Georg Steinrück[2,3], Manuel Johnson[1], Andreas Magerl[2], and •Rainer Fink[1] — [1]FAU Erlangen-Nürnberg, Physical Chemistry 2, Erlangen, Germany — [2]FAU Erlangen-Nürnberg, LS Kristallografie, Erlangen, Germany — [3]present address: SSRL, Menlo Park, USA

The end-functionalized sexithiophene Hex6THex represents a benchmark molecule for organic electronic applications such as OFETs due to its high charge carrier mobility. The latter is mainly related to the high degree of molecular ordering and π-π-stacking within the films. We have employed several probes to investigate the morphologies, molecular order and orientations of such films (thicknesses around 10 layers) prepared by vacuum sublimation at various substrate temperatures on inert SiO2 or Si3N4 substrates. X-ray reflectivity (XRR) probes the vertical electron density distribution that provides information on the thickness and density of individual sublayers. In particular, XRR yields high quality data on the arrangements of both the hexyl functionalities and the thiophene backbone. It is found that the projected length of both film features critically depends on the substrate temperature during deposition. Based on the experimental results, a model proposing the molecular orientation of the Hex6THex molecules with respect to the substrate is derived. These results are in very good agreement with AFM and micro-NEXAFS studies. Some correlations to the electrical transport properties of the films are drawn.

HL 92.34 Thu 16:00 Poster A

Colloidal masking and ion-etched nanochannels on flexible thin foils — •Calvin Brett[1,2], Matthias Schwartzkopf[1], Stephan Roth[1], Michael A. Rübhausen[2], Patrick Kluth[3], Markus Bender[4], Daniel Severin[4], and Christina Trautmann[4] — [1]DESY, Notkestr. 85, 22607 Hamburg — [2]Universität Hamburg, Inst. f. Nanostruktur- und Festkörperforschung, CFEL, APOG, Univ. Hamburg, Luruper Chaussee 149, 22761 Hamburg — [3]Australian National University. Department of Electronic Materials Engineering, Research School of Physics and Engineering, The Australian National University, Canberra, ACT 2601 — [4]: GSI Helmholtzzentrum für Schwerionenforschung GmbH, Planckstraße 1, 64291 Darmstadt

The major issues in the fabrication of periodic nanostructure arrays are the high costs, low patterning speed, and small patterning area. Spray coating of polystyrene colloids (PS) and ion-etched nanochannels on a flexible, chemical resistance polymer (PDMS) thin foil, enable reusable soft masks for deposition and imprinting techniques. Spray coating leads to a self-assembled colloidal film, where every nanosphere can be used as lenses for lithographic fabrication methods. We prove the application principle and the morphology by scattering methods, contact angle analysis and spectroscopic imaging methods. This study offers a novel routine for cost effective nanofabrication which is wide applicable in nanoscale materials.

HL 92.35 Thu 16:00 Poster A

Organic thin film growth on exfoliated hexagonal boron nitride — •Jakob Alexander Genser[1], Markus Kratzer[1], Alexandar Matkovic[2], Rados Galic[2], and Christian Teichert[1] — [1]Institute of Physics, Montanuniversität Leoben, Austria — [2]Institute of Physics, University of Belgrade, Serbia

Hexagonal boron nitride (h-BN) is a two-dimensional insulator. Especially in conjunction with graphene as ultrathin flexible electrode in organic electronics h-BN has great potential as 2D dielectric. Therefore, it is essential to understand organic thin film growth on h-BN.

Here, we use the organic semiconductor molecule para-hexaphenyl

(6P) to study the growth of small, linear, conjugated molecules on h-BN. As substrates, exfoliated h-BN flakes transferred onto a SiO2 support is used. Submonolayer 6P thin films are prepared by vapor deposition in a hot wall epitaxy (HWE) system. The resulting thin film morphologies are investigated as a function of substrate temperature using atomic force microscopy. First results indicate that 6P forms needle like structures consisting of molecules with their long axes oriented parallel to the h-BN plane. The needles show preferential growth directions corresponding to the substrate symmetry.

HL 92.36 Thu 16:00 Poster A

Tailoring Bragg-gratings for light outcoupling of red top-emitting organic light-emitting diodes — •Paul-Anton Will[1], Cornelius Fuchs[1], Frank Boldt[2], Reinhard Scholz[1], Simone Lenk[1], and Sebastian Reineke[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, Germany — [2]Institut für Physik, Technische Universität Chemnitz, Germany

Introducing Bragg-gratings into OLED structures is a promising approach to increase the overall device efficiency. Here, scattering effects lead to a redistribution of internal modes, i.e. wave guided and/or surface plasmon polariton modes, with the benefit of an increased out-coupled mode fraction [1]. The overall emission characteristics of a device depend on the OLED properties like emitter spectrum, device layout, and optical micro cavity order, and also strongly on the shape, period, and height of the incorporated grating structure. We present a detailed analysis of the influence of one dimensional gratings on the emission of various red top-emitting OLEDs by using optical thin film simulations quantifying the emission from periodically perturbated optical micro cavities. AFM measurements of nanoimprinted Bragg-gratings serve as input for the optical simulations. This facilitates the comparison with experimental results from manufactured devices leading to first hints for optimal grating periods in relation to the vertical aspect ratios of the grating structure. Once the optimal parameters are found, the use of Bragg-gratings pose a cheap and up-scalable method to improve the OLED efficiency.

[1] T. Schwab *et al.*, Opt. Express 22, 7524-37, (2014)

HL 92.37 Thu 16:00 Poster A

Growth morphologies of a polar pentacene derivative on SiO_2 and graphene — •Benjamin Kaufmann[1], Markus Kratzer[1], Tony Lelaidier[2], Olivier Siri[2], Aleksandar Matković[3], Radoš Gajić[3], Conrad Becker[2], and Christian Teichert[1] — [1]Institute of Physics, Montanuniversitaet Leoben, Franz Josef Straße 18, 8700 Leoben, Austria — [2]CINaM, Aix Marseille Université, Campus de Luminy Case 913, 13288 Marseille, France — [3]Institute of Physics, Department for Solid State Physics and New Materials, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia

We investigated the growth morphologies of the polar organic molecule dihydrotetraazapentacene (DHTAP) on SiO_2 and exfoliated graphene. The morphology of ultra-thin films grown by hot wall epitaxy was analyzed using atomic force microscopy. The morphologies arising between 290K - 390K exhibit a strong temperature dependence and differ from those found for pentacene. Above substrate temperatures of 330K, the molecules tend to build curved, needle-like structures with lengths of 50nm - 1000nm and heights of a few nanometers. At lower growth temperatures, no needles are present as it is also the case for pentacene growth on SiO_2. On graphene, the islands are reduced in height compared to those grown on SiO_2. Also here, needle-like structures were found.

HL 93: Transport: Spintronics and Magnetotransport (Joint session of DS, HL, MA and TT, organized by TT)

Time: Thursday 16:15–18:30 Location: H23

Invited Talk HL 93.1 Thu 16:15 H23

Non-Abelian gauge theory description of (dynamical) spin-orbit coupling effects in Fermi gases. — •Cosimo Gorini — Institut für Theoretische Physik, Universität Regensburg, Germany

Spin-orbit coupling heavily influences the dynamics of charge carriers in a solid, where its strength can be enhanced by orders of magnitude as compared to the vacuum. Remarkable consequences are phenomena such as the spin Hall and inverse spin galvanic (or Edelstein) effects, where spin currents and polarizations are generated by purely electrical means. The intricacies of such rich spin-charge coupled dynamics can be described within a non-Abelian gauge theory approach [1], based on Keldysh non-equilibrium formalism [2]. Thanks to a symmetric treatment of spin and charge degrees of freedom, and the removal of ambiguities related to spin non-conservation in the presence of (static or dynamical) spin-orbit coupling, a physically transparent picture is achieved [3]. Furthermore, the non-Abelian language, by virtue of its universal character, treats on the same footing standard spin-orbit interaction in solid state systems and exotic forms of (pseudo) spin-orbit coupling which arise, or can be engineered, in different contexts.

[1] H. Mathur and A. D. Stone, PRL **68**, 2964 (1991)
I. V. Tokatly, PRL **101**, 106601 (2008).
[2] C. Gorini et al., PRB **82**, 195316 (2010).
[3] C. Gorini et al., PRL **109**, 246604 (2012)
C. Gorini et al., PRL **115** , 076602 (2015).

HL 93.2 Thu 16:45 H23

Shot noise in magnetic tunnel junctions: effect of the geometric phase — •Tim Ludwig[1] and Alexander Shnirman[1,2] — [1]Institut für Theorie der Kondensierten Materie, Karlsruher Institut für Technologie, 76131 Karlsruhe, Germany — [2]L. D. Landau Institute for Theoretical Physics RAS, Kosygina street 2, 119334 Moscow, Russia

We analyze the current driven dynamics of magnetization and voltage in a magnetic tunnel junction. As predicted in [1, 2], the magnetization can be driven by spin currents. This effect can also be reversed, such that an externally driven magnetization generates a dc voltage [3]. Although both effects are intimately related, so far they have been treated separately. We generalize the approach of [4] to derive an action that contains both effects simultaneously. We employ the Keldysh formalism, which allows us to derive stochastic Landau-Lifshitz-Gilbert-Langevin equations describing the angular dynamics of the magnetization coupled with the voltage dynamics. We identify two low-temperature regimes. In one regime the voltage fluctuations are governed by the applied current only, as expected for the shot noise. In the other regime an excess noise arises, which is governed by the geometric phase of the precessing magnetization.

[1] L. Berger, PRB **54**, 9353 (1996)
[2] J. C. Slonczewski, J. Magn. Magn. Mater. **159**, L1 (1996)
[3] L. Berger, PRB **59**, 11465 (1998)
[4] A. Shnirman, Y. Gefen, A. Saha, I. S. Burmistrov, M. N. Kiselev, A. Altland, PRL **114**, 176806 (2015)

HL 93.3 Thu 17:00 H23

Electron transport through the helical molecules in the presence of spin-orbit coupling — •Volodymyr V. Maslyuk, Rafael Gutiérrez, and Gianaurelio Cuniberti — Institute for Material Science and Max Bergmann Center for Biomaterials, Dresden University of Technology, Hallwachstr. 3, 01069 Dresden, Germany

Recently it was shown [1] that electron transport through systems with helical symmetry shows spin selectivity. Here we present a theoretical investigation of the transport properties through helical molecules placed between magnetic and nonmagnetic leads by using the DFT and NEGF approach. The performed analysis of the data allow us to show that the systems show spin-polarization only because of spin-orbit interaction and the spin polarization is clearly related to the helical symmetry since a change in handedness of the helix changes the sign of the spin-polarization and a linear chain does not display any sizeable polarization.

[1] B. Göhler, V. Hamelbeck, T. Z. Markus, M.Kettner, G. F. Hanne, Z. Vager, R. Naaman, and H. Zacharias, Science **331**, 894 (2011).

15 min. break

HL 93.4 Thu 17:30 H23

Magnetic impurities on Bi thin films - conductivity and surface diffusion — •Philipp Kröger[1], Sergii Sologub[2], An-

dreas Lücke[3], Nora Vollmers[3], Uwe Gerstmann[3], Wolf Gero Schmidt[3], Herbert Pfnür[1], and Christoph Tegenkamp[1] — [1]Leibniz Universität Hannover, Inst. für FKP, Appelstr. 2, 30167 Hannover — [2]Inst. of Ph., Nat. Acad. of Sc., Nauky Av. 46, 03028 Kyiv, Ukraine — [3]Universität Paderborn, Theoretische Materialphysik, Pohlweg 55, 33098 Paderborn

The semimetal bismuth has attracted a lot of interest because of its unique electronic properties such as low carrier concentration and large mobility. The surface states reveal a pronounced Rashba splitting. The surface conductivity can well be discriminated from bulk contributions for ultra-thin films grown epitaxially on Si(111) substrates, so that surface related effects are accessible even in macroscopic conductance measurements.
In this context, the adsorption of Cr with its high magnetic moment on the Bi(111) surface will be discussed. Cr induces a transition from Weak Anti- to Weak Localization. This indicates strong impurity scattering that mixes spin and orbit momenta, with corresponding symmetry breaking on the Bi surface (TRS), in agreement with results from DFT calculations. Contrary to other impurities adsorbed at subsurface sites (Fe,Co,Cr, Sb), Cr shows signs of diffusion processes at low T (T $\approx$ 10 K), as previously observed for Tb which adsorbes on the surface.

HL 93.5 Thu 17:45 H23

Spin-vibronics in interacting nonmagnetic molecular nanojunctions — •Stephan Weiss[1], Jochen Brüggemann[2], and Michael Thorwart[2] — [1]Theoretische Physik, Universität Duisburg-Essen & CENIDE — [2]1. Institut für Theoretische Physik, Universität Hamburg

We show that in the presence of ferromagnetic electronic reservoirs and spin-dependent tunnel couplings, molecular vibrations in nonmagnetic single molecular transistors induce an effective intramolecular exchange magnetic field[1]. It generates a finite spin-accumulation and -precession for the electrons confined on the molecular bridge and occurs under (non)equilibrium conditions. The effective exchange magnetic field is calculated here to lowest order in the tunnel coupling for a nonequilibrium transport setup. Coulomb interaction between electrons is taken into account as well as a finite electron-phonon coupling. For realistic physical parameters, an effective spin-phonon coupling emerges. It is induced by quantum many-body interactions, which are either electron-phonon or Coulomb-like.
[1] S. Weiss, J. Brüggemann and M. Thorwart,
PRB **92**, 045431 (2015).

HL 93.6 Thu 18:00 H23

Coherent Dynamics of Quantum Spins in Magnetic Environments — •Lars-Hendrik Frahm[1], Christoph Hübner[1], Benjamin Baxevanis[1,2], and Daniela Pfannkuche[1] — [1]1. Institut für Theoretische Physik, Universität Hamburg, 20355 Hamburg, Germany — [2]Instituut-Lorentz, Universiteit Leiden, P.O. Box 9506, 2300 RA Leiden, The Netherlands

We investigate equilibration and transport effects of a magnetic atom that is exchange coupled to two electron reservoirs. An effective crystal field, which arises from the substrate the atom is living on gives the spin of the atom an easy axis for alignment. Further, a spin-polarized electron reservoir breaks the rotation symmetry around the spin quantization axis. A proper description of the dynamics of the quantum spin requires to consider the complete density operator, where its knowledge allows to calculate magnetization dynamics and transport properties on an equal footing. We discuss the electron transport through the atomic system by especially focusing on the non-linear influence of the spin torque effect.

HL 93.7 Thu 18:15 H23

Colossal Magnetoresistance observed in Natural Graphite — •Jose Barzola-Quiquia[1], Mahsa Zoraghi[1], Markus Stiller[1], Christian Precker[1], Ana Champi[2], and Pablo Esquinazi[1] — [1]Institute for Experimental Physics II, University of Leipzig, 04103 Leipzig, Germany — [2]Centro de Ciencias Naturais e Humanas Universidade Federal do ABC, Sao Paulo- Brasil

In this work, the electrical transport properties of a bulk natural graphite flake extracted from a mine in Brazil were investigated. The sample showed metallic behavior and the changes in the magnetoresistance (MR) at 5 K and 7 T shows 1123600% change when the field was applied parallel to the *c*-axis. This value was not yet reported in any graphite sample in the literature. Applying constant magnetic field, resistance measurements as a function of the temperature show also a magnetic field induces metal-insulator transition (MIT), with a small critical field $B_0 \approx 10$ mT compared to literature. We observed also that at fields $B > 0.2$ T a metallic reentrance was observed that remains up to $\approx$ 50 K. STEM measurements reveal the presence of interfaces in the investigated material. Therefore, the observed transport properties are not an intrinsic behavior of the graphite sample but due to the presence of these interfaces. Interfaces in the sample are formed at the interfaces between two crystalline regions inside the sample where a two dimensional electron gas (2DEG) system appears. Raman measurements reveal that our samples are free from any other defects.

HL 94: Symposium SYES: Frontiers of Electronic Structure Theory: Focus on Topology and Transport (Joint session of DS, HL, MA, MM and O, organized by O)

Time: Friday 9:30–12:15 Location: H1

Invited Talk HL 94.1 Fri 9:30 H1

Intrinsic Transport Coefficients and Momentum Space Berry Curvatures — •Allan H MacDonald — University of Texas at Austin, Austin TX, USA

The response of a conductor to a bias voltage is normally dominated by repopulation of states near the Fermi level. The transport steady state is fixed by a competition between acceleration in an electric field and disorder-induced scattering which attempts to restore equilibrium. This response of observables to a bias voltage is therefore extrinsic. There is however also response of states away from the Fermi level, which are polarized by the electric field. Provided that the typical band separation is larger than the finite life-time uncertainty in Bloch state energies this response is intrinsic, and for some observables it can be dominant. Intrinsic response coefficients are attractive targets for electronic structure theory because they are readily evaluated. Examples of responses to bias voltages that are sometimes dominantly intrinsic are the anomalous Hall conductivity of ferromagnetic or antiferromagnetic conductors, the spin-Hall conductivity of heavy metals, and current-induced torques in heavy-metal/ferromagnet systems. Intrinsic transport coefficients tend to be large in crystals with large momentum-space Berry curvatures, for example in crystals with topologically non-trivial electronic structure, and remain finite when a gap opens at the Fermi level to eliminate the Fermi surface. I will discuss some important examples of transport coefficients that are dominated by intrinsic contributions, mentioning as an important case the quantum anomalous Hall effect.

Invited Talk HL 94.2 Fri 10:00 H1

Berry phase linked spin-orbit torques in Ferromagnetic and Antiferromagnetic systems — •Jairo Sinova — Johannes Gutenberg Universität Mainz, Staudingerweg 7, 55128 Mainz Germany

As current-driven torques are becoming more relevant in future MRAM technologies, in-plane current magnetization dynamics driven by the so called Rashba spin-orbit torques or through a combination of spin-Hall effect and spin-transfer torque has become more and more important. Understanding these torques is paramount to maximize their use. In recent experiments we have shown that in addition to the intrinsic SHE and STT effect there exists an intrinsic spin-orbit torque originating from the Berry phase of the spin-orbit coupled Bloch electrons analogous to the intrinsic spin Hall effect. This type of torques can be observed through SO-FMR driven experiments. We show this new type of toques in theory and experiments in GaMnAs and show that it can be of similar strength to the strong field-like torque. In addition, we extend these physics to a new type of order-parameter manipulation by currents by examining the combined effect of spin-orbit coupling and anti-ferromagnetic order. We show that in broken

inversion symmetry anti-ferromagnets a current will induced a non-equilibrium Néel-order field that will act directly on the Néel order parameter, hence making the direct manipulation of anti-ferromagnets without auxiliary exchange biased coupling to other ferromagnets a new and exciting possibility. One of these type of Néel torques has been recently experimentally confirmed.

Invited Talk HL 94.3 Fri 10:30 H1

Transport in Topological Insulators and Topological Superconductors: In Search of Majorana Fermions — •Ewelina Hankiewicz — Wuerzburg University

Topological insulators (TIs) have a bulk energy gap that separates the highest occupied band from the lowest unoccupied band and the metallic gapless states at the edge [1]. Similarly, topological superconductors (TSC) have gapless zero energy states protected by the particle-hole symmetry, which in some cases form Majorana bound states. Here, we focus on the proximity-induced superconductivity in TIs [2] as well as on unusual properties of TSC [3] showing that they both can pave a road to find a Majorana state.

Concerning proximity-induced superconductivity in TIs, we describe a novel superconducting quantum spin-Hall effect, which is protected against elastic backscattering by combined time-reversal and particle-hole symmetry even in magnetic fields [2]. We discuss unusual transport properties of this effect and possible Majorana detection schemes.

Finally, we discuss new systems like TSC on the hexagonal lattices. We develop combined microscopic and macroscopic description of these materials that predicts realistic scanning tunneling microscopy signal in these superconductors [3]. Is there a way to measure Majorana state in these systems?

[1] G. Tkachov and E. M. Hankiewicz, Review in Phys. Status Solidi B 250, 215 (2013). [2] R. Reinthaler, G. Tkachov and E.M. Hankiewicz, Phys. Rev. B 92, 161303(R) (2015). [3] L. Elster, C. Platt, R. Thomale, W. Hanke, and E. M. Hankiewicz, Nature Comm. 6, 8232 (2015).

session break

Invited Talk HL 94.4 Fri 11:15 H1

Engineering Topological Quantum States: From 1D to 2D. — •Jelena Klinovaja — University of Basel, Switzerland

I will discuss low-dimensional condensed matter systems, in which topological properties could be engineered per demand. Majorana fermions can emerge in hybrid systems with proximity pairing in which the usually weak Rashba spin-orbit interaction is replaced by magnetic textures. I will discuss candidate materials such as semiconducting nanowires [1] and atomic magnetic chains [2]. One further goal is to go beyond Majorana fermions and to identify systems that can host quasiparticles with more powerful non-Abelian statistics such as parafermions in double wires coupled by crossed Andreev reflections [3,4]. Next, I will focus on 'strip of stripes model' consisting of weakly coupled one-dimensional wires [5-7], where interaction effects in the wires can be treated non-perturbatively via bosonization. Such systems can exhibit the integer or fractional quantum Hall effect, spin Hall effect, and anomalous Hall effect.

[1] J. Klinovaja and D. Loss, Phys. Rev. B 86, 085408 (2012). [2] J. Klinovaja, P. Stano, A. Yazdani, and D. Loss, Phys. Rev. Lett. 111, 186805 (2013). [3] J. Klinovaja and D. Loss, Phys. Rev. B 90, 045118 (2014). [4] J. Klinovaja, A. Yacoby, and D. Loss, Phys. Rev. B 90, 155447 (2014). [5] J. Klinovaja and D. Loss, Phys. Rev. Lett. 111, 196401 (2013); J. Klinovaja and D. Loss, Eur. Phys. J. B 87, 171 (2014). [6] J. Klinovaja and Y. Tserkovnyak, Phys. Rev. B 90, 115426 (2014). [7] J. Klinovaja, Y. Tserkovnyak, and D. Loss, Phys. Rev. B 91, 085426 (2015).

Invited Talk HL 94.5 Fri 11:45 H1

Skyrmions – Topological magnetization solitons for future spintronics — •Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

Ultrathin magnetic films and heterostructures provide a fantastic playground for the stabilization, manipulation and usage of chiral magnetic skyrmions – topological magnetization solitons – magnetic entities described by a micromagnetic energy functional with particle like properties that may open a new vista for spintronics. A crucial quantity for the chiral skyrmion formation is the Dzyaloshinskii-Moriya interaction (DMI), whose presence in thin films could be established in a concerted effort of first-principles theory and spin-polarized scanning tunneling microscopy. It could be shown that the spin-orbit interaction and the structure inversion-asymmetry in these systems result in a DMI that is strong enough to give rise to one- and two-dimensional lattices of chiral spin-textures, chiral domain walls and even single skyrmions. In retrospect, it is surprising how little is known about the DMI in these metallic systems. In this talk I give insight into the DMI, relating first-principles calculations to different models, discussing the transport properties of electrons *e.g.* the topological (THE) and anomalous (AHE) Hall effect in relation to the spin texture of a skyrmion, and discuss possibilities to tailor the magnetic interactions to enlarge the materials base to stabilize single skyrmions. – I acknowledge fruitful collaborations with D. Crum, J. Bouaziz, B. Dupé, S. Heinze, N. Kiselev, S. Lounis, Y. Mokrousov, A. Nandy, and B. Zimmermann.

HL 95: Novel Functional Materials II

Time: Friday 9:30–12:00 Location: H10

HL 95.1 Fri 9:30 H10

Electron traps in disordered Pt/TiO2 hydrogen sensors — Laurin Schnorr[1], •Mihai Cerchez[1], Dieter Ostermann[2], and Thomas Heinzel[1] — [1]Heinrich Heine University Düsseldorf, Universitätsstr. 1D-40225 Düsseldorf — [2]ODB-Tec GmbH & Co. KG, Bussardweg 12, 41468 Neuss, Germany

Hydrogen sensing at disordered Pt/TiO2 interfaces lacks a deep understanding of the physical processes involved. Aspects related to the mechanism of electron conduction in such systems are attributed usually to oxygen vacancies and/or titanium interstitials. From an electronic transport point of view, defects manifest through creation of electronic states in the band gap, position of which is still under debate. Little is known about the effect of hydrogen on the band gap states during the sensing process. This knowledge would bring some more light concerning the physical hydrogen sensing mechanism. Here we make a step in this direction by performing deep level transient spectroscopy experiments [1] before, during, and after exposure to low concentrations of hydrogen. Our findings [2] suggest that two broad trap levels are present before the exposure, while a third level is formed during hydrogen exposure.

[1] D. V. Lang, J. Appl. Phys. 45, 3023 (1974). [2] L. Schnorr, M. Cerchez, D. Ostermann, and T. Heinzel, Phys. Status Solidi B (2015) (in press)

HL 95.2 Fri 9:45 H10

Theoretical and experimental study of the optoelectronic properties of Nb3O7(OH) and Nb2O5 for photochemistry — •wilayat khan[1], Sophia b. Betzler[2], ondrej sipr[1], jim ciston[3], peter blaha[4], christina scheu[5], and jan minar[1,2] — [1]Technologies-Research Center, University of West Bohemia, Univerzitn 8, 306 14 Plzen, Czech Republic. — [2]Department of chemistry and Center for NanoScience, Butenandtstrae 11, 81377 Munchen, Germany — [3]National Center for Electron Microscopy, Lawrence Berkeley National Lab, Berkeley, USA. — [4]Institute of Materials Chemistry, Vienna University of Technology, Getreidemarkt 9/165-TC, A-1060 Vienna, Austria. — [5]Max-Planck-Institut fr Eisenforschung GmbH, Max-Planck-Strae 1, Dusseldorf, Germany.

Nb3O7(OH) and Nb2O5 were proposed as high performing electrode materials in several fields of application such as dye-sensitized solar cells and photoelectrochemical cells. In this work, we present theoretical and experimental studies of Nb3O7(OH) and Nb2O5 to elucidate their optical and electronic properties. The theoretical study was performed using the full potential linearized augmented plane wave method to calculate the electronic band structures, the density of states and optical properties. To verify the results of our calculations energy-loss functions for the low-loss spectral region were calculated and compared to experimental electron energy-loss spectra, featuring a very close agreement between experiment and theory. Our investigations

show that Nb3O7(OH) has more suitable optoelectronic and transport properties for photochemical application than Nb2O5.

HL 95.3 Fri 10:00 H10

Vibrational Properties of Thermoelectric Magnesium Silicides from First Principle: the role of explicit dopants — •Hagen - Henrik Kowalski, Luca Ghiringhelli, Christian Carbogno, and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

Silicides, and particularly Mg_2Si, are simple, prototypical examples for thermoelectric materials and have thus recently attracted remarkable scientific interest. For this material class, most first-principles studies have so far focused on the structural stability, the electronic structure, and the electronic transport coefficients [1,2], viz. on how these properties can be tailored by doping. Little is however known about the effects of doping on the vibrational properties and the associated thermal conductivity, which are of similar importance for the thermoelectric efficiency. Therefore, we have systematically investigated how different dopants (Ca, Ge, Ag, etc.) affect the vibrational harmonic properties; anharmonic effects are analyzed within the quasi-harmonic approximation. We discuss the implications of our findings for the thermoelectric properties and how they can be utilized in a high-throughput framework.

[1] I. Opahle, G. K. H. Madsen, and R. Drautz, *PCCP* **14**, 16197 (2012).

[2] S. Bhattacharya and G. K. H. Madsen, *Phys. Rev. B* **92**, 085205 (2015).

30 min. Coffee Break

Invited Talk HL 95.4 Fri 10:45 H10

Nano-architectures and organic-inorganic hybrid material combinations for novel photovoltaic device concepts — •Silke Christiansen — Helmholtz-Zentrum- Berlin — Max-Planck-Institute for the Science of Light, Erlangen

The implementation of tailored nano-architectures into conventional inorganic and hybrid photovoltaic devices can improve photovoltaic (PV) cells by optimizing charge generation, separation and extraction. The charge generation can be improved through lowly reflective materials such as nano-patterned layers of silicon nanowires (SiNWs) or inverted cones (SiNCs), produced by reactive ion etching combined with nanosphere-lithography. Nanostructures with optimized optical behavior show large surfaces which require proper passivation e.g. by atomic layer deposition (ALD) and more importantly, good charge extraction concepts. These charge extraction concepts seek for novel cheap, transparent and highly conductive materials replacing conventional metal grid-electrodes. Interesting alternatives are solution-processed Ag-nanowire networks, stabilized and protected by e.g. ALD deposited aluminum doped ZnO, showing solar cells with high short circuit currents, low resistivity and small amounts of metal. The present paper shows optical behavior of individual and arrays of SiNWs and SiNCs in finite difference time domain (FDTD) simulations and experiments so that design rules for optimized PV cells can be derived. Experimental confirmation of simulations rely on nano-probing of individual nano-structures and ensembles using a powerful electron-microscopy platform capable of correlative microscopy and spectroscopies.

HL 95.5 Fri 11:15 H10

Electronic properties of freestanding $Ti_3C_2T_x$ MXene monolayers — •Alessio Miranda[1], Joseph Halim[2], Michel W. Barsoum[2], and Axel Lorke[1] — [1]Dep. of Physics, Uni. Duisburg-Essen, Duisburg, 47058, Germany — [2]Dep. of Materials Science and Engineering, Drexel University , Philadelphia, PA19104, USA

Recently, MXenes, 2D early transition metal carbides and carbonitrides, have been produced by the selective etching of A from the MAX phases. The latter are a large family of compounds, with the general formula $M_{n+1}AX_n$ (n = 1-3), where M is an early transition metal, A is an A-group element, and X represents C or N [1]. During the etching process, the MXene surface acquires terminating functional groups, T, (namely -O, -OH, and/or -F), which can have significant effects on the work function and electrical properties of these new compounds. Here we report, on the electrical properties of $Ti_3C_2Ti_x$ freestanding MXene monolayers in the 2.5 K to 300 K temperature range [2]. We show that $Ti_3C_2Ti_x$ samples exhibit metallic behavior, they have a carrier density of 5×10^{14} cm^{-2}, which is relatively high and can be modulated by the application of a gate voltage. MXenes, which have already been demonstrated to be promising candidates for a variety of applications [3], may also be interesting for electronic applications, such as field-effect devices. Magnetotransport measurements are also reported.

[1] M. W. Barsoum, MAX Phases: Properties of Machinable Ternary Carbides and Nitrides (Wiley-VCH, 2013). [2] A. Miranda, et al. submitted (2015). [3] M. Naguib, et al Adv. Mater. 26, 992-1005 (2014).

HL 95.6 Fri 11:30 H10

Vibrational Dynamics of Filled Skutterudites — •Susmita Basak, Christian Carbogno, and Matthias Scheffler — Fritz Haber Institute of the Max Planck Society

Skutterudites are promising candidates for thermoelectric applications, since their cage like structure can be filled with guest atoms to tune the electronic and vibrational properties and so to optimize the thermoelectric transport coefficients. Various conflicting phenomenological models (e.g., incoherent rattling, coherent coupling [1]) have been proposed to explain the interaction between guest and host, but the exact mechanisms are still topic of debate. To clarify this question, we determine the temperature dependence of the geometric, electronic, and vibrational properties for a set of skutterudites ($CoSb_3$, $CoAs_3$) and guests (Ga, In, Sn, etc.) using density-functional theory in the quasi-harmonic approximation. We find different coupling mechanisms to be active depending on the guest, which leads to a drastically different dynamics ranging from localized to coherent phonon modes. These modes, which are robust against doping and defy the common assumption that the guest's mass primarily determines the coupling, also largely influence the structural and electronic properties. Finally, we discuss the implications of our findings for controlling the thermoelectric efficiency. [1] M. M. Koza *et al.*, Nat. Mat. **7**, 805, (2008).

HL 95.7 Fri 11:45 H10

Formation and function of vacancies in Si/Ge Clathrates: The importance of broken symmetries — •Amrita Bhattacharya, Christian Carbogno, and Matthias Scheffler — Fritz Haber Institute of the Max Planck Society

Inclusion compounds, such as clathrates, are cage-like crystal structures that can encapsulate guest atoms. Since this allows to granularly tune their electronic and vibrational properties, they are regarded as interesting materials for thermoelectric applications. Progress in this field is, however, hindered by the fact that filling of group-IV clathrates often results in complex and unexpected structural changes, e.g., the spontaneous formation of vacancies in certain hosts: In Ge_{46} clathrates filled with K or Ba, the most favourable phases K_8Ge_{44}/Ba_8Ge_{43} feature two/three vacancies. Conversely, the framework of the isoelectronic Si_{46} clathrate remains intact (K_8Si_{46}/Ba_8Si_{46}) upon filling with the exact same guests. Our first-principles calculations of the formation energies (including structural disorder as well as geometric and lattice relaxations) and of the thermodynamic phase stabilities (including harmonic free energies and configurational entropies) confirm this experimental scenario and shed light on the underlying mechanisms. Due to the spatially more delocalized $4sp^3$ orbitals in Ge, fundamentally different symmetry breaking distortions become possible to stabilize the vacancies compared to the more localized $3sp^3$ orbitals in Si. Eventually, we discuss the implications of these findings for the thermoelectric properties of clathrates.

HL 96: Magnetic Semiconductors

Time: Friday 9:30–11:30 Location: H13

HL 96.1 Fri 9:30 H13

A systematic investigation of the magnetic anisotropy of III-Mn-V ferromagnetic semiconductors — •Chi Xu[1,3], Ye Yuan[1,3], Maciek Sawicki[2], Manfred Helm[1,3], and Shengqiang Zhou[1] — [1]Helmholtz-Zentrum Dresden Rossendorf, Institute of Ion Beam Physics and Materials Research, Bautzner Landstrasse 400, D-01328 Dresden, Germany — [2]Institute of Physics, Polish Academy of Sciences, Warszawa, Poland — [3]Technische Universität Dresden, D-01062 Dresden, Germany

As one of the most important physical properties of dilute ferromagnetic semiconductors (DFS), the magnetic anisotropy exhibits a complicated character and its origin is under continuous discussion [1]. Due to different physical parameters (e.g. band gap, lattice constant) in various Mn doped III-V DMSs, various magnetic anisotropies are expected and could be tailored by Mn or hole concentrations [2,3]. To investigate this in greater detail, we prepare three typical III-Mn-V DFSs, InMnAs, GaMnAs, and GaMnP by ion implantation and pulsed laser annealing, which is a complementary approach to low-temperature molecular beam epitaxy. We report a systematic investigation on the magnetic anisotropy with the aim to understand its physical origin.

[1]. T. Dietl et al., Rev. Mod. Phys. 86, 187-251 (2014) [2]. M. Sawicki et al., Phys. Rev. B 70, 245325 (2004) [3]. C. Bihler et al., Phys. Rev. B 78, 045203 (2008)

HL 96.2 Fri 9:45 H13

Application of ion beams to fabricate and tune ferromagnetic semiconductors — •Shengqiang Zhou — Helmholtz-Zentrum Dresden Rossendorf, Institute of Ion Beam Physics and Materials Research, Bautzner Landstrasse 400, D-01328 Dresden, Germany

In this talk, I will show how ion beams can be used in fabricating and understanding ferromagnetic semiconductors. First, ion implantation followed by pulsed laser melting (II-PLM) provides an alternative to the widely used low-temperature molecular beam epitaxy (LTMBE) approach [1-7]. Going beyond LT-MBE, II-PLM is successful to bring two new members, GaMnP and InMnP, into the family of III-V:Mn. Both GaMnP and InMnP films show the signature of ferromagnetic semiconductors and an insulating behavior. Second, we use helium ion irradiation to precisely compensate holes in ferromagnetic semiconductors while keeping the Mn concentration constant [8-10]. By this approach, one can tune the magnetic properties of ferromagnetic semiconductor as well as pattern a lateral structure. It also provides a route to understand how carrier-mediated ferromagnetism is influenced by localization.

[1] M. Scarpula, et al. PRL 95, 207204 (2005); [2] D. Bürger, S. Zhou, et al., PRB 81, 115202 (2010); [3] S. Zhou, et al., Appl. Phys. Express 5, 093007 (2012); [4] M. Khalid et al., PRB 89, 121301(R) (2014); [5] Y. Yuan, et al, IEEE Trans. Magn. 50, 2401304 (2014); [6] Y. Yuan, et al. JPD 48, 235002 (2015); [7] S. Zhou, JPD 48, 263001 (2015); [8] Lin Li, et al., JPD 44 099501 (2011); [9] Lin Li, et al., NIMB, 269, 2469 (2011); [10] S. Zhou, et al. PRB, in revision (2015).

HL 96.3 Fri 10:00 H13

Effective Spin Models and Critical Temperatures for Diluted Magnetic Semiconductors. — Richard Bouzerar[1], •Daniel May[2], Ute Löw[2], Denis Machon[1], Patrice Melinon[1], and Georges Bouzerar[1] — [1]Institut Lumière Matière, CNRS et Université Lyon 1, 69622 Villeurbanne Cedex, France — [2]Technische Universität Dortmund, Lehrstuhl für Theoretische Physik II, 44221 Dortmund, Germany

Diluted magnetic semiconductors (DMS) are materials where magnetic ions substitute a small percentage of the host's cations. We use a one-band VJ model with three adjustable parameters to describe DMS and extract long-range spin-spin couplings. These couplings are subsequently used as input to a classical Heisenberg model which is studied by Monte Carlo simulation (MC) and a self-consistent approach based on Green's functions (L-RPA). Both methods treat random lattice configurations beyond the standard Mean Field Approximation and without resorting to an effective medium. Our focus lies mainly on (In,Mn)P for small concentrations $x < 0.1$ of manganese where critical temperatures of 20-40 K are expected. The L-RPA provides us with a self-consistent expression for T_c whereas we use finite size scaling for the MC results to calculate a reliable critical temperature. Our goal is to provide a consistent description of recent experimental results for the magnetic properties of the Mn-doped InP diluted magnetic semiconductor.

30 min. Coffee Break

HL 96.4 Fri 10:45 H13

Long-range p-d exchange interaction in a ferromagnet-semiconductor hybrid structure — •Matthias Salewski[1], Vladimir L. Korenev[1,2], Ilya A. Akimov[1,2], Victor V. Sapega[2,3], Lukas Langer[1], Ina V. Kalitukha[2], Jörg Debus[1], Roslan I. Dzhioev[2], Dmitri R. Yakovlev[1,2], David Müller[1], Chrstoph Schröder[4], Heinz Hövel[4], Grzegorz Karczewski[5], Maciej Wiater[5], Tomasz Wojtowicz[5], Yuri G. Kusrayev[2], and Manfred Bayer[1,2] — [1]Experimentelle Physik 2, Technische Universität Dortmund, D-44221 Dortmund, Germany — [2]Ioffe Physical-Technical Institute, Russian Academy of Sciences, 194021 St. Petersburg, Russia — [3]Physical Faculty of St. Petersburg State University, 198504 St. Petersburg, Russia — [4]Experimentelle Physik 1, Technische Universität Dortmund, D-44221 Dortmund, Germany — [5]Institute of Physics, Polish Academy of Sciences, PL-02668 Warsaw, Poland

The magnetic coupling in hybrid structures composed of semiconductor (SC) nanostructures and ferromagnetic layers (FM) typically depends on the wave function overlap of SC charge carriers (p-system) and FM ions (d-system) and is therefore short-ranged. Here we report on a hybrid system with surprisingly long-ranged, robust coupling that does not vary with spacer width up to more than 30 nm. We suggest that the resulting spin polarization of acceptor-bound holes is induced by an effective p-d exchange that is mediated by elliptically polarized phonons.

HL 96.5 Fri 11:00 H13

Site resolved band structure of a diluted magnetic semiconductor — •Slavomir Nemsak[1], Mathias Gehlmann[1], Cheng-Tai Kuo[2], Tien-Lin Lee[3], Lukasz Plucinski[1], Claus M. Schneider[1], and Charles S. Fadley[2] — [1]Forschungszentrum Juelich, Germany — [2]UC Davis, CA, USA — [3]Diamond Light Source, Didcot, GB

Standing wave (SW) photoemission of core-levels and valence electrons at the density-of-states limit has proven to be a very potent and powerful method, especially for investigating electronic properties of the buried interfaces, either solid/solid [Gray et al., EPL 104, 17004 (2013)], but also solid/liquid and liquid/gas [Nemsak et al., Nat. Comm. 5, 5441 (2014)]. The exceptional depth selectivity provides a key to the depth-resolved information, which is very difficult to extract by other, less direct, methods.

The combination of the SW approach and hard X-ray angle resolved photoelectron spectroscopy (HARPES) [Gray et al., Nature Mat. 11, 957 (2012)] takes these efforts one step further. The strengths of the SW-HARPES method are demonstrated on the example of diluted magnetic semiconductor Ga(Mn)As. A strong SW is generated using hard X-ray excitation of ca. 3 keV using the (111) reflection of the undoped GaAs substrate and the 5% Mn-doped thin film with. Due to the uneven occupancy of (111) planes by either Ga(Mn) or As atoms, the element specific band structure can be obtained with a help of the SW modulation in core levels. Apart from the site specific decomposition of the electronic structure, the SW measurement confirmed a substitutional presence of Mn atoms at the Ga sites.

HL 96.6 Fri 11:15 H13

Modeling Magnetism of Diluted Magnetic Systems using the Gutzwiller Method — •Thorben Linneweber[1], Ute Löw[1], Florian Gebhard[2], and Jörg Bünemann[2] — [1]Technische Universität Dortmund, Lehrstuhl für Theoretische Physik II, 44221 Dortmund — [2]Philipps-Universität Marburg, AG Vielteilchenphysik, 35032 Marburg

Diluted magnetic semiconductors are materials in which magnetic ions substitutionally or interstitially replace a fraction of the cations of the semiconductor host material. We aim to describe the magnetic properties of the prototype substance $Cd_{1-x}Mn_xTe$. We derive a multiband Hubbard model from DFT calculations using the Wannier90 code. Large unit cells (≈ 200 atoms) account for the randomized substitution

of cations by magnetic ions. We analyze the ground state of this model within the framework of the Gutzwiller variational method. We find that the d-shell of the Mn ions resembles an atomic Hund's rule S=5/2 ground state. Due to the superexchange mechanism, there is an effective short-range Heisenberg exchange between the magnetic ions. We estimate the exchange parameters using energy calculations of different magnetic configurations and finally compare them to experimental results.

HL 97: Topological Insulators II (Joint session of DS, HL O and TT, organized by HL)

Time: Friday 9:30–12:00 Location: H15

HL 97.1 Fri 9:30 H15

Signatures of induced superconductivity in a p-n heterostructure comprised of Sb_2Te_3 and Bi_2Te_3 3D topological insulator thin films with in situ Al capping — •Peter Schüffelgen[1], Daniel Rosenbach[1], Martin Lanius[1], Jörn Kampmeier[1], Gregor Mussler[1], Markus Eschbach[1], Ewa Mlynczak[1], Lukasz Plucinski[1], Martina Luysberg[1], Stefan Trellenkamp[1], Martin Stehno[2], Prosper Ngabonziza[2], Alexander Brinkman[2], Yuan Pang[3], Li Lu[3], Thomas Schäpers[1], and Detlev Grützmacher[1] — [1]Peter Grünberg Institut and JARA-FIT, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]TNW and MESA+ Institute for Nanotechnology, University of Twente, 7500 AE Enschede, The Netherlands — [3]Laboratory for Solid State Quantum Information and Computation, Institute of Physics, Chinese Academy of Sciences, 100190 Beijing, China

We investigate the transport properties of Sb_2Te_3/Bi_2Te_3 p-n heterostructure topological insulator film-superconductor junctions. The films are grown by means of molecular beam epitaxy on a Si (111) substrate and capped *in-situ* by a thin layer of aluminum to prevent thin film degradation and to preserve the Dirac-like surface states. Josephson junctions are defined by depositing two niobium electrodes, separated by a few tens of nanometers, onto the Sb_2Te_3/Bi_2Te_3 layer. The transport measurements at cryogenic temperatures showed signatures of Andreev reflections and Josephson supercurrents. For wider junctions a Fraunhofer pattern was observed for the critical current, whereas for the narrow junctions a monotonous decrease was found.

HL 97.2 Fri 9:45 H15

Teraherz-Induced Chiral Edge Photogalvanic currents in 2D HgTe Topological Insulators — •Kathrin-Maria Dantscher[1], Dimitry A. Kozlov[2], Maria-Theresia Scherr[1], Sebastian Gebert[1], Vasily V. Bel'kov[3], Nikolay N. Mikhailov[2], Sergey A. Dvoretskii[2], Ze Dong Kvon[2], and Sergey D. Ganichev[1] — [1]University of Regensburg, Regensburg, Germany — [2]Institute of Semiconductor Physics, Novosibirsk, Russia — [3]Ioffe Institute, St. Petersburg, Russia

We report on the observation of a chiral photogalvanic current generated in the topological protected edge states of 2D topological insulators fabricated on the basis of 8 nm thick HgTe quantum wells. Illuminating the sample with circularly polarized terahertz radiation and picking-up the signal along the edges we detected a photocurrent whose direction reverses by switching radiation polarization from right- to left-handed one. The influence of the magnetic field, the temperature and the angle of incidence of the radiation to these photocurrents are investigated. We demonstrate that circularly polarized radiation, which, according to selection rules, excites only electrons with a certain spin, results in an imbalance of electron distribution in the k-space and causes a spin polarized electric current.

HL 97.3 Fri 10:00 H15

temperature induced shift of the chemical potential of Bi2Te2Se tetradymite topological insulators — •jayita nayak[1], gerhard h fecher[1], siham quardi[1], chandra sekhar[1], claudia felser[1], christian tusche[2], shigenori ueda[3], and eiji ikenaga[4] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden — [2]Max Planck Institute of Microstructure Physics, Halle — [3]Synchrotron X-ray Station at SPring-8National Institute for Materials Science, Hyogo 679-5148, Japan — [4]Japan Synchrotron Radiation Research Institute, SPring-8, Hyogo, 679-5198, Japan

The temperature dependent HAXPES spectra of Bi2Te2Se reveal the appearance of an additional spectral feature above the band gap at low temperature. It appears at 20 K but is absent in the 300 K spectra and the onset of the main features of the spectra is shifted to lower energies. Momentum resolved photoemission electron microscopy (k-PEEM)was carried out using in order to explain the origin of the additional spectral feature. The measurement provides the evidence of the evolution of bulk bands at low temperature which is caused by the shift of the chemical potential. The bulk sensitive HAXPES valence band spectra are in perfect agreement with first principles calculations.

HL 97.4 Fri 10:15 H15

Optical investigation of the three-dimensional Dirac semimetals $CaMnBi_2$ and $SrMnBi_2$ — •Micha B. Schilling[1], Artem V. Pronin[1], Martin Dressel[1], and Youguo Shi[2] — [1]1. Physikalisches Institut, Universität Stuttgart, 70569 Stuttgart, Germany — [2]Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, 100190 Beijing, China

The interest in the measurements of optical conductivity in three-dimensional Dirac semimetals is based on the recent theoretical studies [1, 2], where the interband optical response of such systems has been shown to be very peculiar. Namely, the real part of the interband optical conductivity has been predicted to be linear in frequency with the slope being related to the Fermi velocity of Dirac electrons.

We investigated the optical properties of the three-dimensional Dirac semimetals $CaMnBi_2$ and $SrMnBi_2$ by means of Fourier-transform infrared spectroscopy. We measured the reflectivity over a frequency range from 50 to 25000 cm^{-1} at different temperatures down to 10 K and determined the optical conductivity from these measurements. In the presentation, we will discuss our results on the optical conductivity in comparison with theoretical predictions.

[1] P. Hosur, S. A. Parameswaran, and A. Vishwanath, Phys. Rev. Lett. **108**, 046602 (2012). [2] A. Bácsi and A. Virosztek, Phys. Rev. B **87**, 125425 (2013).

30 min. Coffee Break

HL 97.5 Fri 11:00 H15

Optoelectronic dynamics in nanocircuits based on the topological insulator Bi2Te2Se — •Mariana Hettich[1], Paul Seifert[1], Christoph Kastl[1], Kristina Vaklinova[2], Marko Burghard[2], and Alexander Holleitner[1] — [1]Walter Schottky Institut and Physik-Department, Technische Universität München, Am Coulombwall 4a, D-85748 Garching, Germany — [2]Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany

We report on the optoelectronic dynamics in nanocircuits made of the topological insulator Bi2Te2Se. An on-chip photocurrent pump-probe spectroscopy based on coplanar striplines allows us to identify the different ultrafast photocurrent mechanisms in topological insulators with a picosecond time resolution. We discuss non-equilibrium thermal effects as well as the circular photogalvanic current generation as contributions to the overall photocurrent.

HL 97.6 Fri 11:15 H15

Structural Study of Weak Topological Insulator Bi_1Te_1 Films on Si(111) grown by Molecular Beam Epitaxy — •Martin Lanius[1], Markus Eschbach[1], Ewa Mlynczak[1], Jens Kellner[2], Pika Gospodaric[1], Chengwang Niu[1], Elmar Neumann[1], Martina Luysberg[3], Gregor Mussler[1], Lukasz Plucinski[1], Gustav Bihlmayer[1], Stefan Blügel[1], Markus Morgenstern[2], Claus Michael Schneider[1], and Detlev Grützmacher[1] — [1]Peter Grünberg Institut, Forschungszentrum Jülich, Germany — [2]II. Institute of Physics B and JARA-FIT, RWTH Aachen University, Aachen, Germany — [3]Ernst Ruska-Centre for Microscopy and Spectroskopy with Electrons, Forschungszentrum Jülich, Germany

We have studied the nucleation, growth process and structural composition of the weak topological insulator Bi_1Te_1 on Si(111) substrates by STM and STEM. Bi_1Te_1 is a superlattice of predicted 2D topological insulating materials, one bilayer Bi and two Bi_2Te_3 quintuple layers per unit cell. The van der Waals growth mode of Bi_1Te_1

shows smooth surfaces and a supressed twin domain density. The thin films from several nanometers thickness down to the nucleation regime have been grown by molecular beam epitaxy. STEM measurements of the grown films reveal a high crystalline perfection. Simulations and ARPES measurements show 2D surface states originating from spin-orbit coupling, depending in their structure on the surface termination. Furthermore we will demonstrate the ability to grow n-p heterostructures of n-doped Bi_1Te_1 with the p-doped strong TI Sb_2Te_3.

HL 97.7 Fri 11:30 H15

Bi2Se3-based heterostructures including magnetic layers: the case of n-QLs Bi2Se3 ontop of Mn-doped Bi2Se3 — •J. Honolka[1], M. Valiska[2], J. Warmuth[3], M. Michiardi[4], M. Vondracek[1], A. S. Ngankeu[4], V. Holy[2], M. Bianchi[4], G. Springholz[5], V. Sechovsky[2], P. Hofmann[4], and J. Wiebe[3] — [1]Institute of Physics, ASCR, Prague, CZ — [2]Department of Condensed Matter, Charles University, Prague, CZ — [3]INF, University of Hamburg, Hamburg, DE — [4]Department of Physics and Astronomy, iNANO, University of Aarhus, Aarhus, DK — [5]Institute of Semiconductor Physics and Solid Solid State Physics, Johannes-Kepler University, Linz, AT

Interfaces between ferromagnetic and non-magnetic Bi2Se3 phases are studied as a material platform to investigate the influence of spin degrees of freedom on 3D topological insulator (TI) properties.

An inverted geometry of n quintuple layers (QLs) Bi2Se3 ontop of Mn-doped Bi2Se3 is achieved by molecular beam epitaxy for n=0 to n=24 QLs and allows to unhamperedly monitor the development of electronic and topological properties by surface sensitive key techniques like angular resolved photoemission spectroscopy. A gap at the Dirac point is observed at small n, which is gradually filled with increasing n. The Dirac point is fully reestablished at about n = 9 QLs. Band bending effects due to the proximity of the interface with the ferromagnetic layers are discussed.

HL 97.8 Fri 11:45 H15

Observation of gapped surface states in the topological regime of the quantum-phase transition in Bi-doped Pb-Sn-Se (111) epitaxial films — •Partha Sarathi Mandal[1], Gunther Springholz[2], Valentyn Volobuev[2], Günther Bauer[2], Evangelos Golias[1], Andrei Varykhalov[1], Jaime Sa'nchez-Barriga[1], and Oliver Rader[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — [2]Institut für Halbleiter und Festkörperphysik, Johannes Kepler Universität, Linz, Austria

Topological crystalline insulators are believed to show a straight forward and versatile connection between mirror symmetries and gap opening at the surface Dirac points. Here we systematically studied the trivial-to-topological insulator phase transition [1] of the $Pb_{1-x}Sn_xSe(111)$ surface grown by molecular beam epitaxy and using angle-resolved photoemission spectorscopy (ARPES) under variation of Sn concentration (10 to 28%) and temperature. Differently from the case of the (001) surface [2], we observe two types of Dirac cones centered at $\overline{\Gamma}$ and $\overline{M}$ in the surface Brillouin zone. By comparing the band structure of samples with fixed Sn concentration and different Bi doping, we demonstrate the existence of gapped surface states within the topological regime of the quantum-phase transition at low temperatures [1].

[1] Y. Ando and L. Fu Annual Review of Condensed Matter Physics Vol. 6: 361-381 (2015). [2] Y. Tanaka, T. Shoman, K. Nakayama, S. Souma, T. Sato, T. Takahashi, M. Novak, Kouji Segawa, and Yoichi Ando PHYSICAL REVIEW B 88, 235126 (2013).

HL 98: Focus Session: Functionalization of Semiconductors III

Organizers: Kerstin Volz, Sangam Chatterjee (Universität Marburg), Michael Dürr (Universität Giessen)

Time: Friday 9:30–11:45 Location: H16

HL 98.1 Fri 9:30 H16

MOVPE growth of InGaAs quantum dots in functionalized semiconductor structures — •Matthias Paul, Jan Kettler, Caterina Clausen, Katharina Zeuner, Fabian Olbrich, Michael Jetter, and Peter Michler — Institut für Halbleiteroptik und funktionelle Grenzflächen, Universität Stuttgart and Research Centers SCoPE and IQST, Allmandring 3, 70569 Stuttgart

InGaAs semiconductor quantum dots (QDs) have been studied as sources for single photons and entangled photon pairs with regard to applications in quantum computation and communication. In that regard, the tunability of the QD emission wavelengths and the control of the area density together with the benefits of a solid state system offer a high degree of integration into photonic devices. We present the growth of low density InGaAs QDs on GaAs substrates for wavelengths ranging from below 900 nm to above 1300 nm by metal-organic vapor-phase epitaxy (MOVPE). Single-photon characteristics and radiative decay cascades are demonstrated in correlation measurements. The site-controlled growth of QDs on patterned GaAs substrates promises deterministic implementation into devices and easy addressability of individual QDs. An important step towards quantum computation with photonic integrated circuits is the realization of emitters and detectors on one chip, e.g., based on InGaAs QDs and GaAs waveguides. In addition, the integration of an optical excitation source allows for a compact device design without an electric field or current at the position of the QDs. Finally, the QDs are embedded in resonator structures to increase the extraction efficiency and study coupling phenomena.

HL 98.2 Fri 10:00 H16

Temperature-stable large-bandwidth directly modulated 1.5 μm quantum dot lasers — Saddam Banyoudeh, •Alireza Abdollahinia, and Johann Peter Reithmaier — Technische Physik, Institute of Nanostructure Technologies and Analytics, University of Kassel, Germany

Within the last decade, semiconductor quantum dot (QD) structures have interested notably both fundamental physics and optoelectronic device applications specially QD lasers operating at 1.5 μm, significant for optical fiber communication [1]. Self-assembled semiconductor QDs formed via the Stranski-Krastanov growth mode have provided a robust active medium for optoelectronic devices like lasers [2], essentially needing a base of high QD density with a homogeneous size distribution, preferably round shaped, resulting in properties such as high temperature stability, reduced threshold current, increased spectral and differential gain, and higher modulation bandwidth [3]. Recently we showed improvement in the QD epitaxy by reduction of the inhomogeneous size distribution [4]. In this work recent enhancements for broad area (BA) and ridge waveguide (RWG) lasers show a high modal gain of 14.5 cm^{-1} per QD layer with a temperature-insensitive threshold current density exhibiting T_0 values of 125 K and 152 K for BA and RWG lasers, respectively, with remarkable improvements in the small signal modulation bandwidth of more than 16 GHz.

[1] J.P. Reithmaier et al., J.Phys.D 38, 2088 (2005) [2] D. Gready et al., PTL 24, 809 (2012) [3] K. Akahane et al., PTL 22, 103 (2010) [4] S. Banyoudeh et al., JCG 425, 299 (2015)

HL 98.3 Fri 10:15 H16

Nitrogen incorporation in GaAs using DTBAA, a novel N precursor with no direct C-N bond — •Eduard Sterzer[1], Andreas Beyer[1], Lennart Duschek[1], Lukas Nattermann[1], Benjamin Ringler[2], Bernhard Leube[2], Andreas Stegmüller[2], Ralf Tonner[2], Carsten von Hänisch[2], Wolfgang Stolz[1], and Kerstin Volz[1] — [1]Material Sciences Center and Faculty of Physics — [2]Material Sciences Center and Faculty of Chemistry, Philipps-Universität Marburg, Germany

III/V semiconductors containing small amounts of N are discussed in the context of solar cell and laser applications. MOVPE growth of these alloy is typically complicated as a large excess of the conventional N precursor (UDMHy) is required in the gas phase to incorporate even small amounts of N. Furthermore, applications are hampered by significant C incorporation in the layers during growth, which either stems from the N precursor or the group III sources. Our novel N precursor DTBAA contains no direct C-N bond, which could reduce the C incorporation. We used this molecule - together with TEGa and, in some experiments, also with TBAs and TMIn - in low temperature Ga(NAs) and (GaIn)(NAs) growth. We observed around 10 times higher N incorporation efficiency in Ga(NAs) compared to UDMHy.

For (GaIn)(NAs) growth we didn't observe the decrease of N incorporation with higher In amount as reported for UDMHy in the literature. These studies underline the great potential of DTBAA for the growth of dilute nitride III/V alloys. Support of the DFG in the framework of GRK 1782 "Functionalization of Semiconductors" is greatfully acknowledged.

30 min. Coffee Break

HL 98.4 Fri 11:00 H16

GaN-on-Si(hkl) epitaxy: physics and chemistry — •Andre Strittmatter and Armin Dadgar — Otto-von-Guericke Universitaet Magdeburg

GaN epitaxy on Si substrates is governed by the atomic arrangement on the Si surface and by chemical processes during growth. Thermal stresses, mechanical strain, and a chemical instability of the Si surface are severe problems which need to be controlled throughout the growth. In order to obtain device-quality material certain measures have to be taken in order to achieve stable growth regimes and single phase, highly crystalline layers. GaN layers with specific orientations can be obtained if Si substrates with proper suface orientations are chosen and special preparation steps are applied to these kind of substrates. We will compare the special requirements of GaN growth on Si for surface orientation.

HL 98.5 Fri 11:30 H16

Atomic-scale investigation of photovoltaic GaN/Si(111) hetero-interfaces using photoexcited scanning tunneling microscopy and spectroscopy — •Fei-Man Hsiao[1], Yen-Chin Huang[2], Bo-Chao Huang[3], Philipp Ebert[4], and Ya-Ping Chiu[5] — [1]Dept. of Physics, National Sun Yat-sen University, Kaohsiung 80424, Taiwan — [2]Dept. of Physics, National Cheng Kung University, Tainan 70101, Taiwan — [3]Institute of Physics, Academia Sinica, Taipei 11529, Taiwan — [4]Peter Grünberg Institut, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [5]Dept. of Physics, National Taiwan Normal University, Taipei 11677, Taiwan

Direct observation of the light response across high-efficiency GaN/Si(111) solar cell heterojunctions was spatially resolved at atomic scale by cross-sectional scanning tunneling microscopy and spectroscopy. By employing a laser with a wavelength of 405 nm at the interface, electron/hole pairs are expected to be primarily generated at the Si side. However, the analysis reveals changes of the tunnel currents at both sides of the hetero-interface under illumination, indicating the transport of excited carriers through the interface. This observation was verified by band alignment calculations: While excited electrons can pass the interface due to the flat alignment of the conduction bands, excited holes do not have sufficient energy to overcome the valence band discontinuity.

HL 99: Gallium Nitride: Devices

Time: Friday 9:30–12:30 Location: H17

Invited Talk HL 99.1 Fri 9:30 H17

Multifunctional 3D GaN: strategies for solid state lighting, electronics and sensing — •Andreas Waag[1,4,5], J. Hartmann[1,4], Hao Zhou[1], S. Fündling[1,4], F. Steib[1,4], M. Mohajerani[1], Feng Yu[1], H.-H. Wehmann[1,4], A.E. Gad[1], D. Prades[6], D. Bichler[2], B. Huckenbeck[2], T. Schimpke[3], M. Mandl[3], I. Stoll[3], A. Avramescu[3], M. Strassburg[3], and H.-J. Lugauer[3] — [1]Institut für Halbleitertechnik, TU Braunschweig — [2]OSRAM GmbH, Schwabmünchen — [3]OSRAM Opto Semiconductors GmbH, Regensburg — [4]Epitaxy Competence Center ec2, Braunschweig — [5]Laboratory for Emerging Nanometrology LENA, Braunschweig — [6]Department of Electronics, University of Barcelona

GaN nanorods and related high aspect ratio 3D GaN nanostructures recently attracted a lot of attention since they are expected to be an exciting new route towards extending the freedom for device design in GaN technology. Such structures offer large surfaces, defect free high quality material, as well as non-polar surface orientations, including the possibility to use very large area foreign substrates without implementing large area strain. All of these aspects are difficult or impossible to achieve when planar thin film approaches are used. This talk will give an overview on the state of the art of our 3D GaN research, pointing out the necessity for further epitaxy related research, but also describing the increasingly interesting demonstration of 3D devices like 3D LEDs, 3D nanoFETs and 3D nanosensing devices, and their substantial potential for solid state lighting, power electronics and nanometrology.

HL 99.2 Fri 10:00 H17

Photon Statistics of high–β Nitride Nanobeam Lasers — •Stefan T. Jagsch[1], Noelia Vico Triviño[2], Gordon Callsen[1], Stefan Kalinowski[1], Ian M. Rousseau[2], Jean-François Carlin[2], Raphaël Butté[2], Axel Hoffmann[1], Nicolas Grandjean[2], and Stephan Reitzenstein[1] — [1]Institut für Festkörperphysik, Technische Universität Berlin, D-10623 Berlin, Germany — [2]Institute of Condensed Matter Physics, École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

1D photonic crystal nanobeam cavities feature an ultra–low mode-volume and are thus exciting candidates for the realization of low threshold and high spontaneous emission coupling factor (β) nanolasers. Of particular interest are GaN based nanobeam lasers because they promise room–temperature operation, which is highly attractive from a practical perspective. Promising applications include for instance on–chip silicon integrated photonics [1]. Herein we present a comprehensive temperature dependent quantum optical characterization of continuous wave lasing in a high–β III–nitride nanobeam cavity grown on silicon. In the present structures, with β–factors close to unity, the onset of stimulated emission can hardly be identified from the sole I-O characteristics. Indeed, we show that the analysis of the photon statistics is required to reveal a threshold behaviour. Our results highlight the importance of determining the photon statistics of emission to unambiguously determine the onset of lasing in nanolasers. [1] Triviño et al., Nano Lett. 15 (2), 1259, 2015

HL 99.3 Fri 10:15 H17

Blue LED optimization based on a MOCVD growth parameter sensitivity study — •Michael Heuken, Egidijus Sakalauskas, Xiaojun Chen, Olivier Feron, Hannes Behmenburg, Ralf Leiers, Markus Luenenbuerger, Peter Lauffer, Adam Boyd, and Johannes Lindner — AIXTRON SE, Dornkaulstr 2, 52134 Herzogenrath, Germany m.heuken@aixtron.com

The most important dependencies such as LED wavelength dependence on surface temperature, ammonia flow, group III molar flow, total flow and total pressure was experimentally determined for a state of the art production reactor. Experimentally obtained temperature sensitivity data serve as input to simulate, understand and finally improve the uniformity and performance of LED. Average system uptime higher than 90% is obtained based on routine maintenance procedures with more than 3 production runs per day in a production process flow for competitive LED products. The measured dependencies and the equipment optimizations result in wavelength uniformity of full susceptor load consisting of 4 inch DPSS wafers of 91.8% for a 6nm bin yield centred at 443nm. In a multi growth campaign utilizing 5 runs with 4 inch DPPS wafer loaded the run to run wavelength stability was assessed. On-wafer uniformity is stable with an average standard deviation of 1.48 nm. R2R wavelength standard deviation of 0.23 nm was observed for this series indicating less than 0.2 C standard deviation in average QW temperature. Loading 12 wafer with 6 inch diameter enable additional productivity gains demonstrated as standard deviation in QW emission wavelength of σ=4.5nm.

HL 99.4 Fri 10:30 H17

Impact of Design on the Optical Polarization of AlGaN Quantum Well Deep UV Light Emitters — •Christoph Reich[1], Martin Feneberg[2], Martin Guttmann[1], Frank Mehnke[1], Tim Wernicke[1], and Michael Kneissl[1] — [1]Technische Universität Berlin, Institut für Festkörperphysik, Berlin, Germany — [2]Otto-von-Guericke-Universität Magdeburg, Institut für Experimentelle Physik, Magdeburg, Germany

Light emitting diodes in the deep ultraviolet spectral region are of significant interest for applications in a variety of fields. However, efficient

light extraction is a challenging task for deep UV emitters due to the strong tendency for transverse magnetic (TM, $\boldsymbol{E} \parallel \boldsymbol{c}$) polarized emission at shorter wavelength. The emission pattern for TM-polarized light is in-plane and thus the light extraction of TM-polarized light through a (0001) surface is an order of magnitude weaker compared to transverse electric (TE, $\boldsymbol{E} \perp \boldsymbol{c}$) polarized light. The optical polarization of (0001) oriented AlGaN quantum wells shifts from TE to TM with increasing aluminum mole fraction due to a reordering of valence bands and changing oscillator strengths. Using $\mathbf{k}\cdot\mathbf{p}$ perturbation theory, the influence of strain, quantum well width, barrier height and composition on the optical polarization has been investigated. The theoretical model calculations showed that compressive strain in the growth-plane and barriers with high aluminum mole fraction are beneficial for enhanced TE-polarized emission. Based on these design parameters, dominant TE emission will be demonstrated at wavelengths as short as 240 nm.

HL 99.5 Fri 10:45 H17

Radiative recombination and parasitic luminescence in AlGaN-based UVC-LEDs — •Simon Kapanke[1], Johannes Enslin[1], Frank Mehnke[1], Christian Kuhn[1], Martin Guttmann[1], Christoph Reich[1], Ute Zeimer[2], Tim Wernicke[1], Markus Weyers[2], and Michael Kneissl[1,2] — [1]Technische Universität Berlin, Institut für Festkörperphysik, Berlin — [2]Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, Berlin

Ultraviolet (UV) light emitting diodes (LEDs) exhibit significant advantages compared to conventional UV light sources such as low power consumption and adjustable wavelength. Interesting applications for UVC-LEDs are compact gas sensing systems. However, achieving the required output power levels and high spectral purity is challenging. In this contribution, we present our recent investigations on the origin of parasitic luminescence observable in the electroluminescence measurements of AlGaN multiple quantum well LEDs emitting at 233 nm. The origin of the parasitic emission was located within the p-side of the LED heterostructure and analyzed by photoluminescence and cathodoluminescence measurements. Therefore, the Al-content in the p-side superlattice was varied resulting in a shift of the two main contributions of the parasitic luminescence towards shorter wavelength for higher Al-content. Additionally a reduced Mg-concentration in the p-side of the LEDs results in a reduced parasitic luminescence intensity indicating Mg-related deep level transitions to be involved as observed by Nakarmi et al. A detailed discussion of the experimental findings together with a comparison to recent literature will be provided.

30 min. Coffee Break

HL 99.6 Fri 11:30 H17

Carbon doping of GaN using propane for compensation of n-type GaN layers — •Andreas Lesnik, Marc Hoffmann, Jonas Hennig, Aqdas Fariza, Jürgen Bläsing, Hartmut Witte, Armin Dadgar, and André Strittmatter — Institut für Experimentelle Physik, Otto-von-Guericke-Universität Magdeburg

We investigated propane as source for intentional carbon doping of GaN using metalorganic vapor-phase epitaxy (MOVPE). The effect of carbon incorporation on structural and electrical parameters was studied in the concentration range of 1x10e^{17}-5x10e^{18} cm^{-3}. Carbon doping using propane leads to highly resistive GaN layers. In order to analyze the compensation efficiency of carbon for n-type GaN layers a Si+C co-doping technique was applied. Resistance and Hall effect measurements at room temperature reveal the persistence of the compensation effect over the whole doping range. Further structural analysis was done by secondary ion mass spectroscopy measurements, high-resolution x-ray diffraction, and atomic force microscopy.

HL 99.7 Fri 11:45 H17

Impact of buffer structure on the performance of AlInN/GaN based FETs grown on Si (111) — •Jonas Hennig, Armin Dadgar, Jürgen Bläsing, Annette Dietz, and André Schrittmatter — Otto-von-Guericke Universität,Magdeburg

We present a study on the impact of SiN masks as well as the influence of AlN interlayers on the performance of AlInN/GaN field effect transistors grown on Si(111). Characteristic device parameters such as breakdown voltage, on-resistance, and buffer leakage are analysed with respect to the quality of the underlying buffer structure. Buffer structures on Si(111) substrates are usually optimized for controlling stresses and the dislocation density in the structure. This is on one hand necessary to enable a compensation of thermal stresses which arise after growth during cooling down to room-temperature. On the other hand, device parameters of FET structures improve with reduction of the dislocation density. We have investigated different AlGaN/GaN buffer structures in combination with low-temperature grown AlN interlayers and in-situ deposited SiN-masks for optimum performance of the FET devices.

HL 99.8 Fri 12:00 H17

Smooth and uniform $Al_{0.8}Ga_{0.2}N$:Si superlattice cladding layers for UV-C laser diodes — •C. Kuhn[1], T. Simoneit[1], M. Martens[1], F. Mehnke[1], J. Enslin[1], K. Bellmann[1], A. Knauer[2], T. Wernicke[1], M. Weyers[2], and M. Kneissl[1,2] — [1]Technische Universität Berlin, Institut für Festkörperphysik, Berlin, Germany — [2]Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, Berlin, Germany

For deep UV laser diodes the current injection, light absorption and waveguiding are key challenges. For efficient waveguiding smooth and abrupt interfaces are required, to avoid losses associated with light scattering. This paper investigates the influence of the growth process on the morphology and the conductivity of $Al_{0.8}Ga_{0.2}N$:Si n-cladding layers. We recently demonstrated highly conductive n-AlGaN single layers with sheet resistance of 0.026 Ωcm. However, these AlGaN layers exhibited relatively rough morphologies with large spirals of 30 nm height caused by the high growth rates. Additionally $Al_xGa_{1-x}N$:Si layers with $x \leq 0.8$ exhibit noticeable compositional fluctuations. In this paper we explore the use of AlGaN super lattices (SL), as well as growth interruptions (GRI) between the SL layers in order to reduce the roughness of the surface. XRD measurements exhibit well-ordered growth of the 2 nm/2 nm thick SL layers with average composition of x=0.8 and distinct satellite peaks in the XRD spectrum, without any indication for compositional fluctuations. The RMS roughness on 10x10 μm^2 decreases from 7.0 nm without SL, to 3.7 nm with SL and 2.5 nm with 10 s GRI and obtaining the high conductivity constant.

HL 99.9 Fri 12:15 H17

Impact of a GaN:Ge/GaN based distributed Bragg reflector on the optical properties of an InGaN LED structure — •Andreas Voss, Gordon Schmidt, Christoph Berger, Stefan Sterling, Frank Bertram, Armin Dadgar, André Strittmatter, and Jürgen Christen — Institute of Experimental Physics, Otto-von-Guericke-University Magdeburg, Germany

The Burstein-Moss effect as present in highly Ge-doped GaN leads to a reduction of the refractive index of GaN:Ge as compared to undoped GaN. The resulting refractive index contrast of 2% is sufficient to realize strain free, highly reflective, and narrow band distributed Bragg reflectors (DBR) by combining highly Ge-doped and undoped GaN quarter-wavelength layers.

We report on the optical properties of an InGaN LED structure grown on top of a modulation-doped DBR by metal-organic vapor phase epitaxy (MOVPE) using an AlGaN/sapphire template. The DBR consists of 100 pairs GaN/GaN:Ge $\lambda/4$ layers. An InGaN/GaN multiple quantum well embedded in a pn-junction acts as active region.

Spatially resolved electroluminescence (EL) measurements exhibit a convolution of the MQW luminescence with the DBR reflectivity which leads to a drastically reduced linewidth at 430 nm. Detailed analysis of the local reflectivity on micrometer scale reveals spatial fluctuations of the stopband position.

HL 100: Organic Electronics and Photovoltaics III (Joint session of CPP, DS, HL and O, organized by CPP)

Time: Friday 9:30–12:00 Location: H40

HL 100.1 Fri 9:30 H40

Influence of order and disorder on some photovoltaic properties of AnE-PV polymers - a DFT study — •Chuan-Ding Dong and Wichard J. D. Beenken — Institut für Physik und Institut für Micro- und Nanotschnologie, Technische Universität Ilmenau, Germany

Recently, the copolymer poly(p-anthraceneethynylene-alt-poly(p-phenylenevinylene) (AnE-PV) has turned out to be a promising model for the effect of order and disorder in polymer-based solar cells.[1] By substituting linear octyl or branched 2-ethyl-hexyl sidechains to the conjugated backbone, the structure of AnE-PV can be tuned from order to disorder. Using Grimme's correction for dispersion in our DFT calculations, we will show that the van-der-Waals interaction between the sidechains influences the planarity of the conjugated backbones significantly. Consequently, we found order-dependent shifts of the respective absorption spectra, which are in agreement with the experimental data. Furthermore, we will demonstrate the effect of the alternative sidechain substitution on the stacking of AnE-PV copolymers to semi-crystalline aggregates, which is crucial for the efficiency of polymer solar cells.

[1] Kästner, C.; Egbe, D.; Hoppe, H.: *J. Mater. Chem. A* **3**(2015)395.

HL 100.2 Fri 9:45 H40

Influence of surface characteristics on electronic properties of polymer thin films — •Philipp Ehrenreich, Susanne Birkhold, Alexander Graf, Eugen Zimmermann, Hao Hu, Kwang-Dae Kim, and Lukas Schmidt-Mende — Department of Physics, University of Konstanz, POB M 680, Konstanz 78457, Germany

Many applications in polymer electronics demand not only for a loss-free charge percolation pathway towards electrodes, but also a highly delocalized pi-orbital system for efficient charge generation after exciton dissociation. The latter is especially important for the development of all-polymer solar cells, in order to compete with fullerene-based devices. Within this work the influence of surface characteristics on structural, or rather electronic properties of polymer thin films is investigated by means of an H/J-aggregate analysis on the model polymer Poly(3-hexylthiophene).

HL 100.3 Fri 10:00 H40

Quantum Molecular Dynamical Calculations of Poly(3,4-ethylenedioxythiophene) and its derivatives — •Amina Mirsakiyeva, Håkan W. Hugosson, and Anna Delin — KTH Royal Institute of Technology, Department of Material and Nanophysics, SE-16440, Sweden

Organic thermoelectrics (TE) are materials with the ability to produce an electrical current from a temperature gradient (the so-called Seebeck effect) and the advantages of organic compounds, such as less toxicity. Organic TE are based on conductive polymers where the conjugation between double and single bonds creates the π-bonds overlapping and consequently allows charge carriers transport along the polymer backbone. Up to this date, the most studied organic TE material is poly(3,4-ethylenedioxythiophene) (PEDOT). Its transparency, high stability in the oxidized state and ability to form water-soluble polyelectrolytes bring it to the leading position in industry. The success of PEDOT makes also its selenium (PEDOS) and tellurium (PEDOTe) derivatives promising thermoelectric materials. Here, we present theoretical calculations of PEDOS and PEDOTe. We determined structures of the polymer chains of PEDOS and PEDOTe, investigated HOMO and LUMO and calculated point-charge distributions along the polymer backbone. Our analysis aims at finding the localization of a polaron, i.e. the electronic excitation resulting in localized structural changes and charge accumulation. Such a deeper atomistic understanding of the processes inside thermoelectric materials will hopefully allow an improvement of the thermoelectric qualities of conductive polymers.

HL 100.4 Fri 10:15 H40

How Morphology Affects the Charge Transport: A Case Study for C60 — •Sebastian Schellhammer[1,2,3], Frank Ortmann[1,2], and Gianaurelio Cuniberti[1,2,3] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials, Technische Universität Dresden, 01062 Dresden, Germany — [2]Dresden Center for Computational Materials Science, Technische Universität Dresden, 01062 Dresden, Germany — [3]Center for Advancing Electronics Dresden, Technische Universität Dresden, 01062 Dresden, Germany

The performance of organic electronic devices is significantly influenced by the morphology of the individual layers. However, theoretical studies can cover mostly only highly ordered or completely amorphous systems.

We present a computational algorithm for the construction of arbitrarily ordered films ranging from amorphous to polycrystalline and highly crystalline. We demonstrate its application for a systematic study of the electron mobility in C60 systems depending on the degree of ordering which is based on a full parameterization of the electronic properties. Additionally, we present a generalization for other molecular materials such as pentacene as well as organic blends.

HL 100.5 Fri 10:30 H40

Intermolecular hopping transfer between DPP-based donor-acceptor polymers: A first principle study — •Florian Günther[1,2], Sibylle Gemming[1,3], and Gotthard Seifert[2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Institute of Physical Chemistry and Electrochemistry, Dresden University of Technology, Dresden, Germany — [3]Institute of Physics, Technical University Chemnitz, Germany

Diketopyrrolopyrrole (DPP) based materials have recently been considered as promising candidates for novel organic electronics. Here, we report about our investigation on intermolecular charge transfer between DPP-based polymers. We utilize Marcus transfer theory and evaluate the required quantities, the reorganisation energy and the coupling, by density functional-based tight binding (DFTB) calculations.. Due to its computational efficiency as well as the opportunity to tune some calculation features, the DFTB method is well suited for this purpose. In doing so, the coupling elements have been calculated for various stacking formations. In order to derive a single quantity, which can been used for calculate the transfer rates, an energy-weighted statistical approach has been utilised.

The obtained values allow to analyse the charge carrier mobilities in dependence of isomeric effects as the orientation of the individual units, of the molecular structure as fuctionalization, or the meaning of stacking properties as parallel and anti-parallel.

15 min. break

HL 100.6 Fri 11:00 H40

Comparison of electrostatic, inductive and dispersive excitation energy shifts for the example of a molecular crystal — •Jörg Megow — University of Potsdam, Germany

The description of dispersive excitation energy shifts is necessary whenever different molecules within a supramolecular aggregate experience a different environment. A new approach that is based on an extended dipole approximation for higher transition densities in the sum over states expression [1] allowed for an appropriate description of gas-to-crystal-shifts in thin 3,4,9,10-perylenetetracarboxylic diimide (PTCDI) films [2]. It was also possible to explain the splitting of the main bands in the UV/Vis spectrum of double-walled tubular cyanine aggregates [3] as well as the line shift and broadening of the measured UV/Vis spectrum of pheophorbide *a* dendrimers [4]. For the example of a PTCDI crystal the different contributions to the overall site energy shifts are calculated while approximating the sum over states expressions for the energy shifts due to dispersion and inductive polarization, respectively. It is shown that the dispersive site energy shift dominates the site energy shifts due to electrostatic interaction and inductive polarization.

[1] A. Stone, *The theory of intermolecular forces*, Oxford University Press (2013); [2] J. Megow, T. Körzdörfer, T. Renger et al., J. Phys. Chem. C 119, 5747-5751 (2015); [3] J. Megow, M. I. S. Röhr, M. Schmidt am Busch et al., PCCP 17, 6741-6747 (2015); [4] J. Megow, ChemPhysChem 16, 3101-3107 (2015)

HL 100.7 Fri 11:15 H40

Efficient first-principles based screening for high charge carrier mobility in organic crystals — •Christoph Schober, Karsten Reuter, and Harald Oberhofer — Technische Universität München

In organic electronics, charge carrier mobility is a key performance parameter. Due to the complex manufacturing processes of e.g. organic field effect transistors (OFETs) measured mobilities are often heavily affected by the device preparation. This masks the intrinsic materials properties and therewith hampers the decision whether further device optimization for a given organic molecule is worthwhile or not. We developed a fast and efficient protocol with a descriptor based on electronic coupling values to assess the expected performance of organic materials for application in organic electronic devices. Applying this protocol to experimental structures of organic crystals obtained from the Cambridge Structural Database (CSD), we screened about 40000 structures employing only first principle methods. Out of the 28000 successfully calculated structures we selected 2000 candidates with above- average electronic couplings for additional calculations and in-depth analysis using statistical methods and automated classification based on chemical structure. This allowed us not only to identify a number of specific crystals with exceptionally high electronic coupling values and therefore promising properties, but also possible lead structures which can be the basis for in-depth theoretical and experimental studies of new classes of materials for organic electronics.

HL 100.8 Fri 11:30 H40

In-situ x-ray investigation of the structure formation of metal films on photoactive polymers — •Franziska C. Löhrer[1], Volker Körstgens[1], Matthias Schwartzkopf[2], Alexander Hinz[3], Oleksandr Polonskyi[3], Thomas Strunskus[3], Franz Faupel[3], Stephan V. Roth[2], and Peter Müller-Buschbaum[1] — [1]TU München, Physik-Department, LS Funktionelle Materialien, 85748 Garching, Germany — [2]Deutsches Elektronensynchrotron DESY, 22607 Hamburg, Germany — [3]CAU zu Kiel, Institut für Materialwissenschaft, LS Materialverbunde, 24143 Kiel, Germany

Photoactive polymers have received high attention in recent years due to a large variety of different applications in molecular electronics. Although organic materials are used in the active layers of these devices, typically in many cases the electrodes are still made from metals. Thus, the polymer-metal interfaces are inherently present in all these novel devices. Our work takes a deeper look at the morphology of interfaces between photoactive layers and metal contacts deposited on top of them. We investigate morphological changes during sputter deposition of metal films (electrodes) onto photoactive films using in-situ GISAXS. Probing the sputter process in-situ allows highly time resolved insights into the deposition behavior of the metal depending on the polymer layer's properties. The deposition behaviors of gold and aluminium are compared, as both metals are frequently used as electrodes. The photoactive films consist of the low band gap polymer PTB7 as well as of PTB7:PCBM blends. The final film morphology is characterized via SEM and XRR after sputter deposition.

HL 100.9 Fri 11:45 H40

Charge-Transfer - Solvent Interaction Predefines Doping Efficiency in p-Doped P3HT-Films — •Lars Müller[1,2,6], Diana Nanova[1,2,6], Tobias Glaser[2,6], Sebastian Beck[2,6], Annemarie Pucci[2,6], Anne K. Kast[3,6], Rasmus R. Schröder[3,4,6], Eric Mankel[5,6], Robert Lovrincic[1,6], and Wolfgang Kowalsky[1,2,6] — [1]IHF, TU Braunschweig — [2]KIP, Heidelberg University — [3]BioQuant, Heidelberg University — [4]CAM, Heidelberg University — [5]Surface Science Division, TU Darmstadt — [6]InnovationLab, Heidelberg

Doping of organic semiconductors is a prerequisite for the production of efficient devices such as organic light emitting diodes. Numerous recent publications reveal new insights on doping mechanisms and charge transfer, emphasizing the need for further investigations, especially on polymer systems. In this work, we study p-type doping of poly(3-hexylthiophene) (P3HT) with 2,3,5,6-Tetrafluoro-7,7,8,8-tetracyanoquinodimethane (F4TCNQ), spin coated from the solvents chlorobenzene or chloroform. We find that films prepared from chloroform show a higher conductivity than films prepared from chlorobenzene. To clarify this unintuitive behavior, electron diffraction is used to reveal differences in the structural order within films from the two solvents. Additionally, UV-Vis and infrared spectroscopy help to expand the view to electronic properties such as vibrational or polaronic absorptions. It turns out that structural order and electronic properties in doped films are predefined by the interaction of the solvent with charge-transfer complexes already in solution.

HL 101: Graphene IV: Electronic Properties and Structure

Time: Friday 10:30–13:00 Location: S051

HL 101.1 Fri 10:30 S051

Graphene tunable transparency to tunneling electrons: A direct tool to measure the local coupling. — •Héctor González Herrero[1], Antonio Javier Martínez Galera[2], Miguel Moreno Ugeda[3], Delia Fernández Torre[4], Pablo Pou[4], Rubén Pérez[4], José María Gómez Rodríguez[1], and Iván Brihuega[1] — [1]Dept. Física de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Madrid, Spain — [2]II. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany — [3]CIC nanoGUNE, E-20018 Donostia-San Sebastian, Spain — [4]Dept. Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Madrid, Spain

Graphene grown on metals has proven to be an excellent approach to obtain high quality graphene films. However, special care has to be taken in order to understand the interaction of graphene with the substrate since it can strongly modify its properties.

We have grown one monolayer graphene on Cu (111) by using a new technique. By means of low temperature STM/STS experiments, complemented by density functional theory calculations, we have obtained information about the structural and electronic properties of our graphene samples with atomic precision and high energy resolution. Our work shows that depending on the STM tip apex and the tunnel parameters we can get access to either the graphene layer, the copper surface underneath or even both at the same time. Moreover, this approach can also be applied to investigate the interaction of point defects in the graphene layer with the underlying substrate .

HL 101.2 Fri 10:45 S051

Excitons and the XNLD of higly oriented pyrolytic graphite and graphene - theory and experiment — •Dominik Legut[1], Robert Laskowski[2], Peter M. Oppeneer[3], Christine Jansing[4], Markus Gilbert[4], Andreas Gaupp[4], Hans-Christoph Mertins[4], Andrey Sokolov[5], Suk-Ho Choi[6], Hud Wahab[7], and Heiko Timmers[7] — [1]IT4Innovations Centre, VSB-TU Ostrava, Ostrava, Czech Republic — [2]Institute of High Performance Computing, A*STAR, Singapore — [3]Department of Physics and Astronomy, Uppsala, Sweden — [4]FH Münster, Steinfurt, Germany — [5]HZB, Berlin, Germany — [6]Department of Applied Physics, Kyung Hee University, Korea — [7]University of New South Wales Canberra, Canberra BC, Australia

Reflection spectra of the x-ray natural linear dichroism (XNLD) were calculated on highly oriented pyrolytic graphite (HOPG) and graphene. The π- and σ-excitations stemming from the carbon K-edge are considered. It was computed in the single electron picture within the framework of the standart DFT as the first step. For the better descriptions of the core-hole quasiparticle one can model the Slater transition state employing the supercell calculation with partial hole on one of the carbon atoms with the electron charge distributed over the valence states. Another approach is to solve Bethe-Salpeter equations for the many-body electronic effects. The latter approach clearly identify the excitonic features of π- and σ-excitations HOPG. The spectral shape of the reflectance and XNLD of all three modeles are compared with the experimental data.

HL 101.3 Fri 11:00 S051

Direct measurement of chiral symmetry breaking in strained graphene by STM — Alexander Georgi[1], •Peter Nemes-Incze[1], Ramon Carillo-Bastos[2], Martin Schneider[3], Dinesh Subramaninam[1], Torge Mashoff[4], Daiara Faria[2,5], Silvia Viola Kusminskiy[3], Dawei Zhai[2], Marcus Liebmann[1], Marco

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The breaking of reflection symmetry has important consequences for pseudospin 1/2 particles, such as those used to describe low-energy excitations in graphene. Here we show that forces exerted by the tip of a scanning tunneling microscope induce mechanical strain on sub-nm length scales that acts as a gauge field breaking the chiral symmetry of the system. The parity violation manifests itself as a redistribution of the local density of states between the two sublattices by up to 30%. The effect can be understood as a pseudospin polarization due to a pseudo-Zeeman shift produced by the strain induced pseudo-magnetic field. This interpretation is supported by tight binding simulations and effective Dirac model calculations. The tunable pseudo-magnetic field might be used for the ultra fast separation of electrons of different valleys providing a switchable valley filter as a basic element for valleytronics.

HL 101.4 Fri 11:15 S051

Layer symmetry breaking field and conductivity in graphene twist bilayer — •Nicolas Ray, Sam Shallcross, and Oleg Pankratov — Lehrstuhl für theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7 B2, 91058 Erlangen, Germany

The rich electronic structure of the graphene twist bilayer includes both a decoupled large angle limit and a strongly coupled small angle limit [1]. We consider the in-plane conductivity via a linearised Boltzmann equation [2] over the full angle range, both with and without a layer-perpendicular electric field. The layer perpendicular electric field is shown to lead to a strong suppression of conductivity at certain "hot spots" in the twist angle and energy phase space.

[1] S. Shallcross et al., Phys. Rev. B 87, 245403, 2013; [2] E. Mariani et al., Phys. Rev. B 86, 165448, 2012.

HL 101.5 Fri 11:30 S051

How partial dislocations may make bilayer graphene both an insulator and a conductor — Heiko Weber[1] and •Sam Shallcross[2] — [1]Lehrstuhl für Angewandte Physik, Universität Erlangen-Nürnberg, Staudtstr. 7 A3, 91058 Erlangen, Germany — [2]Lehrstuhl für theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7 B2, 91058 Erlangen, Germany

Recently imaged partial dislocations in bilayer graphene [1] have been shown to have a profound impact on transport properties for the case of bilayer graphene on SiC [2]. We demonstrate that the presence of only a few partial dislocations in high quality suspended bilayer graphene can both destroy the intrinsic minimal conductivity of the structurally perfect bilayer, or even enhance it, depending only on the configuration of the partials. The provides a natural explanation for the peculiar behaviour of suspended bilayer graphene, in which seemingly very similar samples are found to be either insulating or conducting in nature.

[1] B. Butz, C. Dolle, F. Niekiel, K. Weber, D. Waldmann, H. B. Weber, B. Meyer, E. Spiecker, Nature 505, 533 (2014). [2] F. Kisslinger, C. Ott, C. Heide, E. Kampert, B. Butz, E. Spiecker, S. Shallcross, H. B. Weber, Nature Physics 11, 650 (2015).

HL 101.6 Fri 11:45 S051

Electronic structure of partial dislocations in bilayer graphene — Dominik Weckbecker and •Sam Shallcross — Lehrstuhl für theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7 B2, 91058 Erlangen, Germany

We present electronic structure calculations for the partial dislocations recently imaged in bilayer graphene on SiC [1,2]. We use an effective field method which allows us to treat both a realistic experimental situation of many disordered dislocations in a sample area of a square micrometer as well as model systems in which the dislocations are ordered. We find near the Dirac point a charge pooling on the bilayer graphene segments, as well as a curious energy dependent localization on the partial lines and partial nodes. We consider the presence of an external out-of-plane magnetic field and identify current circulations associated with partial lines.

[1] B. Butz, C. Dolle, F. Niekiel, K. Weber, D. Waldmann, H. B. Weber, B. Meyer, E. Spiecker, Nature 505, 533 (2014). [2] F. Kisslinger, C. Ott, C. Heide, E. Kampert, B. Butz, E. Spiecker, S. Shallcross, H. B. Weber, Nature Physics 11, 650 (2015).

HL 101.7 Fri 12:00 S051

Deformation in graphene and few layer graphenes: interlayer gauge fields and optical deformations — •Nicolas Ray[1], Fabian Rost[1], Reena Gupta[2], Sangeeta Sharma[2], Oleg Pankratov[1], and Sam Shallcross[1] — [1]Lehrstuhl für theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7 B2, 91058 Erlangen, Germany — [2]Max-Planck-Institute for Microstructure Physics, Weinberg 2, 06120 Halle, Germany

We present a general theory of deformations in graphene and few layer graphenes. In single layer graphene we consider both acoustic and optical deformations, and show that the latter can generate chiral gap opening fields. For the case of few layer graphenes we derive a general interlayer gauge term that relates the local stacking vector to an off-diagonal non-Abelian field. We show that this general result reduces to well known cases such as the Bernal or twist graphene bilayer, but can also be used to treat more complex situations such as partial dislocations in bilayer graphene.

HL 101.8 Fri 12:15 S051

Substrate nanofacets as a stamp for graphene charge carrier modulations — •Jan Honolka[1], Martin Vondracek[1], Ladislav Fekete[1], Jaromir Kopecek[1], Jan Lancok[1], Dipankar Kalita[2], Johann Coraux[2], and Vincent Bouchiat[2] — [1]Institute of Physics, ASCR, CZ-Prague — [2]Department Nanosciences, CNRS, F-Grenoble

We report on 1D quasiperiodic modulations of graphene electron doping, probed by spatial mapping of the electronic band structure in wave-vector-resolved photoemission microscopy (k-PEEM).

Sampling local topography and diffraction, we show that a nanometer-scale periodic structuration and electronic doping by several 0.1eV can be achieved straightforwardly in graphene, as-grown by CVD on high-index vicinal copper. The pattern consists of a rooftop-like alternance of Cu facets of distinctive symmetries, formed by surface energy minimization at the atomic scale, which drives copper and carbon mass-transfers during high-temperature CVD.

The general concept of this work can be extended towards other chemical vapor deposited 2D systems of current interest such as semiconducting transition metal dichalcogenides, e.g. MoS_2, insulating hexagonal boron nitride (h-BN) monolayers, and respective hybrid structures.

HL 101.9 Fri 12:30 S051

Fermi surface nesting in the graphene twist bilayer — •Maximilian Fleischmann, Dominik Weckbecker, Nicolas Ray, Oleg Pankratov, and Sam Shallcross — Theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7B2, 91058 Erlangen

Two mutually rotated layers of graphene exhibit an electronic structure that depends profoundly on the rotation angle of the two layers [1]. This rich electronic structure invites the possibility of significant band engineering control in the small angle limit [2]. We demonstrate that the small angle limit exhibits a massive Fermi surface nesting in the presence of a perpendicular electric field of strength greater than ~ 100 mV/Å. We describe in detail the unusual band topology in this nested region of the energy field phase space, and discuss some of the many body effects likely to be induced by such strong Fermi surface nesting.

[1] S. Shallcross et al., Phys. Rev. B **87**, 245403, 2013.
[2] D. Weckbecker et al., *submitted*

HL 101.10 Fri 12:45 S051

Force-induced dynamic STM mapping and picking of free-standing graphene membranes — •Bernd Uder, Wolf-Rüdiger Hannes, and Uwe Hartmann — Fachrichtung Experimentalphysik, Universität des Saarlandes, Saarbrücken, Germany

Scanning Tunneling Microscopy (STM) of freely suspended membranes only a few atomic layers thick is inherently challenging. Membrane and tip instabilities are easily induced and must be controlled by careful adjustment of scan and regulation parameters. So far only little STM work has been reported on this surface type. We demonstrate seamless imaging of few-layered suspended graphene, from 10μm x 10μm scan width down to 25nm x 25nm. On the scale of 5 - 10nm, we observe corrugations rippled in one dimension. Larger structures are resolved by choosing scan parameters such that vibrational modes are triggered in certain reproducible regions, possibly corresponding to monolayer regions or fragments. Bias voltage ramps are employed for controlled and reversible membrane picking with the observation of flipping processes of the rippled structure.